STATISTICAL THEORIES OF FRAGMENTATION AND NUCLEAR DISASSEMBLY

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ABSTRACT OF THE DISSERTATION

Statistical theories of fragmentation and nuclear disassembly

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A general statistical study of fragmentation and aggregation processes is presented and applied to the fragmentation and thermodynamics of heated nuclear matter. Emphasis is placed on distinguishing combinatorial aspects from the statistical and thermodynamic ones. Combinatorial objects pertinent to fragmentation include integer, vector and set partitions as well as permutations. Algorithms for enumerating and randomly selecting these objects, important for statistical models invoking these objects, are presented. Statistical concepts introduced include approximate methods such as Monte Carlo sampling and Markov processes, and exact methods such as recursion relations and generating function identities. Statistical models introduced and solved exactly include the equipartition weight and the Gibbs weight. The canonical Gibbs model is studied extensively, and is shown to be related to symmetric functions and Pólya-de Bruijn enumeration theory. These exactly solvable models have been applied to Bose-Einstein condensation, the λ transition in liquid ^{4}He, polymer gelation, Ewens' sampling formula in population genetics, group social dynamics, statistical shattering, and the enumeration of involutions, graphs and digraphs, indicating their flexibility and power. The application of these models to nuclear fragmentation results in a computationally simplified model which contains most of the essential physics. This model

is shown to maintain its structure under coarse graining with suitable conditions on its parameters. The thermodynamics of nuclei allowed to fragment is studied in this context, and predictions are compared with experimental data. A critical comparison of this model to the competing percolation model indicates certain advantages to this approach.

Preface

This dissertation reports on the research which I and my thesis advisor, Dr. Aram Mekjian, have been engaged in for the past three years. As such some of the material has appeared in journal articles before [59, 58, 60, 61], or has been submitted for publication. The dissertation however substantially expands on this previous work and includes material which has not appeared in print before. In particular some of the novel mathematical results and applications have only appeared here. Additionally the presentation and notation used in this dissertation differs somewhat from the journal articles, principally in an effort to improve the clarity of the presentation and to adopt notation in common use in the mathematical literature. Hopefully the reader will welcome both the adoption of a standard notation and the expanded presentation of the results.

Although by nature dissertations involve a fair amount of original research, it is safe to say that all such work builds on the work of others. In the process of research, I found myself drawn to a variety of historical models, ideas, and methods from a wide range of papers in mathematics, physics and biology. Not surprisingly, problems I needed to solve had occurred to others before, and in fact, this research was expedited by recognizing that certain mathematical theories of the nineteenth century could be adopted to the physics of fragmentation today. Recalling Gian-Carlo Rota's remark "The history of mathematics, like all history generally, is replete with injustice"[1] I felt the original ideas had languished too long in obscurity and that this "injustice" needed to be addressed. Rescuing some of these ideas, although not my original aim, now seems all the more important in view of my success in applying them to problems of interest in physics. As a result, throughout this dissertation there are a number of short historical

[1] Stated in the introduction to volume one of Percy A. MacMahon's collected papers

interludes, where occasion is taken to mention and credit substantial early work. This is not by any means a definitive history of the subject of these models, but rather an effort to point out the papers which seem to have the most historical significance to the field. An attempt has been made to be somewhat comprehensive, although omissions are unfortunately all too likely. I accept all blame in these instances, but propose that even an incomplete history is better than no history at all.

Acknowledgements

In the process of researching and writing this dissertation, a number of people have been helpful both professionally and personally. Acknowledging their contributions to this work and to my life is but the least I can do to thank them for all they have provided. Graduate school has been long enough but would have been much longer still if not for timely technical assistance and untimely distractions and occasional craziness provided by a host of friends and colleagues. Thank you all.

Firstly, I need to acknowledge the debt owed to Donald Knuth and Leslie Lamport, who in creating the TEX and LATEX systems for technical document preparation, made the process of writing and revising this dissertation a pleasure. With these programs, equations, citations, tables and figures were added with ease. Without them, I am certain the schedule and quality of the dissertation would have been significantly compromised.

I would like to thank my advisor Professor Aram Mekjian for his constant encouragement and endless supply of ideas to pursue. In many cases he suggested the pursuit of a particular goal, and his confidence that I could reach the goal even though the path to it was often unknown inspired me to find many a clever method so as not to disappoint him. I would also like to thank Professor Larry Zamick, who patiently explained many aspects of the nuclear shell model, allowing me to verify whether the models I was pursuing made sense in the zero temperature limit. Additionally, Professor Michael Stephen answered many of my questions about percolation theory, allowing the percolative and thermodynamic approaches to be compared critically. Also noteworthy was the correspondences from Professor George Andrews of Pennsylvania State University, who answered my queries about the status of vector partition theory. He was able to point out the novel aspects of my results, and encouraged further researches on my part

into this area.

I also want to thank my friends and fellow graduate students at Rutgers. They were all instrumental in bringing this project to a successful conclusion, as much for their technical help as for their wit and wisdom. Andrew Getter and Jack Bennetto were often exposed to a variety of technical problems I was experiencing, and as often suggested an appropriate method of attack, which sometimes meant a quick game of xbattle. Victor Debattista helped me organize my results and ideas by scheduling me as a speaker for several Friday morning graduate student seminars. The donuts may have brought me there, but fortunately the effects on the research were longer lasting than the sugar rush. My day-to-day interactions with students in the TP office area also had an impact on this project. My officemate Mark Raschke, when not peppering me with LaTeX questions, gladly listened to my catalogue of recent writing difficulties and Diana Goubeaud made sure I didn't finish all the bags of peanut M&M's all by myself (sugar rush indeed).

My friends outside of physics also showed interest and gave plenty of encouragement throughout the research. Martí Robb deserves certain credit for keeping my mind both off and on the dissertation during the period when the writing was the most demanding. Janet Doherty's periodic visits to New Jersey first from her sanctuary in Alaska and later from Boston provided several deserved breaks from the dissertation. Nina Jochnowitz and Mohammed Abdel-Hafez, my roommates over the past year and a half during which most of the dissertation was written, provided endless entertainment for the times when I was not writing and proved to be exceptions to the rule; any rule it seems. Without question the environment they provided was different enough from the calm pace of research physics that a return home would quickly allow me to distance myself for a time from the problems of writing. For that I thank them.

Lastly, but not at all leastly, I express my heartfelt thanks to my family for their encouragement and help over the years. Without their support, I would not be where I am today.

Dedication

This work is dedicated to my mother and father.

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List of Abbreviations

δ_{jk}	Kronecker delta function
$B(n)$	Number of set partitions of n (Bell number)
$p(n), p_r(n)$	Number of integer partitions, r-partitions of n
$\pi(n), \pi_r(n)$	Set of integer partitions, r-partitions of n
π_j, π_{jk}	Number of clusters with j objects; with j protons, k neutrons
A, n, Z, N	Total number of nucleons, objects, protons, neutrons
V, T, ρ, d	System volume, temperature, density, spatial dimension
λ_T, x	Thermal wavelength, "tuning" parameter $x = V/\lambda_T^d$.
P, S, U	Pressure, entropy, internal energy
F, G, H	Helmholtz free energy, Gibbs free energy, enthalpy
C_V, κ_T, K	Specific heat, isothermal compressibility, incompressibility
$\langle\bullet\rangle$, $\mathcal{Z}$	Grand canonical expectation value, partition function
$\langle\bullet\rangle_n$, Z_n	Canonical expectation value, partition function
$\langle\bullet\rangle_n^{(r)}$, $Z_n^{(r)}$	Microcanonical expectation value, partition function
$[x]_n$, $(x)_n$	Falling factorial, rising factorial (Pochhammer symbol)
$\binom{n}{k}_q$	Gaussian q-binomial coefficient
$\left[{n \atop k}\right]$, $\left\{{n \atop k}\right\}$	(unsigned) Stirling numbers of the first and second kind
$h, \hbar, k_B$	Planck's constants ($\hbar = h/2\pi$), Boltzmann's constant
EOS	Equation of state
LHS,RHS	Left-hand side, right-hand side
MC,GC	Microcanonical, grand canonical
LSC	Lattice spanning cluster
QGP	Quark-gluon plasma
RHIC	Relativistic heavy-ion collider

Chapter 1

Introduction

In the last twenty years, a large number of experimental and theoretical studies of nuclear matter have been conducted, all essentially motivated by the same question: How does nuclear matter behave well away from typical density and temperature? This question is of crucial importance to nuclear physicists, who want to extend their successful description of nuclear matter under ordinary conditions (the nuclear shell model), as well as to astrophysicists, who are interested in the high-density properties of matter as found in collapsing stars and other stellar objects. The hadronic equation of state (EOS) encapsulates this information and is therefore the focus of intense research.

What assumptions does the nuclear shell model make about nuclear matter? Essentially it treats the ground state of the nucleus as a degenerate Fermi liquid at zero temperature. So we expect that at low temperatures the thermal properties are that of a nearly degenerate homogeneous Fermi liquid. However, as the temperature or density is increased, excitations can fragment nuclei into distinct smaller pieces. At first, single nucleons will be ejected from the central nucleus, but as the average internal energy increases, the fragmentation pattern can become fairly complicated. Eventually, fragmentation dominates the physics and the system again becomes a homogeneous (though dilute) gas of individual nucleons. It is the intermediate region in which the nuclei are far from homogeneous that attracts our attention. In this region the fragmentation effects can have a substantial impact on the hadronic EOS, the most important of which would be the introduction of a hadronic matter phase transition. Such a phase transition would appear as a sharp demarcation between the liquid-like low-temperature phase and the gas-like high-temperature phase. So it is clear that any understanding of heated nuclear matter (i.e. the hadronic EOS) over a large range of temperatures and

densities depends on the resulting fragmentation patterns.

As a result, experimentalists have concentrated on elucidating the properties of fragmenting nuclei in collisions. Large nuclei such as gold or uranium are collided with light energetic protons or heavier ions from accelerators, and the charge, mass and other characteristic variables (momentum, spin) of the outgoing fragments are measured. From this information, the hadronic EOS can be constructed, as conditions in the hot core are inferred from the distribution of sizes and momenta of the final fragments.

One goal of theoretical nuclear physics is thus clearly indicated. A model needs to be developed which agrees substantially with the experimental results. The model's parameters must depend on the thermodynamic variables in such a way as to determine a hadronic EOS compatible with the well understood high- and low- temperature limits. At intermediate temperatures, a phase transition is expected to occur, although finite-size effects may obscure clear signals of such a transition.

A number of theories have been developed toward this goal. Currently the best of these theories of nuclear fragmentation and hadronic matter are statistical. Here we attempt to construct such a statistical theory valid in the physically interesting region. To do this, we distinguish the various problems that need to be solved:

- *Combinatorial.* How are the outcomes of fragmentation events described?
- *Statistical.* What probability should outcomes be assigned?
- *Thermodynamic.* What hadronic EOS do nuclei satisfy?

At first this separation of the problem may seem overly pedantic. The first issue can be dispatched in a paragraph if one so chooses. The second almost as quickly, leaving only the thermodynamic problem to be tackled. The separation serves a two-fold purpose however. For one, the deliberate separation allows us to examine approaches to the problems in their most general setting. Describing the fragmentation events in this philosophy becomes an exercise in the mathematical theory of partitions. In this context, there are several approaches to the problems faced, and each approach has something

different to offer. For example, permutations are sometimes more useful than partitions in describing the fragmenting states. For the other, such a separation helps distinguish effects which are simply due to combinatorial or statistical effects, and are independent of the thermodynamics. This is important, since researchers have sometimes mistaken a combinatorial effect for a thermodynamic signal.[1]

It is our goal to make the model both as simple and accurate as possible. Elsewhere in physics such a goal may be motivated by the notion that the simplest theory is more often the correct one, but in hadronic matter where the competition between different forces is intense, overly simplified models might be expected to fare poorly in explaining some phenomena. For this reason, as more and more computer power has become available, many statistical models of nuclei have become increasingly complicated and computationally intensive. Although the accuracy of the models has often improved with the sophistication, our understanding of the physics has become correspondingly clouded. Isolating effects in such models can become extremely difficult. For this reason, simplified models can be attractive, since it is easier to isolate the effects of their various parameters. However, the predictions of such a model sometimes are more qualitative than quantitative.

One such simplified model in nuclear physics, the percolation model, has enjoyed great success for just this reason. In fact it is claimed that "existing models based on nuclear physics do not describe multifragmentation data as well as [this] simple percolation-based model."[2] Its fragmentation pattern depends only on a single parameter, and can be calculated relatively quickly. The models presented in this work differ substantially from the percolation model, but agree in many predictions; for example, both models predict a hadronic matter phase transition characterized by similar critical exponents. In fact, each model presented here can be computed for a typical nuclear

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[1] For example, log-log correlations between different moments calculated from the distribution of fragments was originally promoted [46] as an indication of a phase transition in nuclear matter. Later [264] it was discovered such correlations are a result of the conservation of mass sum-rule. Intermittency effects, also promoted as a indication of a phase transition [239, 240], similarly may only be due to a finite-size effect [52].

[2] [120], page 1590.

system in a few minutes at most on a computer workstation. This has been accomplished by restricting attention to models of nuclei with an inherent exact solution. Even percolation models are not amenable to exact solution, and so this method has some built-in advantages which when exploited create a compelling argument in favor of these models.

1.1 Fragmentation and aggregation theories

Fragmentation is the process of an object breaking up into smaller pieces. Aggregation or clustering is the inverse process in which objects combine to form larger parts. The fundamental law of statistical clustering theories is the simple statement that when these processes compete, an equilibrium emerges with a characteristic distribution of object sizes, and "the entire subject is either the slide-down from this summit, as the principle is applied to various cases, or the climb-up to where the fundamental law is derived."[3] As to be expected, more time will be spent sliding down than climbing up, but the principle by which we will proceed at all points is clearly stated in the fundamental law.

A few examples serve to indicate the wide range of phenomena which are principally described statically by clusters and dynamically by fragmentation or aggregation. At the astronomical scale, galaxies often congregate together in massive galactic clusters. Galaxies themselves are collections of billions of stars. Within a stellar system, matter collects together to form varying numbers of planets of differing sizes. Planets under gravitational stresses may fragment into large numbers of asteroids. On the atomic level, atoms group together chemically by bonds, forming molecules from the simple (e.g. H_2) to the complicated (e.g. long organic polymers, DNA). At the nuclear scale, clustering is manifest at typical energies seen in nature. Stable nuclei are collections of protons and neutrons clustered together by strong-force interactions. They will fragment into smaller nuclei due to internal perturbations or when collided with a high-energy proton or heavy ion in a particle accelerator. At the quark level, clustering is

[3] [102], page 1. Feynman was referring to the key principle of statistical mechanics, but the statement applies equally well here.

further evident, whereby quarks group in threes to forms baryons, and in twos (quark, anti-quark) to form mesons. It may turn out that quarks themselves have substructure, which if history is any guide, will be composed of clusters of still more fundamental units. So clusters can be seen at many length scales in physics.

Although in these examples there is often more happening than can be described by the degree of clustering, one can often make progress in understanding phenomena by analyzing models in which only the sizes of the clusters in their final configurations is considered. There is more information about the final state one may wish to understand, but by concentrating on the clustering degrees of freedom we hope to explain some of the essential features. Approaching the problem in this way, all questions about the system are reduced to the computation of expectation values of the cluster size variables. The advantage of this statistical approach is that a number of nontrivial models of this type are exactly solvable. The obvious disadvantage is a great deal of useful physical information is lost in the process.

It should be noted however that such dynamical-averaging approaches are applicable only to certain situations in physics. In many phenomena it is sufficient to ignore the mechanisms of clustering and fragmentation altogether, as the time scale of other physical processes is much shorter than the time scale of clustering and fragmentation. For example, it is reasonable to ignore the possibility of nuclear fission in modeling the phenomenon of nuclear magnetic resonance. Fortunately, sometimes it is the case that clustering and fragmentation are the dominant physics. The stability of nuclei is well known, but in energetic collisions a nucleus can be forced far from stability where it fragments into smaller nuclei.

This dissertation considers phenomena in which fragmentation and/or aggregation are the dominant physics. It analyzes a class of models appropriate to describing such phenomena, and separates the combinatorial principles from the physical ones. In particular, the models are defined in terms of the equilibrium distribution of clusters, and are therefore insensitive to the dynamical process which yields the particular clustering pattern. This pattern may be due to a fragmentation process, an aggregation process or (more typically) a competition between two such processes. The details of the process

specify the equilibrium distribution of course, but the distribution itself may be the result of many possible dynamic processes.[4] The clustering pattern being the object of this study, it is reasonable to concentrate solely on this distribution.

The principle phenomenon of interest in this dissertation is that of nuclear fragmentation, but the emphasis on nuclear fragmentation should not be construed to indicate a bias in the method toward this application. Indeed many of the ideas in this paper can be traced back to models proposed in polymer physics, where aggregation is the dominant phenomenon. Moreover, the reader may instead detect a bias against nuclear fragmentation, as it is presented after and makes extensive reference to the other phenomena. This was a choice made by the author, principally because the complications inherent in nuclear fragmentation distract from the inherent simplicity of the canonical Gibbs ensemble approach used. Other phenomena are better introductions to the subject, and the reader is well served by first considering such examples.

1.2 Research retrospective

> Unfortunately, what is little recognized is that the most worthwhile scientific books are those in which the author clearly indicates what he does not know; for an author most hurts readers by concealing difficulties.
>
> *Evariste Galois* [173]

A detailed discussion of all the problems overcome in the process of researching and writing this dissertation, although personally satisfying, would overwhelm and eventually disengage the reader. However, like all research projects, there were times when problems were solved and issues which had been hazy suddenly became clear. A personal reflection on the early stages of this research project when such moments were both frequent and satisfying I hope will interest the reader and perhaps explain how

[4] For example, take n indistinguishable objects and select $1 \leq k \leq n$ uniformly at random of them to form a cluster. Repeat the process with the remaining objects until no objects are left. The distribution of clusters from this process (if repeated a large number of times) is specified by the Gibbs weight with $x_k = x/k$ (section 3.2.1). This distribution can also be achieved by following a Markov binary process which allows the clusters to dynamically combine and split (section 4.2.1) at a certain rate. Dynamically these two processes are quite distinct, but there equilibrium distributions are identical.

much of the material I have chosen to include in this dissertation found its way here. For example, the section on Monte Carlo methods is included so as not to downplay early simulation efforts which were eventually replaced by exact solutions. Additionally, this serves as a chronological guide to the dissertation.

My research on fragmentation began (in 1992) with an attempt to reproduce Professor Mekjian's exact results [215] for a Gibbs model using a Monte Carlo simulation (section 3.1.2). Although the exact results were known, the idea was to apply the simulation later to systems for which no exact results were known. In spite of having some experience with modeling the Ising model in two dimensions this way, I could not at first reproduce the results. After several days of frustration, I realized that my method did not satisfy the detailed balance condition since it violated the symmetry condition discussed in section 3.1.2. The natural resolution of this problem was to modify the transition rates, thus introducing Markov processes (section 4.2.1), but this method was at that time unknown to me.[5] Instead I decided to change the objects I was modeling from integer partitions to permutations and project the permutations onto integer partitions using a cycle decomposition, since it seemed easier to satisfy the symmetry condition on permutations than on partitions. This was feasible because Cauchy's formula determined which weight to choose on permutations to get the correct weight for integer partitions (section 2.1.2). With this correction my simulation gave the correct results.

At this point I became interested in the exact solution, since an exact answer is almost always preferable to a Monte Carlo sampled one. It was easy to generalize the recurrence relations to general parameter vectors, and within a short time I was modeling the physics of systems driven by $x_k = x/k^\tau$, discovering that $\tau \approx 2$ reproduced well some early emulsion data [305] of a fragmenting nuclear system (cf. section 6.2.1), better than the previously considered $\tau = 1$.

One thing bothered me about this agreement, however. The emulsion data measured the charge distribution of fragments, whereas the nuclei actually redistribute both their

[5]It would have been surprising if I would have been able to rediscover it independently at that early date.

neutrons and protons among the clusters. If the model was a correct description, it must be the result of a projection of these two-component states (neutrons and protons) onto one-component states (protons only). The model should be a Gibbs model of two kinds of indistinguishable particles, but it seemed to reduce to a Gibbs model of indistinguishable particles under projection. At first I thought this unlikely, and since I hadn't yet realized the exact solutions were generalizable to models with two types of distinguishable particles, I decided to run a Monte Carlo simulation.

Since I had a working simulation on permutations, it was obvious to modify the existing simulation to project states onto partitions of (Z, N) by a simple cycle decomposition of the permutations, but labeling the first Z numbers as protons and the rest as neutrons. I ran this simulation using the same permutation weight as before, and discovered that the expected distribution of isotopes (same proton number) when summed over all possible neutron configurations appeared to be equivalent to the one-component expected distribution for Z nucleons with the same permutation weight. This was both a surprising and encouraging result. It suggested that the model was exactly solvable as before, and that the connection to the permutation group suggested a way of constructing two-component models which reduce to the one-component models. I realized then I had to do two things. One was to find the exact solution of the two-component Gibbs partition model. The second was to determine the generalization to two-components of Cauchy's formula. With these two facts I could understand why the Monte Carlo simulation invariably reduced to the one-component model.

Each problem took quite a bit of time to solve, although in retrospect this needed not to be the case. The principle difficulty was that I was continuing to work on a variety of issues associated with the one-component models (such as their thermodynamic properties, see section 6.3), and had little time free to concentrate on the two-component models. The exact solution turned out to be a straightforward extension of the method used to solve the one-component model. I was able to determine this after studying carefully the method used to calculate the recursion relations, a result I had until that time taken for granted. Detailed study of the proof indicated that recursion relations could be written for any model in which the partial derivatives of the partition function

are functions only of previously computed partition functions (section 3.1.1). This allowed two-component Gibbs models to be solved recursively, and indicated a number of other models could also be solved, such as the equipartition model (section 3.2.2).

The problem of generalizing the Cauchy formula to two-components took longer to intuit. At first computing the case $Z = 2$, $N = 2$ by hand revealed no simple pattern in the numbers. So I broke the problem into two parts. First, I wrote a computer program which generated all the permutations, and then counted mechanically the number of permutations which mapped to a particular partition. This generated the Cauchy numbers for all Z, N up to $Z + N = 10$ quite quickly. These results I hoped to use to test any formula I might derive. I then worked on computing special cases by combinatorial arguments. For the fragmentation state $(j,k)(1,0)^{Z-j}(0,1)^{N-k}$, which is shorthand for one fragment with j protons, k neutrons and all other protons and neutrons being monomers, I was able to show that the generalized two-component Cauchy formula is given by $\binom{Z}{j}\binom{N}{k}(j+k-1)!$. Assuming that the Cauchy formula had a particular structure, this result uniquely determined the general case. Checking this result against the program's output verified the structure and the result.

With the Cauchy formula generalized and the two-component partition models solved exactly, I was able to make significant progress on the description of nuclear fragmentation. Parenthetically, I worked out the generalization of these results to s-component models, which is a trivial extension of the two-component solution. The principle interesting result was a proof that the reduction of the two-component model to the one-component model for the permutation model was in some sense a happy accident. In fact, most two-component Gibbs models do not reduce to a one-component Gibbs model. I was able to establish a set of sufficient conditions for the reduction to be successful (section 6.2.2). At a later time I changed the projection from isotopes to isobars, which has similar characteristics.

Having started working on the Monte Carlo approach, I was determined to derive some utility from my extensive simulation efforts. When I began an investigation of models with identical partition functions but different weight distributions, I thought that Monte Carlo methods would prove to be essential. I focused on models which weigh

each multiplicity (i.e. the total number of clusters) restricted space of events equally, but events within the spaces unequally. The example I considered was the difference between the Gibbs weight and the equipartition weights, and with the aid of Monte Carlo, I discovered some distinctions. I was mistaken however in my belief that exact methods could not be applied to these models. The subspaces were microcanonical, and easily solvable independently, a fact which eventually became apparent. This was hardly an isolated incident. Every time I found a quantity to measure which appeared to defy exact solution, a determined effort would prove my initial impression wrong. Reduced moments (section 4.3.1) are most noteworthy in this respect, and showed that a percolation analysis of the model can be done exactly by extracting information about the largest fragments in an event from the usual partition functions. The informational entropy (section 4.1.4) of the models can also be evaluated exactly by a similar decomposition of the partition functions. The fruits of Monte Carlo are included here nonetheless, as to omit them would be a disservice to both the writer and the reader.

Looking back, I am amazed by my good fortune. Without the benefit of symmetric function theory (section 2.2.2), I had to rederive a number of results, some of which required mathematical subtlety to establish. That I was able to solve them is indeed fortunate, or my enthusiasm for the program of research may have dimmed. My concern over the question of how to properly take into account the distinguishability of particles led to generalizing the Gibbs model and Cauchy numbers to vector partitions. Making little progress on the second question, I made the fortuitous choice of halting my research in order to conduct a search of the mathematical literature. While unable to locate a generalization of the Cauchy numbers, I discovered symmetric function theory, which provided a completely different context in which the models appear. Slowly I was able to fit the problem I was exploring into the larger theory of partitioning and symmetric functions, and began to discover the ubiquity of the model in problems in physics, biology and mathematics. With this cross-pollination of ideas from mathematics and physics, a conceptual framework for the dissertation built around the mathematical theory of partitions was suggested.

1.3 Reader's guide to the dissertation

This dissertation sets out first to construct a sophisticated mathematical machine whose purpose is to render solvable a wide class of statistical models applicable to the understanding of clustering and fragmenting systems. The application of these models to cases of interesting physics, especially toward the understanding of nuclear fragmentation as a statistical process, clearly the primary aim of this dissertation, follows this mathematical beginning. The dissertation separates the models into their component aspects, namely the combinatorial (chapter two), the statistical (chapters three and four) and the thermodynamic (chapters five and six). Depending on one's prejudices, this is a progression from the fundamental issues to the less fundamental issues, or vice versa. My own prejudice is for the former, which perhaps belies the principal aim of the dissertation, but clearly a decision needed to be made with respect to the organization of this work. As such I decided the importance of distinguishing the principal concepts outweighed the need to begin discussing the physics of fragmenting nuclei.

The shortcomings of this approach are many, including the possibility of losing the reader early on in the more mathematical sections. The reader having been warned, she or he may wish to skip about to sections which are more interesting. Nevertheless, some sections deserve close scrutiny first due to their fundamental importance to the work, and as such sections 2.1.1, 2.1.2 should be read for their introduction to the terminology and notation of clustering and sections 3.1, 3.1.1 for their introduction to statistical models and exact methods. Later chapters will be much more comprehensible if this warning is heeded.

A broad outline of the chapters should suffice to orient the reader for the journey ahead. Chapter two introduces the combinatorial objects and algorithms appropriate for a discussion of fragmenting and clustering systems. It is wholly self-contained, and could be used as a reference for some of the combinatorial concepts. Chapter three introduces the statistical methods required for and the statistical models appropriate to clustering and fragmenting systems. It emphasizes exact methods for solution, but

includes a detailed account of Monte Carlo techniques and their application to fragmenting systems. It depends on chapter two for notation and algorithms. Chapter four concentrates on the canonical Gibbs model and its properties, a model of wide applicability in physics and mathematics. It introduces a variety of mathematical and physical properties which this model has, and emphasizes their special character. Chapter five discusses the historical applications of these models to many areas of physics, biology and mathematics. The ideal Bose gas, polymer theory and the λ transition are discussed here in detail, as well as the Ewens' sampling formula, social dynamics, statistical shattering, and the enumeration of Young tableaux and loop-free graphs. Chapter six introduces statistical nuclear fragmentation models. The range of complications inherent in describing the phenomena is fully discussed, and simplified as well as complex models are proposed to model and analyze particular properties of fragmenting nuclei. Experimental evidence and the thermodynamic properties of nuclei are considered, and a comparison is made to their principal simplified competitive model, percolation theory. The approach taken emphasizes the method, and chapter seven concludes the thesis with an overview of the results and a discussion of the most important aspects of this research, as well as some possible future directions of this research.

Chapter 2

Combinatorial objects, theories and algorithms for fragmentation

In essence the subject of this thesis neatly separates into three issues, one mathematical, one statistical and one physical. This chapter introduces and explores the first of these issues, the variety of combinatorial objects and algorithms relevant to the description of fragmentation and their generalizations. The statistical problems are mostly postponed till the next two chapters, and the physical issue of thermodynamics is discussed in chapters five and six in the context of the individual physical examples. In some sense this is for convenience, since the combinatorial aspects of the problem of fragmentation are of fundamental interest themselves and can be discussed independently of the details of the statistical models or thermodynamic details. Nevertheless the objects and algorithms discussed here are crucial to the development of the thesis, and the separation of the subject from the discussion of the statistical models should not suggest that the study of these issues is of lesser importance. On the contrary, a careful study is required to reveal both the inherent difficulties of general fragmentation theories, and the techniques for circumventing these difficulties in particular models.

Section 2.1 introduces the combinatorial objects of interest in aggregation and fragmentation. These include integer and vector partitions (2.1.1) as well as set partitions and permutations (2.1.2). Generating functions and asymptotic formulae for the enumeration of these objects are derived or quoted from the literature. Section 2.2 introduces some classical combinatorial theory of interest to fragmentation, a natural subject following this discussion of objects. Pólya-de Bruijn enumeration theory (2.2.1) and symmetric function theory (2.2.2) are included because of their utility in solving

combinatorial enumeration problems defined on the above objects, and it is these theories that we will return to for the statistical models in the next chapter. Section 2.3 introduces algorithms which enumerate and randomly select these combinatorial objects, two problems of principle importance in general statistical models on these objects. These include algorithms for integer partitions, set partitions and permutations (2.3.1) as well as some novel algorithms for vector partitions (2.3.2).

2.1 Combinatorial objects

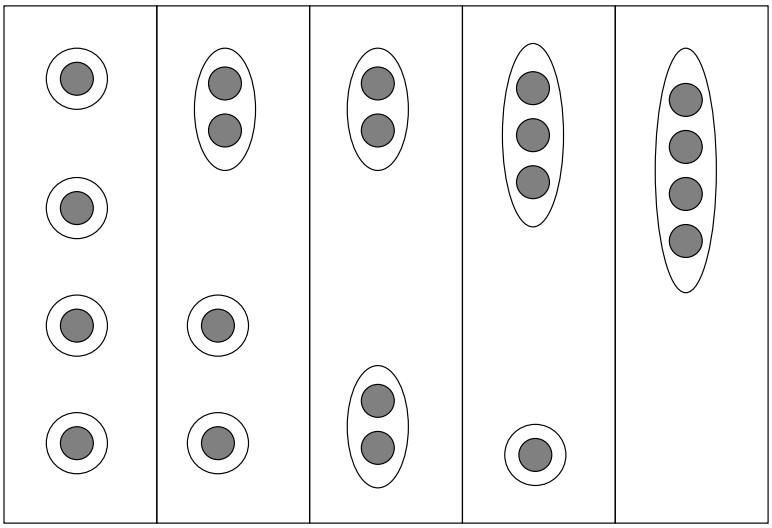
We begin by briefly outlining the combinatorial objects of interest to this research. Fundamentally, we are interested in various ways of partitioning objects under various distinguishability conditions. Particles in physics are generally indistinguishable unless they have some distinguishing characteristic, such as different masses, charges, or spins. For example, in a system of protons there is no real way of distinguishing particles, but in a system of protons and neutrons there is some amount of distinguishability since we can distinguish between neutrons and protons (one is charged, one isn't). Depending on the distinguishability, we shall see that the combinatorial objects which describe the possible fragmentation states are integer partitions and vector partitions (2.1.1), set partitions and permutations (2.1.2). There are many connections between these different combinatorial objects, and exploiting these connections allows us to adopt whichever object is most convenient for a particular calculation.

Much of the material in this section can be found in the mathematical literature, although some results for vector partitions appear to be original. Consequently proofs of some identities will be omitted, but the reader can refer to any of a number of good combinatorial references to supply the missing proofs. A good reference for partitions and vector partitions is George E. Andrews excellent book *Theory of Partitions* [11] and Hansraj Gupta's review article [135]. Set partitions and permutations are discussed in most introductory books on combinatorics. Ioan Tomescu's *Introduction to Combinatorics* [296], Claude Berge's *Principles of Combinatorics* [26] and John Riordan's *An Introduction to Combinatorial Analysis* [255] are all good general references.

2.1.1 Integer and vector partitions

Suppose one is interested in the various ways n indistinguishable objects can form clusters of various sizes. For example, in the case of four indistinguishable objects, there are five possible clusterings as shown by figure 2.1. How can we uniquely describe

Figure 2.1: Cluster configurations for four indistinguishable objects.



any such possible clustering of objects? Clearly if we note how many clusters of a given size occur in a given configuration, then we have uniquely described it, as the indistinguishability of the objects determines that only the sizes of the clusters are pertinent. Let π_k denotes the number of clusters of size k. The vector $\boldsymbol{\pi} = (\pi_1, \pi_2, \ldots)$ therefore uniquely characterizes a particular configuration of the n objects into clusters. Furthermore, $n = \sum_{k>0} k\pi_k$, as counting the number of objects cluster by cluster must result in all objects being accounted for. So the set of all non-negative integer vectors $\boldsymbol{\pi}$ satisfying $\sum_{k>0} k\pi_k = n$ comprises all possible clusterings, which we denote by $\pi(n)$, i.e.

$$\pi(n) = \left\{ \boldsymbol{\pi} \in \mathbb{N}^n \,\middle|\, \sum_{k>0} k\pi_k = n \right\} \quad . \tag{2.1}$$

where $\mathbb{N} = \{0, 1, 2, \ldots\}$ is the set of natural numbers.

How many such clusterings are there? The size of the set $\pi(n)$, denoted $p(n)$, can be determined most readily from a generating function or formal power series method. If

$\{f_0, f_1, \ldots\}$ is a sequence, then the formal power series $f(q) = \sum_n f_n q^n$ is its (ordinary) generating function.[1] Often the generating function can be expressed more compactly than the original sequence. For example, in this case

$$\begin{aligned}\sum_{n=0}^{\infty} p(n)q^n &= \sum_{n=0}^{\infty} q^n \sum_{\pi(n)} 1 = \sum_{n=0}^{\infty} \sum_{\pi(n)} q^{\sum_{k>0} k\pi_k} \\ &= \sum_{\pi \in \mathbb{N}^\infty} \prod_{k>0} q^{k\pi_k} = \sum_{\pi_1=0}^{\infty} q^{\pi_1} \sum_{\pi_2=0}^{\infty} q^{2\pi_2} \cdots \\ &= \prod_{k>0} \frac{1}{1-q^k} =: P(q)\ . \end{aligned} \tag{2.2}$$

By direct expansion of this generating function (or by other methods, see section 2.3.1) one can compute any value of $p(n)$, and table 2.1 lists the first few values.

Table 2.1: Number of integer partitions $p(n)$ for $n = 1(1)15$.

n	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
$p(n)$	1	2	3	5	7	11	15	22	30	42	56	77	101	135	176

Although the above discussion was cast in terms of partitioning indistinguishable objects, one could equally well have discussed partitioning integers into positive parts. If one associates with each cluster of size j in the partition of n indistinguishable objects the part j in the partition of the integer n, a bijection between the two sets is established. For example, the partition $3+2+1 = 6$ is associated with the configuration vector $\boldsymbol{\pi} = (1, 1, 1, 0, 0, \ldots)$. For this reason a particular cluster configuration of n indistinguishable objects is referred to by the corresponding partition of the integer n. Partitions of n are usually specified by $\boldsymbol{\pi}$[2], or alternately by $(\lambda_1, \ldots, \lambda_r)$ where $\lambda_1 \geq \cdots \lambda_r \geq 1$ and $n = \sum_k \lambda_k$. Table 2.2 lists the partitions of the first few integers.

As a mathematical problem, the properties of integer partitions has had a long and interesting history, the early part of which is amply documented in Leonard Dickson's *History of the Theory of Numbers* [77]. He marks the beginning of the subject as a letter

[1] If $q = e^{i\pi x}$ then this is equivalent to a discrete Fourier transform of the sequence. Fast Fourier transform methods can then be applied. We also can (and will) introduce other generating functions, such as exponential generating functions $\sum_n f_n q^n/n!$. See Wilf [310] for details.

[2] Often π is written as $1^{\pi_1}2^{\pi_2}\ldots$ with k^{π_k} omitted if π_k is zero, e.g. $10 = 4 + 2 + 2 + 1$ is written as 12^24.

Table 2.2: Integer partitions for $n = 1(1)5$.

n	1	2	3	4 (cf. figure 2.1)	5
$\pi(n)$	1	2 $1+1$	3 $2+1$ $1+1+1$	4 $3+1$ $2+2$ $2+1+1$ $1+1+1+1$	5 $4+1$ $3+2$ $3+1+1$ $2+2+1$ $2+1+1+1$ $1+1+1+1+1$

from Gottfried Leibniz to John Bernoulli asking him if he had investigated the number of ways a number can be partitioned into two, three, or many parts. This was in 1669. Apparently this question did not encourage further research until Leonard Euler took up the subject around 1740, and proceeded to discover most of the elementary results[3], including the surprising pentagonal number theorem[4], which states that

$$\prod_{k>0}(1-q^k) = \sum_{n=-\infty}^{\infty}(-1)^n q^{n(3n-1)/2} \ , \tag{2.3}$$

i.e. that the infinite product expansion has coefficients restricted to $\pm 1, 0$. This is clearly an unexpected result, but not an unwelcome one. The inverse of this product is the generating function for $p(n)$ (equation (2.2)), so a simple recursive formula for computing $p(n)$ can be derived (see section 2.3.1).

It is clear from table 2.1 that the number of integer partitions grows rapidly with n. In fact, Godfrey H. Hardy and Srinivasa Ramanujan [142, 143] showed using complex analysis that for large n, $p(n)$ grows exponentially with the square root of n, i.e.

$$p(n) \sim \frac{1}{4\sqrt{3}n} e^{\pi\sqrt{2n/3}} \ . \tag{2.4}$$

Actually, they were able to compute a divergent series[5] for $p(n)$ in terms of some

[3] We should follow the advice of Laplace, "Read Euler, read Euler, he is the master of us all" [173], a comment possibly motivated by the sheer volume of Euler's published works, touching all areas of mathematics.

[4] The pentagonal number theorem, although an analytic identity, has a combinatorial interpretation in partition theory, cf. Andrews [11].

[5] Divergent series like Hardy-Ramanujan's are often quite useful since a finite truncation of the series will often give a good approximation. For example, Stirling's approximation for $\Gamma(z) \sim \sqrt{2\pi}e^{-z}z^{z-1/2}$ is the first term of a divergent series for the gamma function. See Hardy [141] for more details.

transcendental functions and Hans Rademacher [244] modified their series slightly to arrive at a convergent series. Paul Erdös [91] has also produced an elementary (though tedious) proof of this asymptotic formula. [6]

How many parts are there in a partition $\boldsymbol{\pi}$? Since each π_k counts how many parts there are of a particular size k, $r = \sum_{k>0} \pi_k$ is the total number of parts. Integer partitions of n with the number of parts fixed are known as r-partitions of n, and are interesting to physicists since oftentimes fragmentation events will be classed by the total number of parts, or *multiplicity*.[7] The set of r-partitions of n are denoted by

$$\pi_r(n) = \left\{ \boldsymbol{\pi} \in \pi(n) \,\middle|\, r = \sum_{k>0} \pi_k \right\} . \tag{2.5}$$

Again, the natural first question[8] is to ascertain the size of $\pi_r(n)$, denoted $p_r(n)$. A generating function can be simply computed

$$\begin{aligned} \sum_{n=0}^{\infty}\sum_{r=0}^{\infty} p_r(n) q^n t^r &= \sum_{n=0}^{\infty}\sum_{r=0}^{\infty} q^n t^r \sum_{\pi_r(n)} 1 = \sum_{n=0}^{\infty}\sum_{r=0}^{\infty}\sum_{\pi_r(n)} q^{\sum_{k>0} k\pi_k} t^{\sum_{k>0}\pi_k} \\ &= \sum_{\pi\in\mathbb{N}^\infty} \prod_{k>0} (tq^k)^{\pi_k} = \sum_{\pi_1=0}^{\infty} (qt)^{\pi_1} \sum_{\pi_2=0}^{\infty} (q^2 t)^{\pi_2} \cdots \\ &= \prod_{k>0} \frac{1}{1-q^k t} =: P(q;t) . \end{aligned} \tag{2.6}$$

If we fix r, another generating function can also be determined.

$$\sum_{n=0}^{\infty} p_r(n) q^n = \frac{q^r}{(1-q)(1-q^2)\cdots(1-q^r)} =: P_r(q) . \tag{2.7}$$

Table 2.3 gives $p_r(n)$ for $n = 1(1)15$. From the table it appears that $p_{n-k}(n) = f(k)$ if n is large enough, and in fact it is easy to show that $p_r(n) = p_{n-r}(2(n-r)) = p(n-r)$ for $r \geq n/2$.[9] This eliminates the need to calculate half the values in an exhaustive

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[6] Equation (2.4) and its relatives sometimes appear in physics, where they are useful in estimating energy level densities, e.g. the Bethe formula for the energy level density in nuclei [29] and similar formulae in Green, Schwarz and Witten [123], section 2.3.5, and Dyson [83].

[7] Nuclear physicists usually use the symbol m for multiplicity. Here we use r since m is reserved for one of the components in bipartite partitions. In chapter six we revert to the common usage in nuclear physics, replacing r, n, n_1, n_2 with m, A, Z, N.

[8] Historically, Euler and many other mathematicians have instead examined the related question of the number of partitions with *at most* r parts $p_{\leq r}(n)$, i.e. $p_r(n) = p_{\leq r}(n) - p_{\leq r-1}(n) = p_{\leq r}(n-r)$. Gupta's tables [134] in fact tabulate this function. Nuclear theorists are more interested in $p_r(n)$ however.

[9] Tomescu's problem book [295] gives this as problem 5.11. Section 2.3.2 proves a generalized formula for bipartite partitions which includes this result as a special case.

table. One can also show that $p_1(n) = 1$ and $p_2(n) = [\frac{n}{2}]$, and that as n tends to infinity, $p_r(n)$ is given asymptotically ($r = o(n^{1/3})$) by

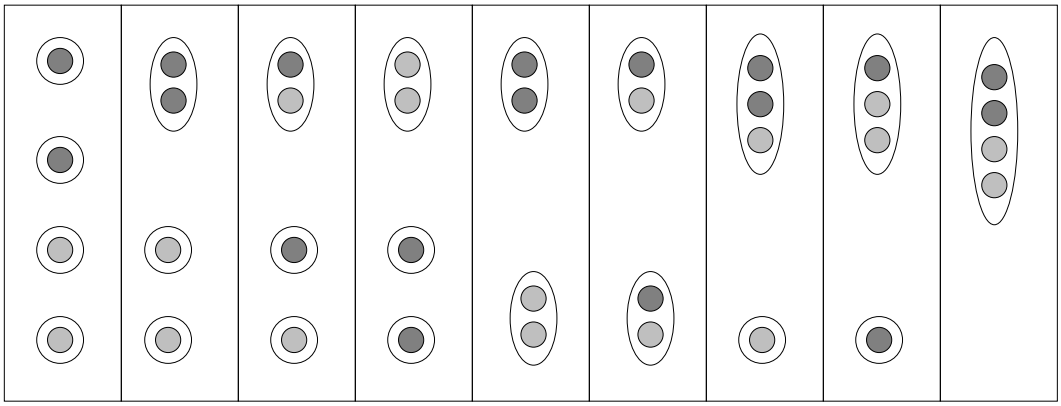
$$p_r(n) \sim \frac{1}{r!}\binom{n-1}{r-1} . \tag{2.8}$$

Table 2.3: Number of integer r-partitions $p_r(n)$ for $1 \leq r \leq n \leq 15$.

$r\backslash n$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
2		1	1	2	2	3	3	4	4	5	5	6	6	7	7
3			1	1	2	3	4	5	7	8	10	12	14	16	19
4				1	1	2	3	5	6	9	11	15	18	23	27
5					1	1	2	3	5	7	10	13	18	23	30
6						1	1	2	3	5	7	11	14	20	26
7							1	1	2	3	5	7	11	15	21
8								1	1	2	3	5	7	11	15
9									1	1	2	3	5	7	11
10										1	1	2	3	5	7
11											1	1	2	3	5
12												1	1	2	3
13													1	1	2
14														1	1
15															1

So for indistinguishable objects there are generating functions which enumerate the possible clusterings both with and without fixing the total number of parts. But the world is not populated exclusively with indistinguishable objects, so clearly the assumption that all the objects in a system are indistinguishable is not always appropriate. Suppose instead of all the objects being indistinguishable, the first n_1 objects are indistinguishable from each other, as are the last $n_2 = n - n_1$ objects, but the two groups of objects are distinguishable from each other. One example from physics where this situation arises is that of a group of n nucleons, n_1 of which are protons, n_2 of which are neutrons. For example, in a helium nucleus there are two protons and two neutrons, and with a little effort we can find the nine possible ways of forming clusters out of these four objects, as is shown in figure 2.2. When all the objects were indistinguishable the configurations could be uniquely specified by the sizes of the clusters. A cluster is now uniquely described by the number of protons (from 0 to n_1) and the number of neutrons

Figure 2.2: Cluster configurations for four objects of two distinguishable types (i.e. $n_1 = 2$, $n_2 = 2$).



(from 0 to n_2). Instead of a vector of n integers characterizing the cluster configuration, one needs a vector of $(n_1 + 1)(n_2 + 1) - 1$ integers, namely $\boldsymbol{\pi} = (\pi_{01}, \pi_{10}, \ldots, \pi_{n_1,n_2})$, such that the two constraints

$$\sum_{jk}(j,k)\pi_{jk} = (n_1, n_2) \tag{2.9}$$

are satisfied. Denote the set of all such vectors by $\pi(n_1, n_2)$, the set of partitions of the integer 2-vector (n_1, n_2),

$$\pi(n_1, n_2) = \left\{ \boldsymbol{\pi} \in \mathbb{N}^\infty \,\middle|\, \sum_{jk}(j,k)\pi_{jk} = (n_1, n_2) \right\} . \tag{2.10}$$

We denote by $n = n_1 + n_2$ the *content* of the system, i.e. the total number of objects. The number of such configurations $p(n_1, n_2) = |\pi(n_1, n_2)|$ can be computed from its generating function

$$\sum_{n_1,n_2\geq 0} p(n_1, n_2) q_1^{n_1} q_2^{n_2} = \prod_{jk} \frac{1}{1 - q_1^j q_2^k} =: P(q_1, q_2) . \tag{2.11}$$

It is easy to see that $p(n_1, n_2) = p(n_2, n_1)$ and $p(n_1, 0) = p(n_1)$, and table 2.4 lists values for the first few pairs of integers.

Mathematically, this generalization of integer partitions has not attracted much attention. In 1912, Percy A. MacMahon [200, 202], applying his earlier work on distributions [198], showed they could be enumerated using existing symmetric function tables. This led him to a series of papers on their enumeration [203–205], and a short

Table 2.4: Number of vector partitions $p(m,n)$ for $1 \le m,n \le 10$.

$r\backslash n$	1	2	3	4	5	6	7	8	9	10
1	2	4	7	12	19	30	45	67	97	139
2		9	16	29	47	77	118	181	267	392
3			31	57	97	162	257	401	608	907
4				109	189	323	522	831	1279	1941
5					339	589	975	1576	2472	3804
6						1043	1752	2876	4571	7128
7							2998	4987	8043	12693
8								8406	13715	21893
9									22652	36535
10										59521

table of $p(m,n)$ for $m \le 10, n \le 8$ appears in [204] (with several errors). In the 1950s, interest in the asymptotic behavior of $p(m,n)$ produced several papers (cited below) by F.C. Auluck, V.S. Nanda, E.M. Wright and M.M. Robertson. M.S. Cheema and T.S. Motzkin [62] extended these studies to r-partitions in 1971, and gave further asymptotic results and algorithms for computation.

Again it is clear that the number of partitions of (n_1, n_2) grows rapidly. Indeed, it is larger than the number of corresponding integer partitions of the same content, i.e. $p(n_1,n_2) \ge p(n_1+n_2)$ and is much greater when $n_1 \sim n_2$. For example, $p(10,10)/p(20) \approx 95$, $p(20,20)/p(40) \approx 8100$. The reason can be seen from the asymptotic expansion of $p(n,n)$, which was first presented by F.C. Auluck [14][10] in 1953

$$p(n,n) \sim \frac{\zeta(3)^{19/36}}{(72\pi^3)^{1/4} n^{55/36}} \exp\left\{ 3\zeta(3)^{1/3} n^{2/3} + \frac{\zeta(2)}{\zeta(3)^{1/3}} n^{1/3} + \zeta'(-1) + \frac{\zeta(2)^2}{4\zeta(3)^{2/3}} + \frac{1}{4} \right\}, \tag{2.12}$$

where $\zeta(z)$ is the Riemann zeta function, and $\zeta'(-1) \approx -0.165421$. So $p(n,n)$ grows

[10] Ignorant at first of this work, I made my own attempt at determining the asymptotics of $p(n,n)$. I was able to determine $\ln p(n,n) \sim Bn^{2/3} + Cn^{1/3}$, and found the correct expression for B (my expression for C was nearly correct). So I guessed $p(n,n) \sim An^{\alpha} \exp(Bn^{2/3} + Cn^{1/3})$, and tried to determine the constants from a table of $p(n,n)$ from $n = 1 - 640$ I had constructed. From this table I estimated $\alpha \approx -1.51$, which is very close to the exact value of $-55/36 \approx -1.52778$. I also estimated $B \approx 3.19$, $C \approx 1.54$ which compares well to the exact values $B = 3.189796$, $C = 1.547059$. The constant term I estimated as greater than $A \approx 0.03$, which is nowhere near $A = 0.317379$ according to Auluck, but as the constant term is the most difficult to estimate, the disagreement is not entirely unexpected. Auluck's result confirmed my hypothesis, but also dissuaded further numerical experiments, which I rather enjoyed. Additionally, unlike the Hardy-Ramanujan result, this was not determined from establishing a series expansion, but rather by applying a Tauberian theorem. As a result it can not be used as the starting point for an exact expression for $p(n,n)$.

exponentially with the 2/3 power of n, whereas $p(2n)$ grows exponentially with the 1/2 power of n. The asymptotics of $p(n_1, n_2)$ is less easily expressed, but still determinable in many cases, see V.S. Nanda [228], E.M. Wright [312, 314, 313], and M.M. Robertson [259, 258, 257, 260] for details.

The total number of clusters in a partition $\boldsymbol{\pi}$ is given by $r = \sum_{jk} \pi_{jk}$ and so the set of partitions of (n_1, n_2) into exactly r parts is defined by

$$\pi_r(n_1, n_2) = \left\{ \boldsymbol{\pi} \in \pi(n_1, n_2) \,\middle|\, r = \sum_{jk} \pi_{jk} \right\} . \tag{2.13}$$

It has size $p_r(n_1, n_2)$ given by the generating function,

$$\sum_{n_1 n_2, r} p_r(n_1, n_2) q_1^{n_1} q_2^{n_2} t^r = \prod_{jk} \frac{1}{1 - q_2^j q_2^k t} =: P(q_1, q_2; t) . \tag{2.14}$$

Similar to the case of integer partitions, $p_r(n_1, n_2) = f(n_1 + n_2 - r)$ if $r \geq \max(n_1 + n_2/2, n_2 + n_1/2)$, where $f(n) = p_{3n}(2n, 2n)$, which eliminates one sixth of the entries in an exhaustive table.[11] It is also asymptotic (as $n_1, n_2 \to \infty$) to

$$p_r(n_1, n_2) \sim \frac{1}{r!} \binom{n_1 - 1}{r - 1} \binom{n_2 - 1}{r - 1} . \tag{2.15}$$

Table 2.5: Number of vector r-partitions $p_r(m, n)$ for $1 \leq r \leq m + n \leq 10$.

	1	2	3	4	5	6	7
1,1	1	1					
2,1	1	2	1				
3,1	1	3	2	1			
2,2	1	4	3	1			
4,1	1	4	4	2	1		
3,2	1	5	6	3	1		
5,1	1	5	6	4	2	1	
4,2	1	7	10	7	3	1	
3,3	1	7	11	8	3	1	
6,1	1	6	9	7	4	2	1
5,2	1	8	15	12	7	3	1
4,3	1	9	18	16	9	3	1

	1	2	3	4	5	6	7	8	9	10
7,1	1	7	12	11	7	4	2	1		
6,2	1	10	21	21	13	7	3	1		
5,3	1	11	26	28	18	9	3	1		
4,4	1	12	29	32	21	10	3	1		
8,1	1	8	16	16	12	7	4	2	1	
7,2	1	11	28	31	23	13	7	3	1	
6,3	1	13	37	45	34	19	9	3	1	
5,4	1	14	42	53	42	23	10	3	1	
9,1	1	9	20	23	18	12	7	4	2	1
8,2	1	13	36	46	37	24	13	7	3	1
7,3	1	15	48	68	57	36	19	9	3	1
6,4	1	17	58	86	75	48	24	10	3	1
5,5	1	17	60	90	80	52	25	10	3	1

[11] See section 2.3.2 for details. A further one twelfth of the entries can be similarly eliminated.

The general case is to consider vector partitions[12] of $(n_1, \ldots, n_s)$, $n = \sum_{k=1}^{s} n_k$, where n_k are the number of indistinguishable objects of type k. We will call such systems s-component or s-partite systems of content n, as there are s types (components) of distinguishable objects and n objects overall. A cluster configuration of such a system is then given by the vector of $\prod_{j=1}^{s}(n_j+1)-1$ integers, $\boldsymbol{\pi} = (\pi_{00\ldots01}, \ldots, \pi_{n_1,\ldots,n_s})$ where $\pi_{k_1\ldots k_s}$, or $\pi_{\mathbf{k}}$ is the number of clusters with k_1 objects of the first type, k_2 objects of the second type, etc. There are s constraints on the cluster configurations, namely

$$\sum_{\mathbf{k}>\mathbf{0}} (k_1, \ldots, k_s)\pi_{\mathbf{k}} = (n_1, \ldots, n_s)\,, \tag{2.16}$$

and the set of all such cluster configurations or vector partitions is (not surprisingly) denoted by

$$\pi(\mathbf{n}) = \left\{ \boldsymbol{\pi} \in \mathbb{N}^{\infty} \,\middle|\, \sum_{\mathbf{k}>\mathbf{0}} \mathbf{k}\pi_{\mathbf{k}} = \mathbf{n} \right\}\,. \tag{2.17}$$

The properties of these vector partitions are generalizations of the 2-vector case, so we will just quickly summarize them. The number $p(\mathbf{n})$ of such configurations is again enumerated by a generating function

$$\sum_{\mathbf{n}\geq\mathbf{0}} p(\mathbf{n}) q_1^{n_1}\cdots q_s^{n_s} = \prod_{\mathbf{k}>\mathbf{0}} \frac{1}{1-q_1^{k_1}\cdots q_s^{k_s}} =: P(q_1, \ldots, q_s)\,. \tag{2.18}$$

The leading term for the asymptotic expansion of $p(\mathbf{n})$ for $n_k = n$, $k = 1, \ldots, s$ is given by

$$\ln p(n, \ldots, n) \sim (s+1)\zeta(s+1)^{1/(s+1)} n^{s/(s+1)}\,. \tag{2.19}$$

The total number of clusters is given by $r = \sum_{\mathbf{k}>\mathbf{0}} \pi_{\mathbf{k}}$ and the set of partitions of $(n_1, \ldots, n_s)$ into r parts is denoted by

$$\pi_r(\mathbf{n}) = \left\{ \boldsymbol{\pi} \in \pi(\mathbf{n}) \,\middle|\, r = \sum_{\mathbf{k}>\mathbf{0}} \pi_{\mathbf{k}} \right\}\,. \tag{2.20}$$

---

[12] Vector partitions have many names in the literature, such as multipartitions, partitions of multipartite numbers, partitions of integer vectors, etc. "Vector partitions" has obvious syntactic advantages, and will be used exclusively throughout this work.

Similarly, the generating function for $p_r(\mathbf{n})$[13] is given by

$$\sum_{\mathbf{n}\geq\mathbf{0},r} p_r(\mathbf{n}) q_1^{n_1}\cdots q_s^{n_s} t^r = \prod_{\mathbf{k}>\mathbf{0}} \frac{1}{1-q_1^{k_1}\cdots q_s^{k_s} t} =: P(q_1,\ldots,q_s;t)\ . \tag{2.21}$$

and its asymptotic behavior is given by

$$p_r(\mathbf{n}) \sim \frac{1}{r!}\prod_{k=1}^{s}\binom{n_k-1}{r-1}\ . \tag{2.22}$$

The important aspect of this rather long mathematical section is that describing the character of a system of objects with varying distinguishabilities is a well defined historical problem that has been solved in the following sense. For any particular distinguishability scheme, we can determine the number of available states, either exactly using generating functions as we will detail in section 2.3, or asymptotically using the Hardy-Ramanujan formula or its kin. The states themselves can be simply and uniquely described by enumerating the number of occurrences of each possible distinguishable cluster. Complicated distinguishability schemes therefore present only accounting difficulties, and are no more intrinsically difficult than the case of completely indistinguishable objects. In fact all of the cases considered in this section are simply examples of a general combinatorial object specified by a nonnegative integer vector $\boldsymbol{\pi} = (\pi_1, \pi_2, \ldots)$ satisfying the set of constraints

$$\sum_{k>0}(f_{k1},\ldots,f_{ks})\pi_k = (n_1,\ldots,n_s)\ . \tag{2.23}$$

The set of all such objects $\pi(\mathbf{n};f)$ is enumerated by the ordinary generating function

$$\sum_{\mathbf{n}\geq\mathbf{0}} p(\mathbf{n};f)\prod_{k=1}^{s} q_k^{n_k} = \prod_{j>0}\frac{1}{1-\prod_{k=1}^{s} q_k^{f_{jk}}}\ . \tag{2.24}$$

---

[13] MacMahon [202] showed that this can be expressed in terms of a sum over ordinary partitions of r, namely

$$\sum_{\mathbf{n}\geq\mathbf{0},r} p_r(\mathbf{n}) q_1^{n_1}\cdots q_s^{n_s} t^r = \sum_r t^r(1-t)\sum_{\pi(r)}\prod_{k>0}\frac{1}{\pi_k!}\left(\frac{1}{k\prod_{j=1}^{s}(1-q_j^k)}\right)^{\pi_k}$$

a formula which is interesting, but not particularly helpful in practical calculations (except when r is small).

2.1.2 Set partitions and permutations

The previous section assumes that all objects are indistinguishable, or that the objects form sets of indistinguishable objects. Suppose instead that all objects are distinguishable. By the above discussion, the states are given by partitions of the n-vector $(1, 1, \ldots, 1)$, but there is another point of view which is useful to consider. Since each object is distinguishable, each cluster is distinguishable and is specified by the set of objects which it contains, so $\pi_{\mathbf{k}} = 0, 1$ for any $\mathbf{k}$. So we might as well only list the clusters which appear. A partition of all the objects into clusters is therefore equivalent to a partition of the set of objects into disjoint subsets (i.e. clusters). In mathematical language, we are interested in partitioning the set of (distinguishable) objects X into subsets $X_1, \ldots, X_r$ such that $X_i \cap X_j = \emptyset, i \neq j$ and $\cup_i X_i = X$. This casting of the problem into mathematical language shows the partitioning of distinguishable objects is the mathematical equivalent of set partitioning, just as the partitioning of indistinguishable objects is equivalent to integer partitioning. Denote the set of all set partitions of n objects by $\beta(n)$ and the set of all set partitions of n objects into exactly r parts, i.e. set r-partitions of n, by $\beta_r(n)$. It is a well known fact that the number of set partitions of n objects is given by the Bell number $B(n)$ and the number of set r-partitions of n objects is given by the Stirling number of the second kind $\left\{ {n \atop r} \right\}$ [296]. Stirling numbers (of both kinds) were introduced by James Stirling [281] in 1730, and Bell numbers were introduced in 1934 by Eric T. Bell [24,23,25]. As in the case of partitions, we can derive generating functions which determine these numbers. Exponential generating functions for these numbers can be found in most combinatorics books, see Tomescu [296] for instance, so we simply quote the results

$$\sum_{n \geq 0} B(n) \frac{q^n}{n!} = e^{e^q - 1} , \tag{2.25}$$

$$\sum_{n \geq 0} \sum_{r \geq 0} \left\{ {n \atop r} \right\} \frac{q^n}{n!} t^r = e^{t(e^q - 1)} . \tag{2.26}$$

Some alternative generating functions for $\left\{ {n \atop r} \right\}$ are

$$\sum_{n\geq 0} \left\{ {n \atop r} \right\} q^n = \frac{q^r}{(1-q)(1-2q)\cdots(1-rq)} , \tag{2.27}$$

$$\sum_{n\geq 0} \left\{ {n \atop r} \right\} \frac{q^n}{n!} = \frac{(e^q-1)^r}{r!} . \tag{2.28}$$

Tables 2.6 and 2.7 list the first few Bell numbers and Stirling numbers of the second kind. Notice that the number of set partitions $B(n)$ grow much more quickly than the corresponding number of integer partitions $p(n)$ (as to be expected), and that $\left\{ {n \atop 1} \right\} = \left\{ {n \atop n} \right\} = 1$, $\left\{ {n \atop 2} \right\} = 2^{n-1}-1$, $\left\{ {n \atop n-1} \right\} = \binom{n}{2}$. Asymptotic results [224,223] with $n \to \infty$ are given by

$$\begin{aligned} B(n) &\sim \frac{e^{n(R+1/R-1)-1}}{(R+1)^{1/2}} \left(1 - \frac{R^2(2R^2+7R+10)}{24n(R+1)^3} \right) , \\ \left\{ {n \atop r} \right\} &\sim \frac{r^n}{r!} , \\ \left\{ {n \atop n-r} \right\} &\sim \frac{n^{2r}}{r!2^r} . \end{aligned} \tag{2.29}$$

where $R + \ln R = \ln n$.

Table 2.6: Number of set partitions or Bell numbers $B(n)$ for $n = 1(1)12$.

n	1	2	3	4	5	6	7	8	9	10	11	12
$B(n)$	1	2	5	15	52	203	877	4140	21147	115975	678570	4213597

Since each set partition of $X = \cup_j X_j$ can be associated with a unique integer partition of $|X|$ by associating each X_j with an integer part of size $|X_j|$, we have a natural map from the set partitions to the integer partitions. Many set partitions can map to the same integer partitions (as expected, since $B(n) \geq p(n)$) but every integer partition has at least one set partition in the map's preimage, so the map is surjective but not bijective. For example, the second column of table 2.8 details such a projection of β_4 onto $\pi(4)$. The number of set partitions which map to a particular integer partition

Table 2.7: Number of set r-partitions or Stirling numbers of the second kind $\left\{ {n \atop r} \right\}$ for $1 \leq r \leq n \leq 12$.

$r \backslash n$	1	2	3	4	5	6	7	8	9	10	11	12
1	1	1	1	1	1	1	1	1	1	1	1	1
2		1	3	7	15	31	63	127	255	511	1023	2047
3			1	6	25	90	301	966	3025	9330	28501	86526
4				1	10	65	350	1701	7770	34105	145750	611501
5					1	15	140	1050	6951	42525	246730	1379400
6						1	21	266	2646	22827	179487	1323652
7							1	28	462	5880	63987	627396
8								1	36	750	11880	159027
9									1	45	1155	22275
10										1	55	1705
11											1	66
12												1

$\boldsymbol{\pi}$ of n is attributed to Cauchy[14], and is equal to

$$\text{Part}(\boldsymbol{\pi}) = n! \prod_{j>0} \frac{1}{\pi_j!(j!)^{\pi_j}} \ . \tag{2.30}$$

This identity will have significant consequences when we discuss statistics in the next chapter (see section 3.1.1).

Note that the cluster decomposition function can be modified to induce instead a map from set partitions of X onto any particular vector partition of content $|X|$. For example, to model partitions of integer 2-vectors, the cycle decomposition can be modified to distinguish between the two kinds of objects, inducing a different surjective map to project out the cycle structure. These kinds of configurations can arise from the set partition picture by mapping a set partition to a cluster exactly as before, only distinguishing the first n_1 elements as different from the last n_2. The third column in table 2.8 shows such a decomposition for β_4 onto $\pi(2,2)$. The number of set partitions which correspond to a specific partition of (n_1, n_2) is given by the generalization of

[14]Many combinatorics texts attribute this result to Cauchy, but none give a reference. Indeed, Sylvester and Jacobi may deserve credit for this result, but it will probably continue to be called the "Cauchy" numbers

Table 2.8: The fifteen set partitions of β_4 and their partition representations in $\pi(4)$ and $\pi(2,2)$.

$\boldsymbol{\beta} \in \beta_4$	$(\pi_1, \ldots, \pi_4)$	$(\pi_{01}, \pi_{02}, \pi_{10}, \ldots \pi_{22})$
{1}{2}{3}{4}	(4, 0, 0, 0)	(2,0,2,0,0,0,0,0)
{1, 2}{3}{4}	(2, 1, 0, 0)	(2,0,0,0,0,1,0,0)
{1, 3}{2}{4}	(2, 1, 0, 0)	(1,0,1,1,0,0,0,0)
{1, 4}{2}{3}	(2, 1, 0, 0)	(1,0,1,1,0,0,0,0)
{2, 3}{1}{4}	(2, 1, 0, 0)	(1,0,1,1,0,0,0,0)
{2, 4}{1}{3}	(2, 1, 0, 0)	(1,0,1,1,0,0,0,0)
{3, 4}{1}{2}	(2, 1, 0, 0)	(0,1,2,0,0,0,0,0)
{1, 2}{3, 4}	(0, 2, 0, 0)	(0,1,0,0,0,1,0,0)
{1, 3}{2, 4}	(0, 2, 0, 0)	(0,0,0,2,0,0,0,0)
{1, 4}{2, 3}	(0, 2, 0, 0)	(0,0,0,2,0,0,0,0)
{1, 2, 3}{4}	(1, 0, 1, 0)	(1,0,0,0,0,0,1,0)
{1, 2, 4}{3}	(1, 0, 1, 0)	(1,0,0,0,0,0,1,0)
{1, 3, 4}{2}	(1, 0, 1, 0)	(0,0,1,0,0,1,0,0)
{2, 3, 4}{1}	(1, 0, 1, 0)	(0,0,1,0,0,1,0,0)
{1, 2, 3, 4}	(0, 0, 0, 1)	(0,0,0,0,0,0,0,1)

Cauchy's number,

$$\mathrm{Part}(\boldsymbol{\pi}) = n_1! n_2! \prod_{jk} \frac{1}{\pi_{jk}!(j!k!)^{\pi_{jk}}} \ . \tag{2.31}$$

Generalizing to the vector partition case is simple enough. Vector partition cluster configurations can be derived surjectively from set partitions by identifying subsets in the set partitions with cluster configurations, treating $1, \ldots, n_1$ as indistinguishable, $n_1 + 1, \ldots, n_1 + n_2$ as indistinguishable, etc. The number of set partitions which map to a particular partition is given by

$$\mathrm{Part}(\boldsymbol{\pi}) = \left(\prod_{j=1}^{s} n_j! \right) \prod_{\mathbf{k}>\mathbf{0}} \frac{1}{\pi_{\mathbf{k}}!(k_1! \cdots k_s!)^{\pi_{\mathbf{k}}}} \ . \tag{2.32}$$

If the objects are not only distinguishable, but within each cluster the sequence of the objects is distinguishable (the first object in the cluster sequence being arbitrary), then the partitions of the objects are identified with permutations and cycle decomposition of the permutation determines the cluster configurations. We denote by S_n the set of all permutations on n objects and $S_n^{(r)}$ the set of permutations with a total of r cycles. Determining the order of these sets is an old problem in combinatorics. The

number of permutations of n objects is simply the factorial number $n!$ and the number of r-permutations is given by $\left[{n \atop r}\right]$, the unsigned Stirling numbers of the first kind [281]. Exponential generating functions for these numbers are given by

$$\sum_{n\geq 0} n!\frac{q^n}{n!} = \frac{1}{1-q}\,, \tag{2.33}$$

$$\sum_{n\geq 0}\sum_{r\geq 0}\left[{n \atop r}\right]\frac{q^n}{n!}t^r = \left(\frac{1}{1-q}\right)^t\,. \tag{2.34}$$

An alternate generating function $\left[{n \atop r}\right]$ is

$$\sum_{n\geq 0}\left[{n \atop r}\right]\frac{q^n}{n!} = \frac{(-\ln(1-q))^r}{r!}\,. \tag{2.35}$$

Tables 2.9 and 2.10 list the first few factorial numbers and unsigned Stirling numbers of the first kind. Again, the table shows the number of permutations grow more quickly than the number of set or integer partitions, and that $\left[{n \atop n}\right] = 1$, $\left[{n \atop 1}\right] = (n-1)!$, $\left[{n \atop n-1}\right] = \binom{n}{2}$. Asymptotic results [225] for $n \to \infty$ are

$$\begin{aligned} n! &\sim \sqrt{2\pi}n^{n+1/2}e^{-n}\,, \\ \left[{n \atop r}\right] &\sim (n-1)!\frac{(\gamma+\ln n)^{r-1}}{(r-1)!}\,, \\ \left[{n \atop n-r}\right] &\sim \binom{n}{r}\left(\frac{n-r}{2}\right)^r\,, \end{aligned} \tag{2.36}$$

where $\gamma \approx 0.5772156649$ is Euler's constant.[15]

Table 2.9: Number of permutations or factorial numbers $n!$ for $n = 1(1)10$.

n	1	2	3	4	5	6	7	8	9	10
$n!$	1	2	6	24	120	720	5040	40320	362880	3628800

As in the case of set partitions, cluster decomposition of the permutations induces a map from the permutations onto the set of integer partitions. In other words, identify a permutation with a particular cluster configuration by decomposing the permutation into its cycles and associating each cycle of length k with a cluster of size k. As with set partitions, this map can be modified to project onto any vector partition space,

[15] More extensive asymptotic formulae for Stirling numbers can be found in [292].

Table 2.10: Number of r-permutations or unsigned Stirling numbers of the first kind $\left[{n \atop r}\right]$ for $1 \leq r \leq n \leq 10$.

$r\backslash n$	1	2	3	4	5	6	7	8	9	10
1	1	1	2	6	24	120	720	5040	40320	362880
2		1	3	11	50	274	1764	13068	109584	1026576
3			1	6	35	225	1624	13132	118124	1172700
4				1	10	85	735	6769	67284	723680
5					1	15	175	1960	22449	269325
6						1	21	322	4536	63273
7							1	28	546	9450
8								1	36	870
9									1	45
10										1

or onto the set partitions. As an example consider the 24 permutations of $n = 4$ and their identification both integer partitions and vector partitions of $(2,2)$ as given in table 2.11. Again this is a surjective map from the permutations to the partitions, and the number of permutations which map to a particular integer partition[16] $\boldsymbol{\pi}$ of n was calculated by Cauchy, who showed it equal to

$$\mathrm{Perm}(\boldsymbol{\pi}) = n! \prod_{j>0} \frac{1}{\pi_j! j^{\pi_j}} \ . \tag{2.37}$$

A similar formula generalizes the map of permutations onto a particular vector partition, giving the generalized Cauchy number

$$\mathrm{Perm}(\boldsymbol{\pi}) = \left(\prod_{j=1}^{s} n_j! \right) \prod_{\mathbf{k}>\mathbf{0}} \frac{1}{\pi_{\mathbf{k}}!} \left(\frac{(k-1)!}{k_1! \cdots k_s!} \right)^{\pi_{\mathbf{k}}} \ . \tag{2.38}$$

where $k = \sum_{j=1}^{s} k_j$.

In conclusion we have extended the notion of distinguishability in such a way so as to naturally identify set partitions and permutations with clustering objects. More importantly, the connection between these objects and integer and vector partitions introduced in the previous section has been made explicit and denumerable by defining the Cauchy numbers. These numbers can be determined quickly from the compact formulas given in the section. Indeed, the form of the Cauchy numbers is fortunate in view

[16] $\mathrm{Perm}(\pi)$ is denoted $M_2(\pi)$ in Abramowitz and Stegun [1].

of the kinds of statistical models we will be interested in analyzing. Figure 2.3 sketches the hierarchical relationship between various representations of clustering states we have introduced, a figure which should reinforce the fact that various distinguishability schemes can be implemented by projecting states out of the more general objects such as permutations or set partitions.

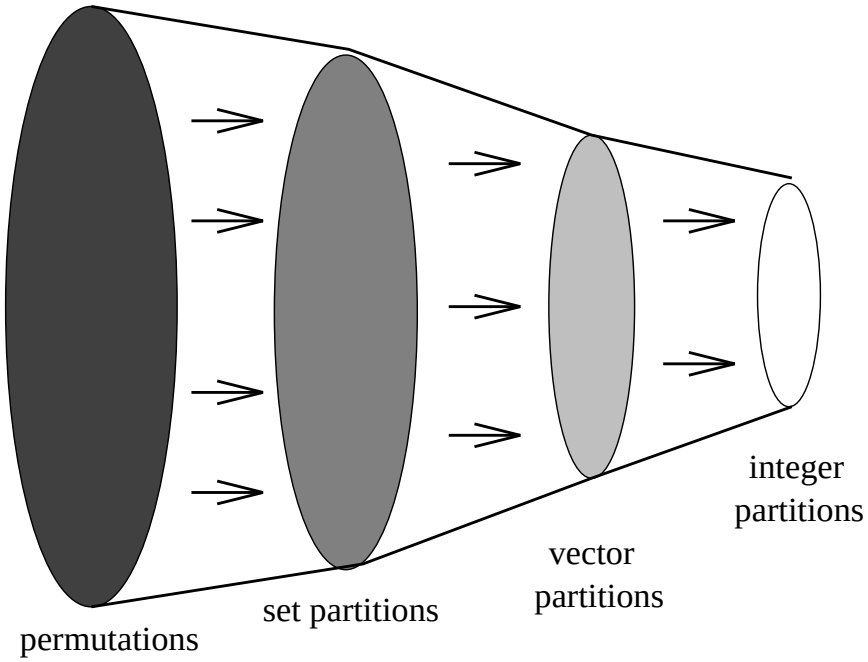
Table 2.11: The twenty four permutations of S_4 (in standard and cycle notation) and their partition representations in $\pi(4)$, $\pi(2,2)$.

p	p	$(\pi_1, \ldots, \pi_4)$	$(\pi_{01}, \pi_{02}, \pi_{10}, \ldots, \pi_{22})$
(1,2,3,4)	(1)(2)(3)(4)	(4,0,0,0)	(2,0,2,0,0,0,0,0)
(1,2,4,3)	(1)(2)(3,4)	(2,1,0,0)	(0,1,2,0,0,0,0,0)
(1,3,2,4)	(1)(2,3)(4)	(2,1,0,0)	(1,0,1,1,0,0,0,0)
(1,4,3,2)	(1)(2,4)(3)	(2,1,0,0)	(1,0,1,1,0,0,0,0)
(3,2,1,4)	(1,3)(2)(4)	(2,1,0,0)	(1,0,1,1,0,0,0,0)
(4,2,3,1)	(1,4)(2)(3)	(2,1,0,0)	(1,0,1,1,0,0,0,0)
(2,1,3,4)	(1,2)(3)(4)	(2,1,0,0)	(2,0,0,0,0,1,0,0)
(1,3,4,2)	(1)(2,3,4)	(1,0,1,0)	(0,0,1,0,1,0,0,0)
(1,4,2,3)	(1)(2,4,3)	(1,0,1,0)	(0,0,1,0,1,0,0,0)
(4,2,1,3)	(1,4,3)(2)	(1,0,1,0)	(0,0,1,0,1,0,0,0)
(3,2,4,1)	(1,3,4)(2)	(1,0,1,0)	(0,0,1,0,1,0,0,0)
(2,3,1,4)	(1,2,3)(4)	(1,0,1,0)	(1,0,0,0,0,0,1,0)
(2,4,3,1)	(1,2,4)(3)	(1,0,1,0)	(1,0,0,0,0,0,1,0)
(3,1,2,4)	(1,3,2)(4)	(1,0,1,0)	(1,0,0,0,0,0,1,0)
(4,1,3,2)	(1,4,2)(3)	(1,0,1,0)	(1,0,0,0,0,0,1,0)
(2,1,4,3)	(1,2)(3,4)	(0,2,0,0)	(0,1,0,0,0,1,0,0)
(3,4,1,2)	(1,3)(2,4)	(0,2,0,0)	(0,0,0,2,0,0,0,0)
(4,3,2,1)	(1,4)(2,3)	(0,2,0,0)	(0,0,0,2,0,0,0,0)
(3,4,2,1)	(1,3,2,4)	(0,0,0,1)	(0,0,0,0,0,0,0,1)
(4,1,2,3)	(1,4,3,2)	(0,0,0,1)	(0,0,0,0,0,0,0,1)
(2,3,4,1)	(1,2,3,4)	(0,0,0,1)	(0,0,0,0,0,0,0,1)
(2,4,1,3)	(1,2,4,3)	(0,0,0,1)	(0,0,0,0,0,0,0,1)
(3,1,4,2)	(1,3,4,2)	(0,0,0,1)	(0,0,0,0,0,0,0,1)
(4,3,1,2)	(1,4,2,3)	(0,0,0,1)	(0,0,0,0,0,0,0,1)

2.2 Combinatorial theories

The objects defined in the previous section adequately describe the states of a fragmenting system, but applying them successfully will require more combinatorial theory than

Figure 2.3: Schematic figure illustrating the relation (generally surjective) between various combinatorial fragmentation objects under projection.



the amount presented already for their enumeration. This section introduces Pólya-de Bruijn enumeration theory (2.2.1) and symmetric function theory (2.2.2), combinatorial theories which will prove to be quite useful in the next chapter when computing statistical functions. Since they can be defined and applied independently of the statistical models, they are presented here in a strictly combinatorial setting. Statistical interpretations of the results will wait till the next chapter.

Good references for this section are numerous, and for Pólya-de Bruijn enumeration theory include the previously mentioned works by Tomescu [296], Berge [26] and Riordan [255] as well as *Graph Theory* by Frank Harary [140]. Symmetric functions are most often discussed in the context of the theory of equations, but MacMahon's *Combinatory Analysis* [201] or more recently *Symmetric functions and Hall polynomials* by Ian MacDonald [195] present them from a combinatoric vantage.

2.2.1 Pólya-de Bruijn enumeration theory

The previous section showed that given the set of set partitions (or permutations) on n objects and an appropriate cluster decomposition function, we can project onto any vector partition space, and hence can describe any distinguishability scheme in the context of set partitioning. In this instance information about the distinguishability of objects is contained in the cluster decomposition function. We can make the distinguishability mapping more formal by encoding it directly in a symmetry group G of permutations on the n objects. For example if all objects are distinguishable, then the group G containing only the identity element encodes the distinguishability, since any nontrivial permutation of a configuration can be detected as all the objects are distinguishable. On the other extreme, if all objects are indistinguishable any permutation on n elements leaves configurations unchanged, so that the symmetry group is $G = S_n$, the complete permutation group on n objects.

This notion of distinguishability defined by a symmetry group is the basis for Pólya-de Bruijn enumeration theory [242, 243, 42]. This theory is a beautiful combination of group theory, partitions and symmetric functions (see next section) which was developed to systematically solve a number of difficult enumeration problems. Although this dissertation has no need to apply it for its designed purpose, the central function of Pólya theory is the same as the canonical Gibbs model partition function in statistical physics (section 3.2.1) which will play a central role in our description of many physical systems, and so a brief discussion of the theory is merited. Proofs of the principal results are omitted, but can be found in the above references. Historically, it should be noted that the essence of George Pólya's 1937 paper is to be found in a paper by J.H. Redfield [251] ten years earlier which for some unfortunate reason languished in obscurity for years before being discovered around 1960 by Frank Harary, a noted graph theorist [139, 140]. Additionally, some of MacMahon's work [201] touches on elements of Pólya theory. A rather modest application of this theory is made in section 5.8 to counting loop-free graphs and digraphs, and the theory has occasionally been applied to problems of physical interest such as the determination of virial expansions in non-ideal

gases [298, 254, 181].

First we will review some basic notions from group theory.[17] A *group* $(G, \bullet)$ is (technically) a set G and a binary operator $\bullet$ which satisfy the group axioms (see figure 2.4). Nontechnically, a group is a way of encoding how a system changes under a set of transformations. For example, if you rotate an n-sided polygon about its center in the plane by an angle $2\pi/n$ repeatedly, you will form a group, known as the cyclic group Z_n. If we add one more rotation about the center through one of its vertices, we double the number of possible arrangements of the vertices, and have constructed the dihedral group D_n. The symmetric group S_n is the group of all bijections on n objects with the operator being function composition, i.e. permutations on n objects, and in this polygon representation is all possible ways of labeling the n vertices.

Figure 2.4: Group theory axioms

- (closure) $\forall g, h \in G, g \bullet h \in G$.
- (associativity) $\forall f, g, h \in G,\ f \bullet (g \bullet h) = (f \bullet g) \bullet h$
- (identity) $\exists e \in G, e \bullet e = e$.
- (inverse) $\forall g \in G, \exists h \in G,\ g \bullet h = h \bullet g = e$

The following definitions are needed for our discussion. The *order* of a group G is the size of the set G, and is denoted $|G|$. A *subgroup* H of a group G is simply a subset of the group which still satisfies the group axioms. Two groups G, H are *isomorphic* if there exists a bijection between them such that the group structure is preserved, i.e. $\exists f : G \to H,\ f(g \bullet_G h) = f(g) \bullet_H f(h)$. The *direct product* of two groups G and H is the set of all ordered pairs of elements (g, h), $g \in G, h \in H$ with the product rule, $(g_1, h_1) \bullet (g_2, h_2) = (g_1 g_2, h_1 h_2)$. By construction $|G \times H| = |G||H|$. If G acts on a set X, the *orbit* of $x \in X$ is the set $\{gx : g \in G\} \subseteq X$.

Suppose we have $n = \sum_{k=1}^{s} n_k$ objects, each n_k being a set of indistinguishable objects, but the groups are separately distinguishable. Within each set, the permutation

[17] There are many good introductory group theory books, but I referred to Herstein [146] to prepare this section.

group S_{n_k} encodes the symmetry, which is independent of the symmetry of any other group of objects. Therefore the overall symmetry group G must contain permutations which permute within the separate sets of objects but not among each other. A direct product of symmetry groups has this property, and we see that the symmetry group for the vector partition scheme $(n_1, \ldots, n_s)$ is encoded in the group $G = S_{n_1} \times \cdots \times S_{n_s}$, with $|G| = \prod_{k=1}^{s} n_k!$. Now this group is in fact a subgroup of S_n[18]. For every element in S_n, and therefore for any element in its subgroup G, we can assign a set of cycle indexes $\pi_1, \pi_2, \ldots$ where π_j is the number of cycles in the permutation of length j, such that if $p \in S_n$ then $\sum_{k>0} k\pi_k(p) = n$ since each element of the group lies in exactly one cycle. In fact, this was just what was done when we defined the Cauchy numbers in the last section. Let X be our set of objects, then the orbits of X are the sets of indistinguishable objects.

We can now write down a simple theorem due to Pólya which generalizes a well known result attributed to Burnside but certainly known to Cauchy and Frobenius much earlier.

Theorem 2.2.1 (Pólya) *Let G be a permutation group acting on a set $X \subseteq [n]$ with orbits $\theta_1, \ldots, \theta_r$ and let w be a function which assigns a weight to each $x \in X$ such that $w(x) = w(\theta_i)$ whenever $x \in \theta_i$. Then the sum of the weights of the orbits is given by*

$$\sum_i w(\theta_i) = \frac{1}{|G|} \sum_{g \in G} \sum_{x = gx} w(x) \, . \tag{2.39}$$

An immediate corollary is the well known Burnside's lemma.

Corollary 2.2.1 (Burnside's lemma) *The number of orbits in a group $G \leq S_n$ is*

$$N(G) = \frac{1}{|G|} \sum_{g \in G} \pi_1(g) \, . \tag{2.40}$$

Proof: Let $w(x) = 1$ and apply Pólya's theorem.

This simple result due to Pólya is the basis of Pólya's theorem which we will now motivate.[19] Suppose we have a set of objects X, $|X| = n$ whose distinguishability is

[18] Cayley's theorem states that every finite group is a subgroup of some permutation group S_m, but in this case $m \leq n$, and for convenience we can think of it as a subgroup of S_n.

[19] The path from the simple result to the more powerful theorem is unfortunately omitted. Interested readers should consult this sections references.

given by a group G and a set of colors R, $|R| = r$. We want to color each object in X with exactly one color from R. Call such a coloring c, which is a map from X to R, i.e. $c : X \to R$. Suppose each color $r \in R$ has *content* $w(r)$ given by a nonnegative integer. Define the content of a coloring as the sum of the contents assigned to the colors of each object, i.e.

$$w(c) = \sum_{x \in X} w(c(x)) \, . \tag{2.41}$$

The combinatorial question which Pólya theory then answers is given R and $w : R \to \{0, 1, 2, \ldots\}$, how many different colorings on X have a given total content w, treating colorings as equivalent if $\exists g \in G$ which transforms one coloring into another.

Theorem 2.2.2 (Pólya's enumeration theorem) *Let X be a set of objects, $|X| = n$ and $G \leq S_n$ a group of permutations acting on X describing the distinguishability of the objects. Let R be a set of colors, and*

$$f(x) = \sum_j f_j x^j \, , \tag{2.42}$$

$$F(x) = \sum_j F_j x^j \tag{2.43}$$

be generating functions, where f_j is the number of colors having content j and F_j is the number of equivalence classes (colorings) of content j. Then,

$$F(x) = Z(G, f(x), f(x^2), \ldots, f(x^n)) \, , \tag{2.44}$$

where

$$Z(G; g_1, \ldots, g_n) := \frac{1}{|G|} \sum_{g \in G} \prod_{j \geq 1} g_j^{\pi_j(g)} \tag{2.45}$$

is the cycle index function.

Nicolaas G. de Bruijn as well as others have extended this theorem in various ways and this theory is generally referred to as Pólya-de Bruijn enumeration. One important generalization is that if the content is given by a vector of nonnegative integers, then the theorem becomes

$$F(x_1, \ldots, x_m) = Z(G, f(x_1, \ldots, x_m), f(x_1^2, \ldots, x_m^2), \ldots f(x_1^n, \ldots, x_m^n)) \, . \tag{2.46}$$

One other important result is that is the group G is a direct product, then the cycle index function is a simple product, i.e.

$$Z(G \times H) = Z(G)Z(H)\,. \tag{2.47}$$

This is all very interesting for the combinatorist, but should a physicist be interested in these counting methods. The short answer is yes. The combinatorial interpretation is easily reinterpreted as a statistical one, and the theorem then provides a method to solve these problems. For example, note that for the full permutation group, the cycle index is given by

$$Z(S_n; g_1, \ldots, g_n) = \sum_{\pi(n)} \prod_{j \geq 1} \frac{1}{\pi_j!} \left(\frac{g_j}{j}\right)^{\pi_j}\,. \tag{2.48}$$

Therefore, for indistinguishable objects, this sum is of critical importance. In fact, we will show in the next section that it is a particular symmetric function of historical significance, and moreover it is related to a statistical model which can be used to describe the fragmentation and aggregation of indistinguishable objects (see section 3.2.1). For now, we will just note that if we have an infinite number of colors, each with a unique content, then $f_j = 1 \Rightarrow f(x) = 1/(1-x)$, and by Pólya's theorem

$$F(x) = \sum_{\pi(n)} \prod_{j \geq 1} \frac{1}{\pi_j!} \left(\frac{1}{j(1-x^j)}\right)^{\pi_j}\,;. \tag{2.49}$$

But $F(x) = \sum_j F_k x^k$ with F_k the number of colorings of content k. Since each color has a unique content and there are only n objects to color, we can say $k = \sum_{j=1}^{n} j\pi_j$, or that $F(x)$ enumerates partitions with maximum part n, i.e.

$$F(x) = \frac{1}{(1-x)(1-x^2)\cdots(1-x^n)}\,. \tag{2.50}$$

Combining equations (2.49) and (2.50) gives a partition identity originally due to Cayley [53, 55, 201], namely,

$$\frac{1}{(1-x)(1-x^2)\cdots(1-x^n)} = \sum_{\pi(n)} \prod_{j \geq 1} \frac{1}{\pi_j!} \left(\frac{1}{j(1-x^j)}\right)^{\pi_j}\,. \tag{2.51}$$

2.2.2 Symmetric function theory

From Pólya theory it is natural to introduce the theory of symmetric functions. A symmetric function is a function on n variables such that under any permutation of the variables the function is invariant. For example, $f(x_1, x_2, x_3) = x_1x_2x_3 + x_1^3 + x_2^3 + x_3^3$ is a symmetric function on three variables. Interest in the theory of symmetric functions arose from the efforts of mathematicians studying polynomial equations. Sir Isaac Newton [230] in 1707 proved that given the polynomial equation

$$x^n + a_1x^{n-1} + \cdots + a_n = 0 \ , \tag{2.52}$$

with roots $x_1, \ldots, x_n$, the following relation between the roots and the coefficients holds,

$$\begin{aligned} -a_1 &= x_1 + x_2 + \ldots + x_n \ , \\ +a_2 &= x_1x_2 + x_1x_3 + \cdots \ , \\ \vdots &\quad \vdots \ , \\ (-1)^n a_n &= x_1x_2 \cdots x_n \ , \end{aligned}$$

i.e., that the coefficients are symmetric functions of the roots. The combinatorial significance of symmetric functions was recognized by Percy A. MacMahon, who used them extensively in his treatise *Combinatory Analysis* [201], which collected results from his earlier published papers. We will see shortly that they also arise in the Pólya theory of indistinguishable objects.

Putting aside historical questions for the moment, the symmetric functions e_n, k_n[20] are defined implicitly by the following two generating functions.

$$E(q) = \prod_{j>0}(1 + x_jq) = \sum_{n\geq 0} e_nq^n \ , \tag{2.53}$$

$$K(q) = \prod_{j>0} \frac{1}{1 - x_jq} = \sum_{n\geq 0} k_nq^n \ , \tag{2.54}$$

[20] k_n is usually denoted h_n for the homogenous symmetric function, i.e. $k_n = h_n$. For vector partitions the generalization of the homogenous symmetric function is different from the generalization we use, i.e. $k_{mn} \neq h_{mn}$, and so forth for other integer vectors, so we have adopted k_n throughout the section to avoid possible confusion.

which are equivalent to the following explicit definitions,

$$e_n := \sum_{j_1<\cdots<j_n} x_{j_1} x_{j_2} \cdots x_{j_n} , \tag{2.55}$$

$$k_n := \sum_{\pi(n)} \sum_{j_1<\cdots<j_n} x_{j_1}^{\pi_1} \cdots x_{j_n}^{\pi_n} . \tag{2.56}$$

Notice that k_n becomes the generating function for $p_r(n)$ if $x_j = t^j$. It is useful to define the elementary symmetric function s_n[21] explicitly by

$$s_n := \sum_{j>0} x_j^n . \tag{2.57}$$

Its generating function is therefore given by

$$S(q) = \sum_{n\geq 0} s_n q^n = \sum_{n\geq 0}\sum_{j>0} x_j^n q^n = \sum_{j>0} \frac{1}{1-x_j q} . \tag{2.58}$$

These three functions are the symmetric functions of principle interest in combinatorics. For our purposes, we are only interested in s_n and k_n, but we will include results for e_n for completeness.

In practice, there are easy ways to compute one symmetric function from another. For example, clearly $K(q)E(-q) = 1$ from the generating function definitions, so we have the following recursion for k_n in terms of the e_j's, and vice versa.

$$k_n = \sum_{j=1}^{n} (-1)^{j+1} e_j k_{n-j} . \tag{2.59}$$

The following computation reveals k_n is also a recursive function of s_j's.

$$\begin{aligned} S(q) - 1 &= \sum_{j>0}\sum_{n\geq 1} x_j^n q^n = \sum_{j>0} \frac{x_j q}{1-x_j q} = q\frac{d}{dq}\sum_{j>0} \ln \frac{1}{1-x_j q} \\ &= q\frac{d}{dq} \ln \prod_{j>0} \frac{1}{1-x_j q} = q\frac{d}{dq} \ln K(q) = \frac{qK'(q)}{K(q)} . \end{aligned} \tag{2.60}$$

This implies (for $n \geq 1$) from a term by term comparison

$$nk_n = \sum_{j=1}^{n} s_j k_{n-j} . \tag{2.61}$$

---

[21] s_n is usually denoted p_n in modern papers. Since this can easily be confused with $p(n)$, the number of integer partitions of n, I have retained the old notation used by MacMahon [201].

Table 2.12: Elementary symmetric function recursion inter-relations.

	$e_n \leftrightarrow k_n$	s_n
e_n	$e_n = \sum_{j=1}^{n}(-1)^{j+1}k_j e_{n-j}$	$ne_n = \sum_{j=1}^{n}(-1)^{j}s_j e_{n-j}$
k_n	$k_n = \sum_{j=1}^{n}(-1)^{j+1}e_j k_{n-j}$	$nk_n = \sum_{j=1}^{n} s_j k_{n-j}$

A similar relation holds for k_n in terms of e_j. Recursion relations for s_n can be obtained by rewriting the already derived expressions, e.g.

$$s_n = nk_n - \sum_{j=1}^{n-1} k_j s_{n-j} \ . \tag{2.62}$$

Table 2.12 summarizes these recursion relations. This last recurrence ($k_n \leftrightarrow s_n$) will be the primary method for constructing partition functions in a section 3.2.1. However, there the identity is motivated not by a generating function identity, but rather from the conservation law. Interestingly, this derivation must therefore be equivalent, and the notion of conservation of objects can be inferred, for example, by giving statistical interpretations to the symmetric functions. The direct derivation of this fact is easier to understand, and so we will not attempt to interpret the above identity in terms of conservation of objects in this section.

These partition identities are possible because of a basic theorem in symmetric functions [11].

Theorem 2.2.3 (Fundamental theorem on symmetric functions) *Every polynomial symmetric function $f(x_1, \ldots)$ can be written as a polynomial in $s_1, s_2, \ldots$.*

In other words, using any of the three sets of "elementary" symmetric functions, any polynomial symmetric function can be expressed.

The principle connection between partitions and symmetric functions which is of interest to this work was suggested by a result due to Edward Waring [306] in 1762, who discovered and proved that the elementary symmetric functions e_n and k_n are

related by a sum over all partitions[22],

$$k_n = \sum_r (-1)^{r+n} r! \sum_{\pi_r(n)} \prod_{j>0} \frac{e_j^{\pi_j}}{\pi_j!} , \tag{2.63}$$

$$e_n = \sum_r (-1)^{r+n} r! \sum_{\pi_r(n)} \prod_{j>0} \frac{k_j^{\pi_j}}{\pi_j!} . \tag{2.64}$$

This result and others established the utility of computing tables of symmetric functions, a task which was started by Meyer Hirsch [148] in 1808 (up to weight 10). Arthur Cayley [54] in 1857 republished these tables (with corrections), noting a number of interesting properties and symmetries. This prompted a number of mathematicians to work on extending the tables. Successively, Francesco Faà Di Bruno [94] (1875, weight 11), Vaclav Řehořovský [252] (1882, weight 12) and William P. Durfee [79,80] (1882, weight 12; 1887, weight 14), P.A. MacMahon [197] (1882, weight 13), and Floyd Decker [73] (1910, weight 15) extended the tables.[23]

Percy A. MacMahon [196] in 1882 extended these relations, showing that the three fundamental symmetric functions additionally satisfy

$$k_n = \sum_{\pi(n)} \prod_{j>0} \frac{1}{\pi_j!} \left(\frac{s_j}{j}\right)^{\pi_j} , \tag{2.65}$$

$$e_n = \sum_r (-1)^{r+n} \sum_{\pi_r(n)} \prod_{j>0} \frac{1}{\pi_j!} \left(\frac{s_j}{j}\right)^{\pi_j} , \tag{2.66}$$

$$\frac{s_n}{n} = \sum_r (-1)^{r+n} (r-1)! \sum_{\pi_r(n)} \prod_{j>0} \frac{e_j^{\pi_j}}{\pi_j!} \tag{2.67}$$

$$= \sum_r (-1)^{r-1} (r-1)! \sum_{\pi_r(n)} \prod_{j>0} \frac{k_j^{\pi_j}}{\pi_j!} . \tag{2.68}$$

In his widely read treatise [201], he summarized these results, explored their combinatorial significance and extended the theory substantially. In essence this was a precursor to Pólya theory, as the relation between k_n and s_n appears in Pólya theory as the cycle index function for the permutation group S_n, i.e. $k_n = Z(S_n; s_1, \ldots, s_n)$. This connects

[22]Notice that these identities can be reexpressed succinctly in terms of determinants, e.g. $e_n = \det(k_{1-i+j})_{1\le i,j\le n}$, but there is no inherent advantage to expressing them this way, and for our purposes, the above expressions are the most useful.

[23]Of course today such table could be constructed in seconds by computer.

the theory of symmetric functions to Pólya theory, allowing a natural combinatorial interpretation of these symmetric functions. MacMahon explored this well before Pólya, but failed to see its generality.[24]

Waring and MacMahon's formulae connect symmetric functions to integer partitions, and hence to clusters configuration of indistinguishable objects. Since we are also interested in cluster configurations on distinguishable objects, it would be useful to have definitions of vector symmetric functions which can be related to vector partitions. Indeed, the theory of symmetric functions, and these identities in particular, can be generalized to vector partitions [199], i.e. for partitions of $\mathbf{n} = (n_1, \ldots, n_s)$, we have the generating functions

$$E(\mathbf{q}) = \sum_{\mathbf{n}} e_{\mathbf{n}} q_1^{n_1} \cdots q_s^{n_s} = \prod_{\mathbf{j}>\mathbf{0}} (1 + x_{\mathbf{j}} q_1^{j_1} \cdots q_s^{j_s}) \,, \tag{2.69}$$

$$K(\mathbf{q}) = \sum_{\mathbf{n}} k_{\mathbf{n}} q_1^{n_1} \cdots q_s^{n_s} = \prod_{\mathbf{j}>\mathbf{0}} \frac{1}{1 - x_{\mathbf{j}} q_1^{j_1} \cdots q_s^{j_s}} \,, \tag{2.70}$$

$$S(\mathbf{q}) = \sum_{\mathbf{n}} s_{\mathbf{n}} q_1^{n_1} \cdots q_s^{n_s} = \sum_{\mathbf{j}>\mathbf{0}} \frac{1}{1 - x_{\mathbf{j}} q_1^{j_1} \cdots q_s^{j_s}} \,, \tag{2.71}$$

and Waring's and MacMahon's identities generalize to

$$\begin{aligned} k_{\mathbf{n}} &= \sum_r (-1)^{r+n} r! \sum_{\pi_r(\mathbf{n})} \prod_{\mathbf{j}>\mathbf{0}} \frac{e_{\mathbf{j}}^{\pi_{\mathbf{j}}}}{\pi_{\mathbf{j}}!} \\ &= \sum_{\pi(\mathbf{n})} \prod_{\mathbf{j}>\mathbf{0}} \frac{1}{\pi_{\mathbf{j}}!} \left(\frac{(j-1)!}{\prod_i j_i!} s_{\mathbf{j}} \right)^{\pi_{\mathbf{j}}} \,, \end{aligned} \tag{2.72}$$

$$\begin{aligned} e_{\mathbf{n}} &= \sum_r (-1)^{r+n} r! \sum_{\pi_r(\mathbf{n})} \prod_{\mathbf{j}>\mathbf{0}} \frac{k_{\mathbf{j}}^{\pi_{\mathbf{j}}}}{\pi_{\mathbf{j}}!} \\ &= \sum_r (-1)^{r+n} \sum_{\pi_r(\mathbf{n})} \prod_{\mathbf{j}>\mathbf{0}} \frac{1}{\pi_{\mathbf{j}}!} \left(\frac{(j-1)!}{\prod_i j_i!} s_{\mathbf{j}} \right)^{\pi_{\mathbf{j}}} \,, \end{aligned} \tag{2.73}$$

$$\begin{aligned} \frac{(n-1)!}{\prod_i n_i!} s_{\mathbf{n}} &= \sum_r (-1)^{r+n} (r-1)! \sum_{\pi_r(\mathbf{n})} \prod_{\mathbf{j}>\mathbf{0}} \frac{e_{\mathbf{j}}^{\pi_{\mathbf{j}}}}{\pi_{\mathbf{j}}!} \\ &= \sum_r (-1)^{r-1} (r-1)! \sum_{\pi_r(\mathbf{n})} \prod_{\mathbf{j}>\mathbf{0}} \frac{k_{\mathbf{j}}^{\pi_{\mathbf{j}}}}{\pi_{\mathbf{j}}!} \,. \end{aligned} \tag{2.74}$$

[24] Or did he? J.H. Redfield's paper was motivated by MacMahon's work on Latin squares. It is possible MacMahon was aware of the general technique, but limited its use to specific examples.

The recursion relations also generalize, for example,

$$\mathbf{n}k_{\mathbf{n}} = \sum_{\mathbf{j}>0} s_{\mathbf{j}} k_{\mathbf{n}-\mathbf{j}} \ . \tag{2.75}$$

2.3 Combinatorial algorithms

It has been implicitly suggested throughout this chapter that the construction of the combinatorial objects of interest is a technical issue of little consequence. While true in a philosophical sense, the constructions are from an algorithmic point of view a highly nontrivial problem, and one must devote some space to their discussion. Simply put, the algorithms determine the feasibility of applying these techniques to actual systems. Without them, we would be in the unenviable position of giving names to objects we cannot practically compute, construct or enumerate.

Given a (possibly infinite) set of combinatorial objects, a set of parameters specifying (finite) subsets of the complete set, and a total order that can be applied to elements of the subsets[25] there are four basic algorithms (following Nijenhuis and Wilf [231]) of interest to a combinatorist, namely:

- *Sequence.* Given a particular combinatorial object from a specified subset, what is the next object according to the ordering?
- *Rank.* Given a particular combinatorial object from a specified subset, what is r such that the object is the rth element in the set according to the total order?
- *Unrank.* Given an integer r, what is the combinatorial object which is the rth member of the set according to the total order?
- *Select randomly.* Select an object from a specified subset uniformly at random.

Of these algorithms, only the last is particularly useful to a physicist interested in statistical models based on these objects. This is because in the typical cases a physicist

[25]For example, given the set of all integer partitions, take the subsets to be sets of partitions of a particular integer n and the order to be reverse lexicographic. Alternatively, take the subsets to be partitions of n into r distinct parts and the order to be minimum change (i.e. a Gray code (see Wilf [309] for a brief introduction to Gray codes).)

is interested in the size of the subsets is so large as to preclude the kind of individual analysis the first three algorithms would suggest. A random sampling however can be used to test hypotheses and estimate global functions. The determination of the size of the subsets is an algorithm which we will additionally be interested, both for its own value and since most random selection algorithms depend on having an enumeration of the objects. For this reason we add it to Nijenhuis and Wilf's list as a fundamental algorithm.

- *Enumerate.* How many of the objects are there in a specified subset?

This section provides algorithms for the enumeration and random selection of all the combinatorial objects introduced in section 2.1. Section 2.3.1 reviews established algorithms for the enumeration and random generation of integer partitions, set partitions and permutations. Section 2.3.2 tackles the implementation of these algorithms for the case of partitions of bipartite numbers, the combinatorial objects of principal interest to nuclear fragmentation. These algorithms can be extended to other vector partitions with little difficulty.

The principle reference for this section is the excellent book *Combinatorial Algorithms* by Albert Nijenhuis and Herbert S. Wilf [231]. Additional information on computational aspects of combinatorics can be found in *Elements of Combinatorial Computing* by Mark B. Wells [308] and *Implementing Discrete Mathematics* by Steven Skiena [272].

2.3.1 Algorithms for integer partitions, set partitions and permutations

This chapter introduced three common combinatorial objects, namely integer partitions, set partitions and permutations. In this section algorithms from the combinatorial literature [231, 296] are presented which enumerate and randomly select these objects, since our interest is principally on these algorithms. Algorithms for sequencing, ranking and unranking these objects can be found in Nijenhuis and Wilf [231].

Integer partitions are enumerated by $p(n)$, and $p_r(n)$, whose generating functions are given by equations (2.2) and (2.6). Euler's pentagonal number theorem (equation (2.3))

and the generating functions can be used to derive the following recursion relations [11],

$$p(n) = \sum_{k\geq 1}(-1)^{k+1}(p(n-k(3k-1)/2)+p(n-k(3k+1)/2)) , \quad (2.76)$$

$$p_r(n) = p_{r-1}(n-1)+p_r(n-r) , \quad (2.77)$$

with $p(0)=1$, $p(k)=0, k<0$, and $p_0(n)=\delta_{n0}$. As mentioned before, $p_r(n) = p_{n-r}(2(n-r)) = p(n-r)$ if $r \geq n/2$, so some entries can be avoided in an exhaustive computation.[26] The second identity can easily be proved as follows. An r partition of n either does or does not have a one as one of its parts. If it does, it can be formed by adding a one to an $(r-1)$-partition of $n-1$. If it does not, it can be formed by adding a one to every part of an r-partition of $n-r$.

Historically, the computation of $p(n)$ prompted substantial research. MacMahon, using the above recursion, tabulated $p(n)$ up to $n=200$ in 1918. This table was examined by Ramanujan [245], who noted empirically some interesting congruence relations which $p(n)$ appeared to satisfy, for example $p(5m+4) \equiv 0 \pmod 5$. He and others were able to prove these congruences, but it was the physicist Freeman Dyson [81, 82], by inventing the idea of a partition's *rank*, who showed that the division of partitions into equivalence classes implicit in the above example could be realized.[27] A.O.L. Atkin and P. Swinnerton-Dyer [13] provided the first proof however. Hansraj Gupta later extended MacMahon's table by another method successively to $n=300$ [132] in 1935, $n=600$ [133] in 1937, and finally to $n=1000$ [134] in 1958. By then, electronic computers were available which could have calculated these numbers rapidly, and today it is relatively simple task to compute the first several thousand cases of $p(n)$.[28]

---

[26] Some other recursive identities for $p_r(n)$ are

$$p_r(n) = \sum_{k=0}^{r} p_k(n-r)$$

$$rp_r(n) = \sum_{js} jp_{r-s}(n-sj)$$

[27] This is not an isolated incident. Freeman Dyson has published articles on partition theory at several points in his career [84, 85].

[28] In fact it is a built-in function in Wolfram Research, Inc.'s Mathematica™ [311], a popular symbolic and numerical mathematics package.

Selecting a partition $\boldsymbol{\pi} \in \pi(n)$ uniformly at random requires knowledge of $p(n)$. The algorithm is explained in Nijenhuis and Wilf and is a special case of the algorithm for selecting random vector partitions given in the next section, so we will just give the result in figure 2.5.

Figure 2.5: Algorithms for generating random integer partitions $\boldsymbol{\pi} \in \pi(n), \pi_r(n)$.

random_partition$(n, \boldsymbol{\pi})$
- $\pi_j = 0, \forall j$
- $q \leftarrow n$
- While $q > 0$
  - Choose (m, j) randomly with $\Pr(m, j) = \frac{jp(q-mj)}{qp(q)}$
  - $\pi_j \leftarrow \pi_j + m$
  - $q \leftarrow q - mj$

random_r-partition$(n, r, \boldsymbol{\pi})$
- $\pi_j = 0, \forall j$
- $q \leftarrow n$, $s \leftarrow r$
- While $q > 0$
  - Choose (m, j) randomly with $\Pr(m, j) = \frac{p_{s-m}(q-mj)}{sp_s(q)}$
  - $\pi_j \leftarrow \pi_j + m$
  - $q \leftarrow q - mj$, $s \leftarrow s - m$

Set partitions are enumerated by the Bell numbers $B(n)$ and the Stirling numbers of the second kind $\left\{ {n \atop r} \right\}$. Exponential generating functions were given in equations (2.25), (2.26), and from these we have the following recurrence relations

$$B(n) = \sum_{k=0}^{n-1} \binom{n-1}{k} B(k) , \tag{2.78}$$

$$\left\{ {n \atop r} \right\} = \left\{ {n-1 \atop r-1} \right\} + r \left\{ {n-1 \atop r} \right\} , \tag{2.79}$$

with $B(0) = 1$, and $\left\{ {n \atop 0} \right\} = \delta_{n0}$. The recurrence for $B(n)$ can be derived from $B(n) = \sum_{\pi(n)} \mathrm{Part}(\boldsymbol{\pi})$ and applying results from section 3.2.1. The recurrence for $\left\{ {n \atop r} \right\}$ can be proved by an argument similar to the one given for integer r-partitions.

An algorithm for the random generation of set partitions is given in figure 2.6 from Nijenhuis and Wilf. It depends on having the Bell numbers $B(n)$ and an algorithm for randomly permuting a vector, which we give in figure 2.7. A detailed explanation of why it works is given in Nijenhuis and Wilf, but the reasons are similar to the explanation for the vector partition algorithm given in the next section.

Permutations are enumerated by $n!$ and $\left[{n \atop r} \right]$, the unsigned Stirling numbers of the first kind. Their generating functions were given in equations (2.33), (2.34), which

Figure 2.6: Algorithms for generating random set partitions $\boldsymbol{\beta} \in \beta_n, \beta_n^{(r)}$.

```
random_set_partition(n, β)
    q ← n, i ← 0
    While q > 0
        Choose j randomly with
            Pr(j) = C(q-1, j-1) B(q-j)/B(q)
        i ← i + 1
        β_k ← i, k = q - j + 1, ..., q
        q ← q - j
    random_permutation(n, β)
```

```
random_set_r-partition(n, r, β)
    q ← n, s ← r, i → 0
    While q > 0
        Choose j randomly with
            Pr(j) = (1/s) C(q, j) {q-j; s-1} / {q; s}
        i ← i + 1
        β_k ← i, k = q - j + 1, ..., q
        q ← q - j, s ← s - 1
    random_permutation(n, β)
```

imply the following recurrence relations,

$$n! = n(n-1)!\,, \tag{2.80}$$

$$\begin{bmatrix} n \\ r \end{bmatrix} = \begin{bmatrix} n-1 \\ r-1 \end{bmatrix} + (n-1)\begin{bmatrix} n-1 \\ r \end{bmatrix}\,, \tag{2.81}$$

with $0! = 1$, $\left[\begin{smallmatrix} n \\ 0 \end{smallmatrix}\right] = \delta_{n0}$. The first recurrence is in fact the definition of the factorial numbers, whereas the second is an obvious consequence of splitting the r-permutations into sets with and without fixed points.

The shuffle algorithm provides a simple random selection algorithm for permutations. Suppose $k \to p_k$ under the action of p, and consider $(p_1, \ldots, p_n)$ as the representation of the permutation. Starting with the first position in the permutation, exchange it with a uniformly at random chosen member from the entire vector. Do the same for p_2, except exclude the first entry in the vector. in general he kth position is chosen uniformly at random from the last $n - k$ numbers in the vector. This algorithm[29] clearly produces another permutation, and all permutations are equally likely outcomes. Figure 2.7 summarizes the algorithm.

[29] With a good unranking algorithm, we could simply pick a number from 1 to $n!$ uniformly at random and unrank it to obtain a random permutation. Such a method would likely be faster (unranking can be done in $O(\ln n)$ time I believe) than this one, but this method has two clear advantages: it avoids the problem of unranking and (more importantly) it avoids picking a number uniformly at random from a huge space of numbers.

Figure 2.7: Algorithm for generating random permutations $p \in S_n$

```
random_permutation(n, p)
    For k = 1, ..., n − 1
        Choose j randomly with
            Pr(j) = θ(j−k)/(n−k+1)
        p_j ↔ p_k
```

2.3.2 Algorithms for vector partitions

Algorithms for the enumeration and random selection of partitions of vector partitions appear to be not available in the combinatorial literature. Since bipartite partitions are so important to the discussion of nuclear fragmentation, it is important to introduce effective algorithms for their enumeration and random selection. The algorithms are easily generalized to other vector partitions, but for simplicity in notation, we will restrict our attention to the bipartite case.

The enumeration of bipartite partitions can be accomplished in a variety of ways, and several algorithms will be presented, recursive and direct. A recursive algorithm uses the results of previous computations to compute a result, calling itself repeatedly until the results are reduced to some known cases. It is the result of a generating function identity or a constraint relation. A direct algorithm on the other hand computes all the values directly from the generating function. It is often the most efficient method, though it requires one to start in ignorance.[30] All of the methods presented here apply equally well to ordinary partitions and are in fact generalizations of known partition algorithms, but it should be noted that the usual algorithm for computing the values of $p(n)$ cannot be generalized since Euler's pentagonal number theorem does not generalize to higher dimensions.[31] These algorithms are therefore in some sense poor

[30] In other words, a preexisting table of values can not be used to expedite the evaluation of entries outside the table. All values must be computed ab initio in a direct algorithm, and are evaluated in some sense in parallel (though often the parallelism is difficult to exploit).

[31] Euler's pentagonal number theorem can be applied to the problem however, but it is not especially helpful, i.e.

$$\prod_{jk}(1-x^j y^k) = \prod_{\gcd(j,k)=1}\prod_{r=1}^{\infty}(1-(x^j y^k)^r) = \prod_{\gcd(j,k)=1}\left(\sum_{n=-\infty}^{\infty}(-1)^n (x^j y^k)^{n(3n-1)/2}\right).$$

cousins of the integer partition algorithm, but they get the job done nonetheless.

A simple recursive algorithm just implements the following recursive identity for $p(m,n)$ from section 3.2.2 (setting $x_j = 1$),

$$(m,n)p(m,n) = \sum_{jk} \sum_{r\geq 0} (j,k)p(m-rj, n-rk) \ , \tag{2.82}$$

with $p(0,n) = p(n)$, and recalling $p(m,n) = p(n,m)$ to reduce the number of computations. This algorithm has time complexity $O(N^4 \ln N)$ to compute all the $p(m,n)$ up to $p(N,N)$, and is simple to implement in a recursive environment such as Mathematica$^{\text{TM}}$.

Typically, a table of $p(m,n)$ is wanted up to (N,N), in which case the following direct algorithm is significantly faster. Given the generating function,

$$\sum_{n_1 n_2} Z(n_1,n_2) q_1^{n_1} q_2^{n_2} = \prod_{jk} \frac{1}{1 - x_{jk} q_1^j q_2^k} \ , \tag{2.83}$$

we wish to expand this up to order $(uv)^N$ directly from the product expansion. Suppose $G(q_1,q_2) = \sum_{kl} g(k,l) q_1^k q_2^l$, $F(q_1,q_2) = \sum_{kl} f(k,l) q_1^k q_2^l$ are polynomials in q_1, q_2 with $G(q_1,q_2) = F(q_1,q_2)/(1 - x_{mn} q_1^m q_2^n)$. Then the coefficients satisfy the following identity,

$$\begin{aligned} g(k,l) &= f(k,l) + x_{mn} f(k-m, l-n) + x_{mn}^2 f(k-2m, l-2n) + \ldots \\ &= f(k,l) + x_{mn} g(k-m, l-n) \ . \end{aligned} \tag{2.84}$$

This suggests an effective algorithm is to start with $P(q_1,q_2) = 1$ and use the above identity to compute the effect of multiplying the partially determined generating function by the factors $(1 - q_1^j q_2^k)^{-1}$ for all j,k up to N,N. This seems to require extra storage space for the temporary polynomial G, but in computing $F(q_1,q_2) \leftarrow F(q_1,q_2)/(1 - x_{mn} q_1^m q_2^n)$ it is possible to avoid the extra storage by keeping k,l strictly nondecreasing as we update $f(k,l)$[32], i.e.

$$f(k,l) \leftarrow f(k,l) + x_{mn} f(k-m, l-n) \ . \tag{2.85}$$

Now if the number of integer $j,k \leq N$ with $\gcd(j,k) = 1$ was less than $O(N^2)$, then this decomposition would be helpful. However, $\sum_{\gcd(j,k)=1}^{N} 1 \sim \frac{6}{\pi^2} N^2$ and so there is no inherent advantage (and several disadvantages) to this approach.

[32] Matrix multiplication algorithms use a similar trick to avoid having to use extra storage space.

Applying this technique to compute $p(m,n)$ up to $m = n = N$ yields the algorithm given in figure 2.8. This algorithm has time complexity $O(N^4)$ and is probably as efficient as possible.[33]

Figure 2.8: Direct algorithm for enumerating partitions of (m,n)

```
calculate_P(N, p)
    p(0,0) ← 1
    p(m,n) ← 0, (m,n) = (0,1),(1,0),...,(N,N)
    for (m,n) = (0,1),(1,0),...,(N,N)
        for k = m,...,N
            for l = n,...,N
                p(k,l) ← p(k,l) + p(k−m, l−n)
```

If we are interested in computing $p_r(m,n)$, the number of partitions of (m,n) into exactly r parts, we could use the recurrence from section 3.2.2

$$rp_r(m,n) = \sum_{jk} \sum_{s>0} p_{r-s}(m-js, n-ks) \ , \tag{2.86}$$

but the following recursive approach due to F.N. David, M.G. Kendall and D.E. Barton [71] is more efficient.[34] The generating function $P(q_1, q_2; t)$ for bipartite partitions into a fixed number of parts given by equation (2.14) satisfies the following identity

$$(1 - q_1 t)P(q_1, q_2; t) = P(q_1, q_2; q_1 t)P(q_2; t) \ , \tag{2.87}$$

where $P(q;t)$ is the generating function for integer partitions into a fixed number of parts. Expanding both sides of this identity implies the recurrence relation

$$p_r(m,n) = p_r(m-r,n) + p_{r-1}(m-1,n) + \sum_{i=1} \sum_{j=r-i} p_i(m-i, n-j)p_{r-i}(j) \ , \tag{2.88}$$

with $i \leq \min(r-1, m-1)$, $j \leq \min(n-1, m+n-2i)$ and $p(m,n;0) = \delta_{m0}\delta_{n0}$. This algorithm has time complexity $O(N^5)$, and is a generalization of equation (2.77). In this case, the direct approach is also possible and of the same time complexity.

---

[33] Actually, it is straightforward to show that this method requires exactly $N(N+1)^2(N+4)/4$ additions. A similar method for tripartites require $N(N+1)^3(N^2+6N+12)/8$ additions.

[34] Curiously Kim Sneppen [274] when treating the problem in 1987 in a nuclear physics context missed both methods and developed another method from a combinatorial argument. There may be no limit to the number of possible recurrence relations.

The above recursive algorithms can be speeded up since if $r > n + m/2$ then $p_r(m,n) = p_{m-r+2n}(2(m+n-r),n)$. It is simple to extend this result to any vector partition. Since this fact apparently is not in the combinatorial literature, I include a proof.

Lemma 2.3.1 *Let $\boldsymbol{\pi} \in \pi_r(m,n)$ with $r > n + m/2$. Then $\pi_{10} > 0$.*

Proof: Let $r = \sum_{jk} \pi_{jk} = \alpha + \beta + \gamma + \pi_{01} + \pi_{10}$, where

$$\alpha = \textstyle\sum_{k>1} \pi_{0k} \ , \quad \beta = \sum_{k>1} \pi_{k0} \ , \quad \gamma = \sum_{j,k\geq 1} \pi_{jk} \ .$$

It is clear we have the following lower bounds on m, n.

$$\begin{aligned} m &= \sum_{jk} j\pi_{jk} \geq \pi_{10} + 2\beta + \gamma \ , \\ n &= \sum_{jk} k\pi_{jk} \geq \pi_{01} + 2\alpha + \gamma \ . \end{aligned}$$

Now by assumption $r = \alpha + \beta + \gamma + \pi_{10} + \pi_{01} > n + m/2$, so we have by the lower bounds on m, n.

$$\alpha + \beta + \gamma + \pi_{10} + \pi_{01} > \pi_{01} + 2\alpha + \gamma + (\pi_{10} + 2\beta + \gamma)/2 \ ,$$

which gives after some manipulation

$$\pi_{10} > 2\alpha + \gamma \geq 0 \ .$$

□.

Remark: If $r > m + n/2$ then $\pi_{01} > 0$ by a similar argument.

An immediate corollary is

Corollary 2.3.1 *If $r > n + m/2$, then*

$$p_r(m,n) = p_{r-1}(m-1,n) \ . \tag{2.89}$$

Proof: Since every $\boldsymbol{\pi} \in \pi_r(m,n)$ has at least one $(1,0)$ part, we can eliminate exactly one $(1,0)$ from every partition $\boldsymbol{\pi}$, giving $\boldsymbol{\pi}' \in \pi_{r-1}(m-1,n)$. Clearly this is a bijection, So $p_r(m,n) = p_{r-1}(m-1,n)$. □.

Remark: If $r > m + n/2$ then $p_r(m,n) = p_{r-1}(m,n-1)$ by a similar argument.

Theorem 2.3.1 *If* $r > n + m/2$, *then*

$$p_r(m,n) = p_{m-r+2n}(2(m+n-r),n)\ . \tag{2.90}$$

Proof: Apply the above corollary as often as possible, eliminating x $(1,0)$s. Then we have $p_r(m,n) = p_{r-x}(m-x,n)$. Since we can no longer apply the corollary, we must have $r - x = n + (m-x)/2$, which has the solution

$$x \quad = \quad 2(r-n) - m\ ,$$

So we see that

$$\begin{aligned} r - x &= r - 2(r-n) + m = m - r + 2n\ , \\ m - x &= m - 2(r-n) + m = 2(m+n-r)\ , \end{aligned}$$

which proves the theorem. □

Corollary 2.3.2 *If* $r > \max(m + n/2, n + m/2)$ *then*

$$p_r(m,n) = p_{3(m+n-r)}(2(m+n-r), 2(m+n-r))\ . \tag{2.91}$$

Proof: Apply the theorem once, then apply $p_r(m,n) = p_r(n,m)$ and use the theorem a second time.

Using the above theorems, about one quarter of the entries can be avoided in the construction of a table of all the $p_r(m,n)$, a substantial computational savings. Table 2.13 lists the first few entries for $p_{3n}(2n,2n)$, which appear quite frequently in an exhaustive table (about one sixth of the table).

Table 2.13: Number of $3n$-partitions of $(2n,2n)$, $f(n) = p_{3n}(2n,2n)$ for $n = 1(1)12$.

n	1	2	3	4	5	6	7	8	9	10	11	12
$f(n)$	3	10	27	70	166	382	835	1778	3665	7389	14550	28138

The selection of random vector partitions is an obvious modification to the algorithm for generating random partitions given in Nijenhuis and Wilf [231]. The idea is to build up the partition iteratively by adjoining clusters. If each term in the identity

$$1 = \sum_{jk} \sum_{r=1}^{\infty} \frac{(j+k)p(m-rj, n-rk)}{(m+n)p(m,n)}\ , \tag{2.92}$$

(derived from equation (2.82)) is interpreted as the probability of the event that r copies of (j,k) were adjoined to a partition of $(m-rj, n-rk)$ to form a partition of of (m,n), we have a natural algorithm for generating random partitions. Start with (m,n) and extract off r (j,k) clusters with probability as suggested above. Repeat until there are no objects left.

It is easy to see that all partitions of (m,n) have equal probabilities of being chosen by this method. Let

$$(m,n) = \sum_{k=1}^{r} \mu_k (d_{1k}, d_{2k}) \ , \tag{2.93}$$

where (d_{1k}, d_{2k}) are distinct bipartites and μ_k are the multiplicities. This partition is chosen in $\sum_{k=1}^{r} \mu_k$ ways by adjoining s copies of of (d_{1i}, d_{2i}) to $(m,n) - s(d_{1i}, d_{2i})$. Inductively, each of these latter partitions have equal a priori probability of $1/p(m - sd_{1i}, n - sd_{2i})$. The a priori probability of the above partition is therefore

$$\begin{aligned}
&\sum_{i=1}^{r} \sum_{s=1}^{\mu_i} \frac{(d_{1i}+d_{2i})p(m-sd_{1i}, n-sd_{2i})}{(m+n)p(m,n)} \frac{1}{p(m-sd_{1i}, n-sd_{2i})} \\
&\quad = \frac{1}{(m+n)p(m,n)} \sum_{i=1}^{r} \sum_{s=1}^{\mu_i} (d_{1i}+d_{2i}) \\
&\quad = \frac{1}{(m+n)p(m,n)} \sum_{i=1}^{r} \mu_i (d_{1i}+d_{2i}) = \frac{1}{p(m,n)} \ .
\end{aligned}$$

In summary, we have the following algorithm

Figure 2.9: Algorithm for generating random vector partitions $\boldsymbol{\pi} \in \pi(m,n), \pi_r(m,n)$

random_partition$((m,n), \boldsymbol{\pi})$
- $\pi_{jk} = 0, \forall j,k$
- $(p,q) \leftarrow (m,n)$
- While $p+q > 0$
  - Choose (r,j,k) randomly with $\Pr(r,j,k) = \frac{(j+k)p(p-rj,q-rk)}{(p+q)p(p,q)}$
  - $\pi_{jk} \leftarrow \pi_{jk} + r$
  - $(p,q) \leftarrow (p-rj, q-rk)$

random_r-partition$((m,n), r, \boldsymbol{\pi})$
- $\pi_{jk} = 0, \forall j,k$
- $(p,q) \leftarrow (m,n)$, $s \leftarrow r$
- While $p+q > 0$
  - Choose (d,j,k) randomly with $\Pr(d,j,k) = \frac{p_{s-d}(p-dj,q-dk)}{sp_s(p,q)}$
  - $\pi_{jk} \leftarrow \pi_{jk} + d$
  - $(p,q) \leftarrow (p-dj, q-dk)$
  - $s \leftarrow s-d$

Chapter 3

Statistical methods and models for fragmentation

The previous chapter introduced the combinatorial objects and algorithms necessary for the development of a statistical approach to fragmentation, but postponed discussing the details of the statistics, which we now address. The statistical approach is in essence a simplification of matters so that the problems are tractable. We assign to each possible outcome a probability, preferably with an a priori structure such that the expected outcomes are specified by a small number of parameters related to the physics of the processes. Alternately a structure with a large number of parameters can be adjusted a posteori to the experimental results. The important idea is to specify the partition structure ahead of time so that the effect of the parameters on observables is determined. It will become evident that certain structures are more amenable to analysis than others. Fortunately, the structures which are easiest to analyze are the ones motivated by the various physical problems. This chapter will introduce the formalism, and then identify some classes of solvable models. Chapter four explores the properties of one of these models and applying the models to actual physical situations is postponed until chapter five.

Section 3.1 outlines the methods for solving models, both exact (3.1.1) and Monte Carlo sampling methods (3.1.2). Section 3.2 applies the exact methods to solve some useful models, including the Gibbs model (3.2.1), the equipartition model (3.2.2), the separable model (3.2.3) and the interacting Gibbs model (3.2.4).

3.1 Statistical methods

Consider a system of identical particles which can form clusters of various sizes, or equivalently a set of states represented by integer partitions according to the discussion

of section 2.1.1. Statistical models for such systems are simple to introduce. Suppose we have a Hamiltonian which describes the physics, $H = H(\boldsymbol{\pi}, \mathbf{q})$, where $\mathbf{q}$ includes all the degrees of freedom not associated with partitioning (e.g. the position and velocity of the fragments), and $\boldsymbol{\pi}$ specifies the partition. Suppose also that the system is coupled to a heat bath at temperature T. Then the statistical weight of a particular configuration is given by the Boltzmann weight,[1]

$$W(\boldsymbol{\pi}, \mathbf{q}) = e^{-H(\boldsymbol{\pi},\mathbf{q})/k_B T} \ . \tag{3.1}$$

If we complete the sums over the variables $\mathbf{q}$, we can reformulate the problem in terms of the free energy of the configuration $F(\boldsymbol{\pi}, V, T)$, where

$$e^{-F(\boldsymbol{\pi},V,T)/k_B T} = \sum_{\mathbf{q}\in Q} e^{-H(\boldsymbol{\pi},\mathbf{q})/k_B T} \ , \tag{3.2}$$

in other words we can assign the weight

$$W(\boldsymbol{\pi}) = e^{-F(\boldsymbol{\pi},V,T)/k_B T} \ , \tag{3.3}$$

to each partition. The partition function is given by the sum of the weights over the members of the ensemble, and it is this function which determines the details of the statistical physics. There are three ensembles we will consider, namely the microcanonical, canonical, and grand canonical ensembles. Microcanonical models have the number of particles and the number of clusters conserved[2], canonical models have only the number of particles conserved, and grand canonical models have neither conservation law, in

[1] See Huang [149] for an introduction to statistical physics and an explanation of the origins of the Boltzmann weight.

[2] This is a somewhat misleading name as usually a microcanonical ensemble indicates a conservation of energy. If the energy of a cluster of size j is given by $a + bj$, then this is equivalent to conservation of clusters, and the two definitions are equivalent. This is true in the case of polymers, but we will adopt the terminology that microcanonical means conservation of cluster number unless otherwise stated.

other words, the partition functions are given by[3]

$$\begin{aligned} Z_n^{(r)} &:= \sum_{\pi_r(n)} W(\boldsymbol{\pi}) \,, \\ Z_n &:= \sum_{r=1}^{n} Z_n^{(r)} \,, \\ \mathcal{Z} &:= \sum_{n\geq 0} Z_n \,. \end{aligned} \tag{3.4}$$

and ensemble averages or expectation values $\langle \bullet \rangle$ are given by

$$\begin{aligned} \langle f \rangle_n^{(r)} &:= \frac{1}{Z_n^{(r)}} \sum_{\pi_r(n)} f(\boldsymbol{\pi}) W(\boldsymbol{\pi}) \,, \\ \langle f \rangle_n &:= \frac{1}{Z_n} \sum_{\pi(n)} f(\boldsymbol{\pi}) W(\boldsymbol{\pi}) = \frac{1}{Z_n} \sum_{r=1}^{n} Z_n^{(r)} \langle f \rangle_n^{(r)} \,, \\ \langle f \rangle &:= \frac{1}{\mathcal{Z}} \sum_{n\geq 0} \sum_{\pi(n)} f(\boldsymbol{\pi}) W(\boldsymbol{\pi}) = \frac{1}{\mathcal{Z}} \sum_{n\geq 0} Z_n \langle f \rangle_n \,. \end{aligned} \tag{3.5}$$

Notice that even if we are interested in a particular ensemble, computing partition functions and expectation values for ensembles with stricter conservation laws is still useful since they can be used to compute these functions for other ensembles.

In principle, we can now compute any expectation value or thermodynamic function for this system. Since the number of partitions grows exponentially with $\sqrt{n}$ (equation (2.4)), it quickly becomes impractical to compute the partition functions and ensemble averages directly, so in practice, one either chooses weights which are exactly solvable by some faster technique (e.g. of polynomial time complexity), or engages in statistical sampling to obtain estimates of particular expectation values. Both of these methods are detailed in the next subsections.

3.1.1 Exact methods

Consider the following approach, which oftentimes yields a practical method for evaluating the partition functions. Without loss of generality we can assume that

$$W(\boldsymbol{\pi}) = W'(\boldsymbol{\pi}) \prod_{j>0} x_j^{\pi_j} \,, \tag{3.6}$$

[3] I'm assuming any chemical potential terms needed to "tune" these ensembles to the correct expectation values are already included in the weights. For example, if $W(\pi) \propto \prod_j x_j^{\pi_j}$, the choice $x_k = tz^j b_k$ allows z to control $\langle n \rangle$ and t to control $\langle r \rangle_n$. See section 3.2.1 for details.

since x_j can be set identically to one and the effect of the additional terms is nil. For this weight, it is easy to derive formulas for the expectation values of π_k in the various ensembles, namely

$$\begin{aligned} \langle \pi_k \rangle_n^{(r)} &= \frac{x_k}{Z_n^{(r)}} \frac{\partial Z_n^{(r)}}{\partial x_k} , \\ \langle \pi_k \rangle_n &= \frac{x_k}{Z_n} \frac{\partial Z_n}{\partial x_k} , \\ \langle \pi_k \rangle &= \frac{x_k}{\mathcal{Z}} \frac{\partial \mathcal{Z}}{\partial x_k} , \end{aligned} \tag{3.7}$$

or in general for $\prod_{j>0} [\pi_j]_{p_j}$,

$$\begin{aligned} \left\langle \prod_{k>0} [\pi_k]_{p_k} \right\rangle_n^{(r)} &= \left(\prod_{k>0} x_k^{p_k} \right) \frac{1}{Z_n^{(r)}} \frac{\partial^p Z_n^{(r)}}{\partial x_1^{p_1} \dots x_n^{p_n}} , \\ \left\langle \prod_{k>0} [\pi_k]_{p_k} \right\rangle_n &= \left(\prod_{k>0} x_k^{p_k} \right) \frac{1}{Z_n} \frac{\partial^p Z_n}{\partial x_1^{p_1} \dots x_n^{p_n}} , \\ \left\langle \prod_{k>0} [\pi_k]_{p_k} \right\rangle &= \left(\prod_{k>0} x_k^{p_k} \right) \frac{1}{\mathcal{Z}} \frac{\partial^p \mathcal{Z}}{\partial x_1^{p_1} \dots x_n^{p_n}} , \end{aligned} \tag{3.8}$$

where $p = \sum_{k>0} p_k$ and we define the falling factorial

$$[z]_k := \begin{cases} 1 & k = 0 , \\ z(z-1)\cdots(z-k+1) & k > 0 . \end{cases} \tag{3.9}$$

For the canonical and microcanonical ensembles, the two constraints on $\boldsymbol{\pi}$ due to the conservation of objects and clusters hold individually for every partition in the ensemble. Therefore, they must also hold for the expectation values, i.e. $\sum_{k>0} k \langle \pi_k \rangle_n = n$ and $\sum_{k>0} \langle \pi_k \rangle_n^{(r)} = r$, which imply[4]

$$n Z_n = \sum_{k=1}^{n} k x_k \frac{\partial Z_n}{\partial x_k} , \tag{3.10}$$

$$r Z_n^{(r)} = \sum_{k=1}^{n} x_k \frac{\partial Z_n^{(r)}}{\partial x_k} . \tag{3.11}$$

[4]There is a third identity, $\sum_{k>0} k \langle \pi_k \rangle_n^{(r)} = n$, which implies

$$n Z_n^{(r)} = \sum_{k=1}^{n} k x_k \frac{\partial Z_n}{\partial x_k}$$

but the above two are sufficient for implementing all the needed recurrence relations.

If the derivatives in the above equations can be reduced to earlier computed partition functions, the above identities imply recursive algorithms for generating the partition functions. Although nothing we have done so far has suggested that this will turn out to be the case, it is in fact true that several useful weight schemes satisfy this requirement, and are therefore amenable to this kind of analysis. This is the crucial point. If the weight schemes appropriate to the physics did not satisfy this requirement, the models would be not be solvable for large values of n. For small values of n, the partition functions could be evaluated by direct enumeration, but this approach rapidly breaks down since the number of partitions grows exponentially with the square root of n. At larger values of n, the only method generally applicable is Monte Carlo methods, which oftentimes takes tremendous computer resources to attain reasonable accuracy.[5] Exactly solvable models on the other hand will prove to be physically sufficiently flexible and computationally efficient, a fact we will exploit repeatedly in this work.

We can generalize these definitions easily to vector partitions of $\mathbf{n}$. For the weight $W(\boldsymbol{\pi})$, the partition functions are defined by

$$\begin{aligned} Z_{\mathbf{n}}^{(r)} &= \sum_{\pi_r(\mathbf{n})} W(\boldsymbol{\pi}) \,, \\ Z_{\mathbf{n}} &= \sum_{r=1}^{n} Z_{\mathbf{n}}^{(r)} \,, \\ \mathcal{Z} &= \sum_{\mathbf{n}\geq\mathbf{0}} Z_{\mathbf{n}} \,. \end{aligned} \tag{3.12}$$

and the ensemble averages are given by

$$\begin{aligned} \langle f\rangle_{\mathbf{n}}^{(r)} &= \frac{1}{Z_{\mathbf{n}}^{(r)}} \sum_{\pi_r(\mathbf{n})} f(\boldsymbol{\pi}) W(\boldsymbol{\pi}) \,, \\ \langle f\rangle_{\mathbf{n}} &= \frac{1}{Z_{\mathbf{n}}} \sum_{\pi(\mathbf{n})} f(\boldsymbol{\pi}) W(\boldsymbol{\pi}) = \frac{1}{Z_{\mathbf{n}}} \sum_{r=1}^{n} \langle f\rangle_{\mathbf{n}}^{(r)} Z_{\mathbf{n}}^{(r)} \,, \\ \langle f\rangle &= \frac{1}{\mathcal{Z}} \sum_{\mathbf{n}\geq\mathbf{0}} \sum_{\pi(\mathbf{n})} f(\boldsymbol{\pi}) W(\boldsymbol{\pi}) = \frac{1}{\mathcal{Z}} \sum_{\mathbf{n}\geq\mathbf{0}} \langle f\rangle_{\mathbf{n}} Z_{\mathbf{n}} \,. \end{aligned} \tag{3.13}$$

We then specify a weight by

$$W(\boldsymbol{\pi}) = W'(\boldsymbol{\pi}) \prod_{\mathbf{k}>\mathbf{0}} x_{\mathbf{k}}^{\pi_{\mathbf{k}}} \,. \tag{3.14}$$

---

[5] Generally in Monte Carlo, doubling the number of samples only reduces the absolute error by $2^{-1/2}$. Halving the error requires four times as much effort, and diminishing returns quickly sets in.

For the various ensembles, it is easy to derive formulas for the expected values of $\pi_{\mathbf{k}}$, namely

$$\begin{aligned} \langle \pi_{\mathbf{k}} \rangle_{\mathbf{n}}^{(r)} &= \frac{x_{\mathbf{k}}}{Z_{\mathbf{n}}^{(r)}} \frac{\partial Z_{\mathbf{n}}^{(r)}}{\partial x_{\mathbf{k}}} \, . \\ \langle \pi_{\mathbf{k}} \rangle_{\mathbf{n}} &= \frac{x_{\mathbf{k}}}{Z_{\mathbf{n}}} \frac{\partial Z_{\mathbf{n}}}{\partial x_{\mathbf{k}}} \, , \\ \langle \pi_{\mathbf{k}} \rangle &= \frac{x_{\mathbf{k}}}{\mathcal{Z}} \frac{\partial \mathcal{Z}}{\partial x_{\mathbf{k}}} \, , \end{aligned} \tag{3.15}$$

and our constraints, $\sum_{\mathbf{k}>\mathbf{0}} \mathbf{k} \langle \pi_{\mathbf{k}} \rangle_{\mathbf{n}} = \mathbf{n}$ and $\sum_{\mathbf{k}>\mathbf{0}} \langle \pi_{\mathbf{k}} \rangle_{\mathbf{n}}^{(r)} = r$ imply two identities,

$$\mathbf{n} Z_{\mathbf{n}} = \sum_{\mathbf{k}>\mathbf{0}} \mathbf{k} x_{\mathbf{k}} \frac{\partial Z_{\mathbf{n}}}{\partial x_{\mathbf{k}}} \, , \tag{3.16}$$

$$r Z_{\mathbf{n}}^{(r)} = \sum_{\mathbf{k}>\mathbf{0}} x_{\mathbf{k}} \frac{\partial Z_{\mathbf{n}}^{(r)}}{\partial x_{\mathbf{k}}} \, . \tag{3.17}$$

Introducing statistical models for objects described by set partitions and permutations proceeds along similar lines. For example, consider statistical models of permutations. In this case we propose a Hamiltonian $H = H(p, \mathbf{q})$ where $\mathbf{q}$ includes all degrees of freedom not associated with permutations (e.g. translations, rotations), and p specifies the particular permutation. We then construct the free energy for a cluster configuration by summing the weight over $\mathbf{q}$

$$W(p) = e^{-F(p,V,T)/k_B T} = \sum_{\mathbf{q} \in Q} e^{-H(p,\mathbf{q})/k_B T} \, , \tag{3.18}$$

and build the partition functions from these weights,

$$\begin{aligned} Z_n^{(r)} &= \sum_{p \in S_n^{(r)}} W(p) \, , \\ Z_n &= \sum_{p \in S_n} W(p) \, , \\ \mathcal{Z} &= \sum_n \sum_{p \in S_n} W(p) \, . \end{aligned} \tag{3.19}$$

Now usually it is the case that the Hamiltonian of a permutation is invariant for all permutations with the same cycle structure, i.e. $H(p) = H(\boldsymbol{\pi}(p))$, in which case the free energy is the same for all p in the cycle class $\boldsymbol{\pi}$ and we reduce the problem to the case of statistical models defined on partitions, i.e.

$$Z_n = \sum_{p \in S_n} e^{-F(p,V,T)/k_B T} = \sum_{\pi(n)} \mathrm{Perm}(\boldsymbol{\pi}) e^{-F(\pi,V,T)/k_B T} \, . \tag{3.20}$$

As a result, many models on permutations and set partitions reduce to models on partitions, and as such we can usually restrict our attention to various models defined over integer and vector partitions.

3.1.2 Monte Carlo methods

As we shall soon see, there are a number of exactly solvable models for weights defined on integer and vector partitions. These solutions apply equally well to appropriate permutation models when the weights are functions only of the cycle structure of the permutations. However, these models are not always the ones we wish to study, and in the absence of exact methods, we will resort to statistical sampling methods, otherwise known as Monte Carlo methods. Sampling is necessary, since for typical problems the size of the space is sufficiently vast that it precludes direct enumeration. For definiteness, we will restrict our attention to models defined over the permutations on n objects. This is motivated by several factors.

- Since permutation models contain integer, vector and set partition models in subsets defined by simple projection operators (see section 2.1.2) this method is more general than a method applied directly to partitions.

- In practice it is usually easier to manipulate permutations than integer or vector partitions. Additionally the task of projecting onto the partition states often can be done at low computational cost, sometimes making this method more efficient than a direct method.

- There is a natural mapping from permutation models onto canonical Gibbs ensemble models (section 3.2.1) which simplify some of the calculations for this important class of models.

- A Monte Carlo method which operates directly on partitions can be derived from the discussion of Markov processes (section 4.2.1) if one is interested in simulating models only on partitions.

The basic idea behind Monte Carlo is simple. If one knows the overall probability distribution of states, it is possible to measure expectation values by generating a subset of states chosen from the distribution and measuring on the subset. If the subset is representative and the measure taken is not pathologically dependent on some particular set of configurations, the values obtained should approximate the expectation over the whole set.

Monte Carlo algorithms choose their samples by dynamically changing states in a way that emulates the statistical equilibrium process. The equilibrium condition of statistical mechanics states that once a system is in equilibrium the probability of moving in and out of states should be balanced so that the equilibrium is maintained. Given this "detailed" balance condition, one can sample the equilibrium distribution by only allowing changes in the configuration which satisfy (statistically) the detailed balance condition, insuring that the equilibrium distribution will be maintained. In other words, if u and u' are two states of the system, and $\Pr(u)$ is the equilibrium distribution, then the transition rate $q(u \to u')$ of the Monte Carlo simulation must satisfy

$$q(u \to u') \Pr(u) = q(u' \to u) \Pr(u') \ . \tag{3.21}$$

The Metropolis algorithm [220] is the most common of the various Monte Carlo algorithms due to its simplicity. Suppose the system is in a state u, and we consider moving to another state u' selected in some random fashion from the set of all possible states. To be definite, suppose the state u' is selected with probability $p(u \to u')$, with $\sum_{u'} p(u \to u') = 1$. Define the "action" function by

$$S(u) := -\ln \Pr(u) \ , \tag{3.22}$$

i.e. $\Pr(u) =: e^{-S(u)}$. If the move reduces the action ($\Delta S < 0$) accept the move always. If the move increases the action, accept the move with probability $e^{-\Delta S}$. This leads to the following transition rates

$$q(u \to u') = \begin{cases} p(u \to u') & \Delta S < 0 \ , \\ p(u \to u') e^{-\Delta S} & \Delta S \geq 0 \ . \end{cases} \tag{3.23}$$

This method satisfies detailed balance assuming that

$$p(u \to u') = p(u' \to u) \;, \tag{3.24}$$

is true for all u, u'. Applying this algorithm repeatedly produces a set of equilibrium states which can be used to determine any ensemble average by simple sampling. Figure 3.1 details this algorithm.

Figure 3.1: Metropolis algorithm for randomly sampling a statistical system.

```
Metropolis_Algorithm(u)
    Select u' randomly with
        Pr(u, u') = Pr(u', u)
    ΔS = S(u') − S(u).
    If ΔS ≤ 0
        u ← u'
    If ΔS > 0
        Choose q ∈ [0, 1] uniformly at random
        If q < e^{−ΔS}
            u ← u'
```

There are many ways to achieve the symmetry condition of equation (3.24). There are two ways in the context of permutations which are useful and fairly simple to describe and implement, namely by transpositions and shuffles. Consider the permutation p as a vector of numbers, $(p_1, p_2, \ldots, p_n)$, such that under the permutation the number k goes to p_k ($k \to p_k$), i.e. the standard representation. In a transposition, uniformly at random pick a number k from 1 to n and then transpose p_k and p_{k+1} (p_1 if $k = n$) in the permutation vector, which is equivalent to modifying the permutation such that $k \to p_{k+1}$, $k+1 \to p_k$. This transition is obviously symmetric, and can generate any permutation in S_n in some finite number of transpositions[6]. This transition will in the cycle (or partition) picture either join two cycles together (if the number $k+1$ is not in the cycle generated by p acting on k) or split a cycle into two cycles (if the number $k+1$ is in the cycle generated by p acting on k). A possible generalization is to randomly

[6]Possibly as many as $\binom{n}{2}$, since this is the inverse of sorting by adjacent transposition, i.e. bubble sort.

choose two elements in the permutation vector to swap, however tests show that this method appears to be no better than the method described above.

Alternately, we can consider shuffles as our transitions. In a shuffle, the permutation is transformed to another permutation by shuffling the numbers in the permutation vector like a deck of cards. This transition is symmetric so long as all states are equally likely outcomes of the shuffling procedure, which is easy to arrange. The method usually used is for every position in the "deck" of the permutation to be sequentially swapped with a uniformly at random chosen element beneath that "card" in the "deck" order. This method has the advantage that it is possible to move in one step from one element to any other element in the set. Notice that this transition in the cycle picture will convert one partition into another partition with no relation between the two states. The motivation for shuffles which are computationally more costly to implement than transpositions is given by the case in which the action over the permutation space has many local minima. In this case, the action of a transposition on the permutation may keep the permutation "close" to a particular local minimum for a large number of transitions, suggesting that the actual equilibrium configuration has been reached. That conclusion would lead to incorrect results. So to avoid that result, a comparison of the local move simulation should be made with a simulation employing global moves as a check.

3.2 Exactly solvable statistical models

Although the proceeding section illustrates how to proceed in general to "solve" a given statistical clustering or fragmenting system, we are motivated for various reasons to reject the Monte Carlo method when other methods are available, such as exact solutions. This section outlines several nontrivial models which can be solved exactly by analytical techniques. Specifically, four models will be introduced, namely the Gibbs, equipartition, separable and interacting Gibbs models. The Gibbs and equipartition models are suggested by models in physics and mathematics, and are special cases of separable models. The distinction is useful since these two models are somewhat simpler to treat than the general case. Interacting Gibbs models are a generalization of the

Table 3.1: Recursion relations for canonical model partition functions.

$W(\boldsymbol{\pi})$	Z_n
$\prod_{j>0} \frac{x_j^{\pi_j}}{\pi_j!}$	$nZ_n = \sum_{j>0} j x_j Z_{n-j}$
$\prod_{j>0} x_j^{\pi_j}$	$nZ_n = \sum_{j>0} \sum_{s\geq 1} j x_j^s Z_{n-js}$
$\prod_{j>0} \frac{x_j^{\pi_j}}{\pi_j!} \prod_{k>0} y_{jk}^{\pi_j(\pi_k - \delta_{jk})/2}$	$nZ_n = \sum_{j>0} j x_j Z_{n-j}(x_k \to x_k y_{jk})$

Gibbs model which includes a cluster interaction term. The solution for the interacting Gibbs model is usually much more difficult to implement than the noninteracting cases, but can be accomplished in some interesting special cases. Table 3.1 summarizes some of the recursive solutions which will be derived in the following subsections.

3.2.1 Gibbs models

To motivate the Gibbs model, consider the following simple picture (unrigorous, but will be made rigorous later when we introduce Markov process models (section 4.2.1)). Let the (indistinguishable) objects initially be unclustered, and form a particular partition by taking groups of individual objects and clustering them. Suppose the probability of forming a j-cluster is proportional to x_j. If these probabilities are independent (which they are not) then the weight $W(\boldsymbol{\pi}) \propto \prod_j x_j^{\pi_j}$. However, in forming π_j j-clusters, there is an overcounting since the clusters are indistinguishable. As in the case of the ideal gas, we modify the weight by $1/\pi_j!$ to correct for the indistinguishability of the clusters, a rule which is also known as "correct Boltzmann counting."[7] The weight for a partition is therefore given by

$$W(\boldsymbol{\pi}, \mathbf{x}) = \prod_{j>0} \frac{x_j^{\pi_j}}{\pi_j!} , \tag{3.25}$$

where $\mathbf{x}$ is a vector of parameters. We denote these models Gibbs models[8], and as we shall soon see they have some very nice properties.

---

[7] Huang [149], pg. 141. The quotation marks are used in Huang, probably to indicate that the rule is not due to Boltzmann.

[8] The 1/n! correction to the partition function is originally due to Gibbs and therefore my choice of nomenclature.

The grand canonical partition function for this weight can be determined explicitly,

$$\begin{aligned} \mathcal{Z}(\mathbf{x}) &= \sum_{n\geq 0}\sum_{\pi(n)}\prod_{j>0}\frac{x_j^{\pi_j}}{\pi_j!} = \sum_{\pi_1\geq 0}\frac{x_1^{\pi_1}}{\pi_1!}\sum_{\pi_2\geq 0}\frac{x_2^{\pi_2}}{\pi_2!}\cdots \\ &= \exp\left\{\sum_{j>0} x_j\right\} . \end{aligned} \tag{3.26}$$

from which the first derivative is given by

$$\frac{\partial \mathcal{Z}}{\partial x_k} = \mathcal{Z}(\mathbf{x}) , \tag{3.27}$$

Setting $x_k = tz^k b_k$ allows the derivatives for the canonical and microcanonical partition functions to be extracted from the above identity (since then $\mathcal{Z} = \sum_{n\geq 0} z^n Z_n(t\mathbf{b}) = \sum_{n\geq 0}\sum_r z^n t^r Z_n^{(r)}(\mathbf{b})$), or alternately we can compute them directly,

$$\frac{\partial Z_n^{(r)}}{\partial x_k} = \sum_{\pi_r(n)}\frac{x_k^{\pi_k-1}}{(\pi_k-1)!}\prod_{j\neq k}\frac{x_j^{\pi_j}}{\pi_j!} = Z_{n-k}^{(r-1)}(\mathbf{x}) , \tag{3.28}$$

$$\frac{\partial Z_n}{\partial x_k} = \sum_{\pi(n)}\frac{x_k^{\pi_k-1}}{(\pi_k-1)!}\prod_{j\neq k}\frac{x_j^{\pi_j}}{\pi_j!} = Z_{n-k}(\mathbf{x}) , \tag{3.29}$$

where it is understood that $Z_n(\mathbf{x}) = 0$ for $n < 0$, $Z_n^{(r)}(\mathbf{x}) = 0$ for $r > n$ or $n, r < 0$. Applying these identities repeatedly obtains the generalization:

$$\begin{aligned} \frac{\partial^p Z_n^{(r)}}{\partial x_1^{p_1}\cdots\partial x_n^{p_n}} &= Z_{n-\sum_{k>0} kp_k}^{(r-p)}(\mathbf{x}) , \\ \frac{\partial^p Z_n}{\partial x_1^{p_1}\cdots\partial x_n^{p_n}} &= Z_{n-\sum_{k>0} kp_k}(\mathbf{x}) , \\ \frac{\partial^p \mathcal{Z}}{\partial x_1^{p_1}\cdots\partial x_n^{p_n}} &= \mathcal{Z}(\mathbf{x}) , \end{aligned} \tag{3.30}$$

where $p = \sum_{k>0} p_k$.

Equations (3.29) and (3.10), (3.10) allow the determination of the following recursion relations for the canonical and microcanonical ensembles,

$$nZ_n(\mathbf{x}) = \sum_{k=1}^{n} kx_k Z_{n-k}(\mathbf{x}) , \tag{3.31}$$

$$rZ_n^{(r)}(\mathbf{x}) = \sum_{k=1}^{n-r+1} x_k Z_{n-k}^{(r-1)}(\mathbf{x}) . \tag{3.32}$$

These recursions bottom out at $Z_0(\mathbf{x}) = 1$ and $Z_n^{(1)}(\mathbf{x}) = x_n$, respectively, so these relations can be used to generate all the partition functions iteratively in polynomial

time complexity. For example, computing Z_n requires $\sum_{k=1}^{n}(n-k) = \binom{n}{2}$ additions and a similar number of multiplications. Alternately, the canonical recursion relation could have been derived by exploiting the fact that Z_n and kx_k are symmetric functions (section 2.2.2) by comparing equations (2.65) and (3.25) and applying equation (2.61)

The above derivatives allows us to compute the expectation values of π_k, or in general any expectation value.

$$\begin{aligned} \langle \pi_k \rangle_n^{(r)} &= x_k \frac{Z_{n-k}^{(r-1)}(\mathbf{x})}{Z_n(\mathbf{x})} , \\ \langle \pi_k \rangle_n &= x_k \frac{Z_{n-k}(\mathbf{x})}{Z_n(\mathbf{x})} , \\ \langle \pi_k \rangle &= x_k . \end{aligned} \tag{3.33}$$

Specializing to microcanonical partition functions for a moment, if r is near n, we can compute the microcanonical partition functions exactly in a small number of terms since there are only a small number of partitions with a large number of parts[9], namely:

$$\begin{aligned} Z_n^{(n)} &= \frac{x_1^n}{n!} , \\ Z_n^{(n-1)} &= \frac{x_1^{n-2}x_2}{(n-2)!} , \\ Z_n^{(n-2)} &= \frac{x_1^{n-3}x_3}{(n-3)!} + \frac{x_1^{n-4}x_2^2}{2(n-4)!} , \\ Z_n^{(n-3)} &= \frac{x_1^{n-4}x_4}{(n-4)!} + \frac{x_1^{n-5}x_2x_3}{(n-5)!} + \frac{x_1^{n-6}x_2^3}{6(n-6)!} , \\ Z_n^{(n-4)} &= \frac{x_1^{n-5}x_5}{(n-5)!} + \frac{x_1^{n-6}}{(n-6)!}\left(x_2x_4 + \frac{x_3^2}{2}\right) + \frac{x_1^{n-7}x_2^2x_3}{2(n-7)!} + \frac{x_1^{n-8}x_2^4}{24(n-8)!} , \\ Z_n^{(n-5)} &= \frac{x_1^{n-6}x_6}{(n-6)!} + \frac{x_1^{n-7}(x_2x_5 + x_3x_4)}{(n-7)!} + \frac{x_1^{n-8}(x_2^2x_4 + x_2x_3^2)}{2(n-8)!} \\ &\quad + \frac{x_1^{n-9}x_3x_2^3}{6(n-9)!} + \frac{x_1^{n-10}x_2^5}{120(n-10)!} . \end{aligned} \tag{3.34}$$

[9]Originally, I derived these first few relations from the canonical recurrence relation while exploring the high temperature properties of this model. Clearly if $x_k = tb_k$, then $Z_n = \sum_r t^r Z_n^{(r)}$. However, in this case I noticed $Z_n^{(n-k)}$ appeared to be simple for k small. So I worked out the first few examples completely from the canonical recurrence relation, a quite tedious exercise in algebra. Only later did I realize the by setting $x_k = tb_k$ I was breaking the integer partitions into groups specified by the total number of parts, i.e. integer r-partitions, and that the simplicity of the results was a reflection on the paucity of partitions with a large number of parts. This is a good example of how a little combinatorial knowledge saves a great amount of computations.

In general $Z_n^{(n-k)}(\mathbf{x})$ depends only on $x_1, \ldots, x_{k+1}$ for $k < n/2$.[10]

These microcanonical partition functions are useful in computing high temperature expansions of some canonical models as we now show. Suppose $x_k = tb_k$, then $Z_n(t) = \sum_r Z_n^{(r)}(\mathbf{b})t^r$, since $\prod_k t^{\pi_k} = t^r$ where $r = \sum_k \pi_k$. If t is large, then this expression is dominated by the microcanonical partition functions listed above. For example, we can expand $\ln Z_n$ in inverse powers of t with the aid of the above expressions, i.e.

$$\begin{aligned}\ln Z_n = &\ln Z_n^{(n)} + n\ln t \\ &+\frac{1}{t}\frac{Z_n^{(n-1)}}{Z_n^{(n)}} + \frac{1}{2t^2}\left(\frac{2Z_n^{(n-2)}}{Z_n^{(n)}} - \frac{(Z_n^{(n-1)})^2}{(Z_n^{(n)})^2}\right) \\ &+\frac{1}{3t^3}\left(\frac{3Z_n^{(n-3)}}{Z_n^{(n)}} - \frac{3Z_n^{(n-2)}Z_n^{(n-1)}}{(Z_n^{(n)})^2} + \frac{(Z_n^{(n-1)})^3}{(Z_n^{(n)})^3}\right) + \ldots .\end{aligned} \tag{3.35}$$

Similarly, if t is small, we can expand in terms of $Z_n^{(r)}$ where r is small.

$$\begin{aligned}\ln Z_n = &\ln Z_n^{(1)} + \ln t \\ &+t\frac{Z_n^{(2)}}{Z_n^{(1)}} + \frac{t^2}{2}\left(\frac{2Z_n^{(3)}}{Z_n^{(1)}} - \frac{(Z_n^{(2)})^2}{(Z_n^{(1)})^2}\right) \\ &+\frac{t^3}{3}\left(\frac{3Z_n^{(4)}}{Z_n^{(1)}} - \frac{3Z_n^{(3)}Z_n^{(2)}}{(Z_n^{(1)})^2} + \frac{(Z_n^{(2)})^3}{(Z_n^{(1)})^3}\right) + \ldots .\end{aligned} \tag{3.36}$$

A consequence of these expansions is a simplified approach to the virial expansion of non-ideal gases (section 5.1).

Generalizing these results to vector partitions is relatively uncomplicated. Suppose there are $n = \sum_{k=1}^{s} n_k$ objects, n_k of type k, for a total of s-components ($n_k > 0, \forall k$). Assume the weight for the cluster configuration is given by

$$W(\boldsymbol{\pi}, \mathbf{x}) = \prod_{k_1 \ldots k_s} \frac{x_{\mathbf{k}}^{\pi_{\mathbf{k}}}}{\pi_{\mathbf{k}}!} , \tag{3.37}$$

where $\mathbf{x}$ is a parameter vector. Partial derivatives of the partition functions are then given by

$$\begin{aligned}\frac{\partial Z_{\mathbf{n}}^{(r)}}{\partial x_{\mathbf{k}}} &= Z_{\mathbf{n}-\mathbf{k}}^{(r-1)}(\mathbf{x}) , \\ \frac{\partial Z_{\mathbf{n}}}{\partial x_{\mathbf{k}}} &= Z_{\mathbf{n}-\mathbf{k}}(\mathbf{x}) , \\ \frac{\partial \mathcal{Z}}{\partial x_{\mathbf{k}}} &= \mathcal{Z}(\mathbf{x}) ,\end{aligned} \tag{3.38}$$

[10] An interesting application of these formulas is to determine exact expressions for the Stirling numbers, Lah numbers, and C-numbers, see section 4.1.2 for details.

The grand canonical partition function for these partition functions is given by the closed form expression

$$\mathcal{Z}(\mathbf{x}) = \exp\left\{\sum_{k_1 \ldots k_s} x_{\mathbf{k}}\right\} . \tag{3.39}$$

The canonical and microcanonical partition functions are determined by the recursion relations,

$$\mathbf{n} Z_{\mathbf{n}}(\mathbf{x}) = \sum_{k_1 \ldots k_s} \mathbf{k} x_{\mathbf{k}} Z_{\mathbf{n}-\mathbf{k}}(\mathbf{x}) , \tag{3.40}$$

$$r Z^{(r)}_{\mathbf{n}}(\mathbf{x}) = \sum_{k_1 \ldots k_s} x_{\mathbf{k}} Z^{(r-1)}_{\mathbf{n}-\mathbf{k}}(\mathbf{x}) , \tag{3.41}$$

with $Z_{\mathbf{0}} = 1$, $Z^{(1)}_{\mathbf{n}} = x_{\mathbf{n}}$.

3.2.2 Equipartition models

Consider now a set of models which do not suppress phase space by $1/\pi_k!$ factors. These models are called equipartition models, since for the choice of $\mathbf{x} = (1, 1, \ldots)$, they reduce to a model of fragmentation in which every partition is equally likely.[11] Although these models are not well motivated by many examples in physics, they are useful in the general study of partitions. For example, one can use the results here for the choice $x_k = 1$, $k = 1, \ldots, n$ to determine the values for $p(n)$, $p_r(n)$, independent of the recurrence relations mentioned in section 2.3.1.

Suppose the weight for a partition is given by

$$W(\boldsymbol{\pi}, \mathbf{x}) = \prod_{j>0} x_j^{\pi_j} . \tag{3.42}$$

The grand canonical partition function is therefore given by

$$\begin{aligned} \mathcal{Z}(\mathbf{x}) &= \sum_{n \geq 0} Z_n(\mathbf{x}) = \sum_{n \geq 0} \sum_{\pi(n)} \prod_{j>0} x_j^{\pi_j} = \sum_{\pi_1 \geq 0} x_1^{\pi_1} \sum_{\pi_2 \geq 0} x_2^{\pi_2} \cdots \\ &= \prod_{j>0} \frac{1}{1 - x_j} , \end{aligned} \tag{3.43}$$

[11] Such a model is analyzed in section 5.6.

The partition functions, defined in the usual way, therefore have the following derivatives (using the $x_k = tz^k b_k$ trick):

$$\begin{aligned} \frac{\partial Z_n^{(r)}}{\partial x_k} &= \sum_{i\geq 1} x_k^{i-1} Z_{n-ik}^{(r-i)}(\mathbf{x}) , \\ \frac{\partial Z_n}{\partial x_k} &= \sum_{i\geq 1} x_k^{i-1} Z_{n-ik}(\mathbf{x}) , \\ \frac{\partial \mathcal{Z}}{\partial x_k} &= \frac{1}{1-x_k}\mathcal{Z}(\mathbf{x}) , \end{aligned} \tag{3.44}$$

or in general for the grand canonical partition function

$$\frac{\partial^p \mathcal{Z}}{\partial x_1^{p_1} \ldots \partial x_n^{p_n}} = \left(\prod_{j>0} \frac{p_j!}{(1-x_j)^{p_j}} \right) \mathcal{Z}(\mathbf{x}) . \tag{3.45}$$

The microcanonical and canonical partition functions can now be determined by recursion relations[12], namely

$$n Z_n(\mathbf{x}) = \sum_{k=1}^{n} k \sum_{i\geq 1} x_k^i Z_{n-ik}(\mathbf{x}) , \tag{3.46}$$

$$r Z_n^{(r)}(\mathbf{x}) = \sum_{k=1}^{n-r+1} \sum_{i\geq 1} x_k^i Z_{n-ik}^{(r-i)}(\mathbf{x}) , \tag{3.47}$$

where $Z_0(\mathbf{x}) = 1$, $Z_n^{(1)}(\mathbf{x}) = x_n$. Determining expectation values of π_k in the various ensembles is now possible, for example

$$\begin{aligned} \langle \pi_k \rangle_n^{(r)} &= \sum_{i\geq 1} x_k^i \frac{Z_{n-ik}^{(r-i)}(\mathbf{x})}{Z_n^{(r)}(\mathbf{x})} , \\ \langle \pi_k \rangle_n &= \sum_{i\geq 1} x_k^i \frac{Z_{n-ik}(\mathbf{x})}{Z_n(\mathbf{x})} , \\ \langle \pi_k \rangle &= \frac{x_k}{1-x_k} . \end{aligned} \tag{3.48}$$

As in the Gibbs model, if r is near n, the microcanonical partition functions can be

[12]The direct algorithm discussed in section 2.3.2 for computing $p(m,n)$ and $p_r(m,n)$ can also be applied to computing the canonical and microcanonical partition functions in these models. As before, this method is more efficient than applying the constraint recursion relations.

computed exactly in a small number of terms, namely:

$$\begin{aligned}
Z_n^{(n)} &= x_1^n \,, \\
Z_n^{(n-1)} &= x_1^{n-2} x_2 \,, \\
Z_n^{(n-2)} &= x_1^{n-3} x_3 + x_1^{n-4} x_2^2 \,, \\
Z_n^{(n-3)} &= x_1^{n-4} x_4 + x_1^{n-5} x_2 x_3 + x_1^{n-6} x_2^3 \,, \\
Z_n^{(n-4)} &= x_1^{n-5} x_5 + x_1^{n-6}(x_3^2 + x_2 x_4) + x_1^{n-7} x_2^2 x_3 + x_1^{n-8} x_2^4 \,, \\
Z_n^{(n-5)} &= x_1^{n-6} x_6 + x_1^{n-7}(x_5 x_2 + x_4 x_3) \\
&\quad + x_1^{n-8}(x_4 x_2^2 + x_3^2 x_2) + x_1^{n-9} x_3 x_2^3 + x_1^{n-10} x_2^5 \,.
\end{aligned} \tag{3.49}$$

In fact, $Z_n^{(n-k)}(\mathbf{x}) = x_1^n Z_k(x_2/x_1^2, x_3/x_1^3, \ldots)$ for $k < n/2$.

Generalizing these results to vector partitions proceeds as expected. Suppose that the weight for a configuration is given by

$$W(\boldsymbol{\pi}, \mathbf{x}) = \prod_{k_1 \ldots k_s} x_{\mathbf{k}}^{\pi_{\mathbf{k}}} \,. \tag{3.50}$$

The derivatives are given by

$$\begin{aligned}
\frac{\partial Z_{\mathbf{n}}^{(r)}}{\partial x_{\mathbf{k}}} &= \sum_{i \geq 1} x_{\mathbf{k}}^{i-1} Z_{\mathbf{n}-i\mathbf{k}}^{(r-i)}(\mathbf{x}) \,, \\
\frac{\partial Z_{\mathbf{n}}}{\partial x_{\mathbf{k}}} &= \sum_{i \geq 1} x_{\mathbf{k}}^{i-1} Z_{\mathbf{n}-i\mathbf{k}}(\mathbf{x}) \,, \\
\frac{\partial \mathcal{Z}}{\partial x_{\mathbf{k}}} &= \frac{1}{1 - x_{\mathbf{k}}} \mathcal{Z}(\mathbf{x}) \,,
\end{aligned} \tag{3.51}$$

or in general for the grand canonical partition function

$$\frac{\partial^p \mathcal{Z}}{\partial x_{10\ldots0}^{p_{10\ldots0}} \ldots \partial x_{n_1 \ldots n_s}^{p_{n_1 \ldots n_s}}} = \left(\prod_{\mathbf{k}} \frac{p_{\mathbf{k}}!}{(1 - x_{\mathbf{k}})^{p_{\mathbf{k}}}} \right) \mathcal{Z}(\mathbf{x}) \,. \tag{3.52}$$

The grand canonical partition function is explicitly given by

$$\mathcal{Z}(\mathbf{x}) = \prod_{k_1 \ldots k_s} \frac{1}{1 - x_{\mathbf{k}}} \,, \tag{3.53}$$

and the microcanonical and canonical partition functions are given by the recursion relations

$$\mathbf{n} Z_{\mathbf{n}}(\mathbf{x}) = \sum_{k_1 \ldots k_s} \mathbf{k} \sum_{i \geq 1} x_{\mathbf{k}}^i Z_{\mathbf{n}-i\mathbf{k}}(\mathbf{x}) \,, \tag{3.54}$$

$$r Z_{\mathbf{n}}^{(r)}(\mathbf{x}) = \sum_{k_1 \ldots k_s} \sum_{i \geq 1} x_{\mathbf{k}}^i Z_{\mathbf{n}-i\mathbf{k}}^{(r-i)}(\mathbf{x}) \,, \tag{3.55}$$

where $Z_{00\ldots00} = 1$, $Z_{\mathbf{n}}(\mathbf{x}) = x_{\mathbf{n}}$.

3.2.3 Separable models

Gibbs and equipartition models are special cases of a class of models I refer to as separable models, since the weights separate into products over functions of π_j. The development is essentially an elaboration of the equipartition case, Suppose the weight for a partition is given by

$$W(\boldsymbol{\pi}, \mathbf{x}, \mathbf{f}) = \prod_{j>0} f_j(\pi_j) x_j^{\pi_j} \ . \tag{3.56}$$

Let us define generating functions derived from the functions $f_j(n)$, namely

$$F_j(x) \ := \ \sum_{n\geq 0} f_j(n) x^n \ , \tag{3.57}$$

$$G_j(x) \ := \ \frac{\partial}{\partial x} \ln F_j(x) = \sum_{n\geq 0} g_j(n) x^n \ . \tag{3.58}$$

The grand canonical partition function is then given explicitly by

$$\mathcal{Z}(\mathbf{x}, \mathbf{f}) = \prod_{j>0} F_j(x_j) \ , \tag{3.59}$$

and its derivatives are given by

$$\frac{\partial \mathcal{Z}}{\partial x_k} = G_k(x_k) \mathcal{Z}(\mathbf{x}, \mathbf{f}) \, . \tag{3.60}$$

From this identity we compute the partial derivatives of the canonical and microcanonical partition functions.

$$\frac{\partial Z_n^{(r)}}{\partial x_k} \ = \ \sum_{i\geq 1} g_k(i-1) x_k^{i-1} Z_{n-ik}^{(r-i)}(\mathbf{x}, \mathbf{f}) \, , \tag{3.61}$$

$$\frac{\partial Z_n}{\partial x_k} \ = \ \sum_{i\geq 1} g_k(i-1) x_k^{i-1} Z_{n-ik}(\mathbf{x}, \mathbf{f}) \, , \tag{3.62}$$

which imply the microcanonical and canonical partition functions are given by the recurrence relations

$$n Z_n(\mathbf{x}, \mathbf{f}) \ = \ \sum_{k=1}^{n} k \sum_{i\geq 1} g_k(i-1) x_k^i Z_{n-ik}(\mathbf{x}, \mathbf{f}) \, , \tag{3.63}$$

$$r Z_n^{(r)}(\mathbf{x}, \mathbf{f}) \ = \ \sum_{k=1}^{n-r+1} \sum_{i\geq 1} g_k(i-1) x_k^i Z_{n-ik}^{(r-i)}(\mathbf{x}, \mathbf{f}) \, , \tag{3.64}$$

where $Z_0(\mathbf{x},\mathbf{f}) = 1$, $Z_n^{(1)}(\mathbf{x},\mathbf{f}) = f_n(1)x_n$.

This gives us formulas for various expectation values of π_k, for example

$$\begin{aligned} \langle \pi_k \rangle_n^{(r)} &= \sum_{i\geq 1} g_k(i-1)x_k^i \frac{Z_{n-ik}^{(r-i)}(\mathbf{x},\mathbf{f})}{Z_n^{(r)}(\mathbf{x},\mathbf{f})} , \\ \langle \pi_k \rangle_n &= \sum_{i\geq 1} g_k(i-1)x_k^i \frac{Z_{n-ik}(\mathbf{x},\mathbf{f})}{Z_n(\mathbf{x},\mathbf{f})} , \\ \langle \pi_k \rangle &= x_k G_k(x_k) . \end{aligned} \tag{3.65}$$

For the microcanonical partition functions, if r is near n, we can compute these functions exactly in a small number of terms,

$$\begin{aligned} Z_n^{(n)} &= f_1(n)x_1^n , \\ Z_n^{(n-1)} &= f_2(1)x_2 f_1(n-2)x_1^{n-2} , \\ Z_n^{(n-2)} &= f_3(1)x_3 f_1(n-3)x_1^{n-3} + f_2(2)x_2^2 f_1(n-4)x_1^{n-4} , \\ Z_n^{(n-3)} &= f_4(1)x_4 f_1(n-4)x_1^{n-4} + f_3(1)x_3 f_2(1)x_2 f_1(n-5)x_1^{n-5} \\ &\quad + f_2(3)x_2^3 f_1(n-6)x_1^{n-6} , \\ Z_n^{(n-4)} &= f_5(1)x_5 f_1(n-5)x_1^{n-5} + f_3(2)x_3^2 f_1(n-6)x_1^{n-6} \\ &\quad + f_4(1)x_4 f_2(1)x_2 f_1(n-6)x_1^{n-6} + f_3(1)x_3 f_2(2)x_2^2 f_1(n-7)x_1^{n-7} \\ &\quad + f_2(4)x_2^4 f_1(n-8)x_1^{n-8} . \end{aligned} \tag{3.66}$$

The vector partition case is an obvious generalization of the integer partition case just developed.

3.2.4 Interacting Gibbs models

In this section, we introduce a two-body interaction term to the Gibbs model already considered. Interaction terms can be added to the equipartition and separable models as well, but they are more difficult to analyze. The motivation of the terminology comes from the following example. Suppose the free energy defined over permutations is given by

$$F(p,V,T) = \sum_{k>0} \pi_k(p) F_k(V,T) + \frac{1}{2} \sum_{j,k>0} \pi_j(p)(\pi_k(p) - \delta_{jk}) F_{jk}^i(V,T) . \tag{3.67}$$

The second term in this free energy can be thought of as an interaction energy due to clusters of size j interacting with clusters of size k (the delta function introduced to exclude self-interaction terms). This free energy induces the integer partition weight given by

$$W(\boldsymbol{\pi}, \mathbf{x}, Y) = \prod_{j>0} \frac{x_j^{\pi_j}}{\pi_j!} \prod_{k>0} y_{jk}^{\pi_j(\pi_k - \delta_{jk})/2} \ , \tag{3.68}$$

where $\mathbf{x}$ is a parameter vector, and $Y = (y_{jk})_{1 \le j,k \le n}$ is a parameter matrix characterizing an interaction between clusters. It will be assumed that this matrix is symmetric, i.e. $y_{jk} = y_{kj}$, for if it isn't, it can be symmetrized without changing the physics.

As in the non-interacting case, we proceed by computing the partial derivatives of the partition function.

$$\begin{aligned}
\frac{\partial Z_n^{(r)}}{\partial x_k} &= \sum_{\pi_r(n)} \frac{x_k^{\pi_k - 1}}{(\pi_k - 1)!} \left(\prod_{j \neq k} \frac{x_j^{\pi_j}}{\pi_j!} \right) \prod_{ij} y_{ij}^{\pi_i(\pi_j - \delta_{ij})/2} \\
&= \sum_{\pi_r(n)} \frac{x_k^{\pi_k - 1}}{(\pi_k - 1)!} y_{kk}^{(\pi_k - 1)(\pi_k - 2)/2 + (\pi_k - 1)} \\
&\quad \times \prod_{j \neq k} \frac{x_j^{\pi_j}}{\pi_j!} y_{jk}^{(\pi_k - 1)\pi_j + \pi_j} \prod_{i \neq k} y_{ij}^{\pi_i(\pi_j - \delta_{ij})/2} \\
&= \sum_{\pi_r(n)} \frac{(x_k y_{kk})^{\pi_k - 1}}{(\pi_k - 1)!} y_{kk}^{(\pi_k - 1)(\pi_k - 2)/2} \\
&\quad \times \prod_{j \neq k} \frac{(x_j y_{jk})^{\pi_j}}{\pi_j!} y_{jk}^{\pi_j(\pi_k - 1)} \prod_{i \neq k} y_{ij}^{\pi_i(\pi_j - \delta_{ij})/2} \\
&= Z_{n-k}^{(r-1)}(x_j \to x_j y_{jk}, Y) \ , \\
\frac{\partial Z_n}{\partial x_k} &= Z_{n-k}(x_j \to x_j y_{jk}, Y) \ , \\
\frac{\partial \mathcal{Z}}{\partial x_k} &= \mathcal{Z}(x_j \to x_j y_{jk}, Y) \ ,
\end{aligned} \tag{3.69}$$

and in general

$$\begin{aligned}
\frac{\partial^p Z_n^{(r)}}{\partial x_1^{p_1} \ldots x_n^{p_n}} &= \left(\prod_{jk} y_{jk}^{p_j(p_k - \delta_{jk})/2} \right) Z_{n - \sum_{k>0} k p_k}^{(r-p)}(x_j \to x_j \prod_{k>0} y_{jk}^{p_k}, Y) \ , \\
\frac{\partial^p Z_n}{\partial x_1^{p_1} \ldots x_n^{p_n}} &= \left(\prod_{jk} y_{jk}^{p_j(p_k - \delta_{jk})/2} \right) Z_{n - \sum_{k>0} k p_k}(x_j \to x_j \prod_{k>0} y_{jk}^{p_k}, Y) \ , \\
\frac{\partial^p \mathcal{Z}}{\partial x_1^{p_1} \ldots x_n^{p_n}} &= \left(\prod_{jk} y_{jk}^{p_j(p_k - \delta_{jk})/2} \right) \mathcal{Z}(x_j \to x_j \prod_{k>0} y_{jk}^{p_k}, Y) \ .
\end{aligned} \tag{3.70}$$

It is interesting that the interaction terms seems to induces a "scaling" transformation of the parameters $\mathbf{x}$ when the partition function is differentiated, at least when the expressions are compared to the ordinary Gibbs model. The operator $\frac{\partial}{\partial x_k}$ when applied to the canonical system of n objects, could be interpreted as destroying k objects[13] and rescaling the primary parameter vector by interactions with k sized objects. Another quirk of the model is the identity

$$\frac{1}{2}x_j x_k \frac{\partial^2 Z_n}{\partial x_j \partial x_k} = y_{jk} \frac{\partial Z_n}{\partial y_{jk}} , \tag{3.71}$$

or more generally

$$\frac{1}{2^p} \prod_{k=1}^{n} x_k^{p_k} \frac{\partial^{2p} Z_n}{\partial x_1^{p_1} \cdots \partial x_n^{p_n}} = \prod_{j,k=1}^{n} y_{jk}^{p_{jk}} \frac{\partial^p Z_n}{\partial y_{11}^{p_{11}} \cdots \partial y_{nn}^{p_{nn}}} , \tag{3.72}$$

where $p = \sum_{jk} p_{jk}$, $p_k = \sum_j p_{jk} + p_{kj}$. These identities are useful in some calculations, and indicate the extent to which the interactions and the parameters are closely related in the partition functions.

Unlike the Gibbs model, we cannot construct the grand canonical partition function explicitly, however we can derive recursion relations for the canonical and microcanonical partition functions which are of some utility

$$r Z_r(\mathbf{x}, Y) = \sum_{k>0} x_k Z_{n-k}^{(r-1)}(x_j \to x_j y_{jk}, Y) , \tag{3.73}$$

$$n Z_n(\mathbf{x}, Y) = \sum_{k>0} k x_k Z_{n-k}(x_j \to x_j y_{jk}, Y) , \tag{3.74}$$

where $Z_0(\mathbf{x}, Y) = 1$, $Z_n^{(1)}(\mathbf{X}, Y) = x_n$ anchor the recursions. Working in a symbolic math system such as Mathematica$^{\text{TM}}$ allows these recursions to be brought to bear for a particular choice of parameters.

In practice, the only interacting Gibbs model of utility is specified by $y_{jk} = y$, a constant, since then the weight reduces to a Gibbs weight times $y^{r(r-1)/2}$. A microcanonical decomposition of the canonical case allows us to quickly compute the partition functions and related expectation values. Without this simplification, the recursion relations for this model become hopeless since the number of terms in the partition function grows

[13] The ordinary Gibbs model has this property as well, and it is fully explored in section 4.1.1.

exponentially and each term must be maintained to implement the "scaling" transformations in the recursions. The recursion relations can be useful in computing small cases, however, and possibly in computing the effects of a weak interaction.

As in the other models, the microcanonical partition functions for n near r can be determined in a small number of terms, for example

$$
\begin{aligned}
Z_n^{(n)} &= \frac{x_1^n y_{11}^{n(n-1)/2}}{n!} , \\
Z_n^{(n-1)} &= \frac{(x_1 y_{11}^{(n-3)/2} y_{12})^{n-2} x_2}{(n-2)!} , \\
Z_n^{(n-2)} &= \frac{(x_1 y_{11}^{(n-4)/2} y_{13})^{n-3} x_3}{(n-3)!} + \frac{(x_1 y_{11}^{(n-5)/2} y_{12}^2)^{n-4} x_2^2 y_{22}}{2(n-4)!} , \\
Z_n^{(n-3)} &= \frac{(x_1 y_{11}^{(n-5)/2} y_{14})^{n-4} x_4}{(n-4)!} + \frac{(x_1 y_{11}^{(n-6)/2} y_{12} y_{13})^{n-5} x_2 x_3 y_{23}}{(n-5)!} \\
&\quad + \frac{(x_1 y_{11}^{(n-7)/2} y_{12}^3)^{n-6} x_2^3 y_{22}^3}{6(n-6)!} , \\
Z_n^{(n-4)} &= \frac{(x_1 y_{11}^{(n-6)/2} y_{15})^{n-5} x_4}{(n-5)!} \\
&\quad + \frac{(x_1 y_{11}^{(n-7)/2})^{n-6}}{(n-6)!} \left(\frac{x_3^2 y_{33} y_{13}^{2(n-6)}}{2} + x_2 x_4 y_{24} (y_{12} y_{14})^{n-6} \right) \\
&\quad + \frac{(x_1 y_{11}^{(n-8)/2} y_{12}^2 y_{13})^{n-7} x_2^2 x_3 y_{22} y_{23}^2}{2(n-7)!} + \frac{(x_1 y_{11}^{(n-9)/2} y_{12}^4)^{n-8} x_2^4 y_{22}^6}{24(n-8)!} .
\end{aligned}
\tag{3.75}
$$

Generalizing this model to vector partitions is an uncomplicated elaboration (thankfully omitted) on the above procedure.

Chapter 4

The canonical Gibbs fragmentation model

Of the exactly solvable models introduced in the previous chapter, the Gibbs model is both the simplest and the most useful. It is the natural model in the context of equipartitioning of set partitions or permutations as can be seen from the Cauchy numbers of section 2.1.2. It is also the natural model for the statistical physics of indistinguishable particles because of its inclusion of the Gibbs factor, $\prod_j 1/\pi_j!$. As such, a detailed investigation of its properties, especially under the canonical ensemble, is warranted.

This chapter discusses properties of the Gibbs model which are both mathematically (section 4.1) and physically (sections 4.2, 4.3) interesting, although the distinction is somewhat arbitrary as they are all mathematical properties, some just more physically relevant than others. Among the mathematical properties, section 4.1.1 explores the curious fact that the canonical Gibbs model partition functions are a representation of the eigenstates of a bosonic creation-annihilation algebra. Although of little practical utility, this fact establishes a conceptual framework for thinking about the model, and gives an operator-theoretic method of constructing the partition functions. On the other hand section 4.1.2 which outlines a number of closed-form and alternate recurrence relations for these models is of great utility. Many of these special cases are of historical significance, and all can be used to expedite computations. Section 4.1.3 explores the various identities connecting vector and integer partition sums. These identities reduce certain vector partition sums to integer partition sums, a process which speeds their computation immensely. Section 4.1.4 defines the informational entropy of the Gibbs model, which is a measure of the diversity of clustering patterns. Its maximum point is of clear interest as it specifies the point where the patterns are most unpredictable.

Physical (or less mathematical) properties are equally helpful and are explored in section 4.2. Section 4.2.1 introduces a simple Markov process which has the canonical Gibbs model as its equilibrium distribution. This Markov process serves both as a possible microscopic picture of the dynamics of the Gibbs model, and as a physical process motivating the equilibrium distribution in real-world systems. Section 4.2.2 investigates the distribution of cluster sizes (the "mass yield") of the Gibbs model for various parameter vectors of the form $x_k = xb_k$, which are representative of the parameters of interest in many physical situations. Section 4.2.3 opines briefly on the origins of the Gibbs model and why it applies to so many different physical problems.

Section 4.3 attempts to specify under what conditions a phase transition occurs in a fragmenting system, defined in such a way as to be independent of the thermodynamic considerations, which often are absent from the models. From this point of view, several (but not all) of the critical exponents of transition can be related simply to the clustering properties of the models around the point where large clusters disappear. Specifically the reduced moments (4.3.1) are introduced to characterize such a phase transition. In the Gibbs models however, the variance of the multiplicity and higher-order multiplicity fluctuations (4.3.2) also indicate the location and behavior of the phase transition and this is explored in depth, which improves our understanding of phase transitions in these models and allows a comparison of the canonical Gibbs model to the microcanonical and grand canonical Gibbs models. The connection of this phase transition to the location of the zeros of the partition functions in the complex plane (4.3.3) is also considered.

4.1 Mathematical properties of the Gibbs model

The purpose of this section is to explore some of the purely mathematical properties of the Gibbs models which permit either additional insight or better algorithms for the evaluation of particular partition functions. The creation-annihilation algebra (4.1.1) implicit in the Gibbs model provides some such insight into the nature of its partition functions, and also provides a computational algorithm for their evaluation, although it is impractical in general. The existence of closed-form solutions and alternate recursive

techniques (4.1.2) on the other hand provides tremendously improved algorithms for the evaluation of certain partition functions. Similarly, vector partition invariants help relate particular vector partition models to integer partition models, which vastly simplifies their computation. Alas, none of these algorithms can be applied generally, and so we can expect that for most models we are restricted to the simple (but effective) techniques of section 3.2.1.

4.1.1 Creation-Annihilation algebras

One of the most widely applied models in physics is the quantum harmonic oscillator, specified by the Hamiltonian $\hat{H} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2$, where x is the position of the particle moving in a potential field $V(x) = \frac{1}{2}x^2$.[1] The eigenstates ψ_n determined by $\hat{H}\psi_n = E_n\psi_n$ can be constructed by a creation-annihilation algebra, and in the standard Schrödinger representation, these eigenfunctions are essentially Hermite polynomials times an exponential decay factor. Specifically, the Hamiltonian can be rewritten as $\hat{H} = \hat{a}^\dagger\hat{a} + \frac{1}{2}$, where $\hat{a}^\dagger, \hat{a}$ are creation and annihilation operators, $\hat{a}^\dagger\psi_n \propto \psi_{n+1}$, $\hat{a}\psi_n \propto \psi_{n-1}$. But the harmonic oscillator wavefunctions or equivalently their creation-annihilation algebra can have many possible representations, and in fact as shall soon be shown the canonical Gibbs ensemble partition functions is one possible representation of this algebra.

Consider the behavior of the canonical Gibbs partition functions $Z_n(\mathbf{x})$ under differentiation. Equation (3.29) suggests that $\frac{\partial}{\partial x_k}$ takes a Gibbs system with n objects, destroys k objects, returning a Gibbs system with $n-k$ objects. Considering the partition functions as forming a set of eigenstates of some (yet to be determined) operator, $\frac{\partial}{\partial x_1}$ "lowers" the eigenstate $Z_n(\mathbf{x})$ to $Z_{n-1}(\mathbf{x})$. So we can define a lowering operator $\hat{L}$ as follows.

$$\hat{L} := \frac{\partial}{\partial x_1}\,, \tag{4.1}$$

[1] I'm assuming the reader is familiar with the quantum mechanical harmonic oscillator. If not, a quick glance at any introductory quantum mechanics book should answer any questions, e.g. Liboff [189].

since

$$\hat{L}Z_n(\mathbf{x}) = \frac{\partial Z_n}{\partial x_1} = Z_{n-1}(\mathbf{x}) \; . \tag{4.2}$$

Similarly we can define a creation operator which "raises" the partition function $Z_n(\mathbf{x})$ to $Z_{n+1}(\mathbf{x})$. Indeed, consider the differential operator $\hat{R}$ defined by

$$\hat{R} := x_1 + \sum_{k>1} k x_k \frac{\partial}{\partial x_{k-1}} \; . \tag{4.3}$$

This operator raises canonical Gibbs partition functions as seen by the following computation:

$$\begin{aligned} \hat{R}Z_n(\mathbf{x}) &= \left(x_1 + \sum_{k>1} k x_k \frac{\partial}{\partial x_{k-1}} \right) Z_n(\mathbf{x}) \\ &= x_1 Z_n(\mathbf{x}) + \sum_{k=2}^{n+1} k x_k Z_{n+1-k}(\mathbf{x}) \\ &= \sum_{k=1}^{n+1} k x_k Z_{n+1-k}(\mathbf{x}) = (n+1) Z_{n+1}(\mathbf{x}) \; , \end{aligned} \tag{4.4}$$

where we have used equations (3.31) and (3.29). So we could use $\hat{R}$ to produce the partition functions. However, this method quickly becomes cumbersome as the exact form of the partition function (with $p(n)$ terms) must be maintained to apply the operator. Interestingly, this method was anticipated in symmetric function theory, where differential operators called Hammond operators were used by some mathematicians to generate tables of symmetric functions [201][2]

Computation of the commutator of these two operators reveals that the algebra induced by the operators is equivalent to the algebra for a system of bosons. Specifically,

$$\hat{L}\hat{R}Z_n(\mathbf{x}) = (n+1)Z_n(\mathbf{x}) \; , \tag{4.5}$$

$$\hat{R}\hat{L}Z_n(\mathbf{x}) = nZ_n(\mathbf{x}) \; , \tag{4.6}$$

---

[2]The Hammond operator [137,138] given by

$$D_1 = e_1 + \sum_{k>0} e_k \frac{\partial}{\partial e_{k+1}}$$

defines a lowering operator on k_n, i.e. $D_1 k_n = k_{n-1}$. Realizing that in terms of symmetric functions, $Z \leftrightarrow k$, $kx_k \leftrightarrow s_k$, we can reexpress $\hat{L}, \hat{R}$ in terms of symmetric functions also, i.e. $\hat{L} = \partial/\partial s_1$, $\hat{R} = s_1 + \sum_{k>1}(k-1)s_k \frac{\partial}{\partial s_{k-1}}$.

or in other words, on the space of functions spanned by the canonical Gibbs partition functions,

$$[\hat{L}, \hat{R}] = 1 \ , \tag{4.7}$$

which is the commutation relation for creation and annihilation operators of bosons. Quantum mechanically speaking, the partition functions form a set of eigenfunctions (unnormalized) of the Hamiltonian operator $\hat{H} = \hat{R}\hat{L}$, which are a representation of a system of bosons. We can even interpret $\hat{L}$, $\hat{R}$ in terms of position and momentum operators. These functions span a subspace of symmetric functions, since the canonical Gibbs partition functions are themselves symmetric functions (see section 2.2.2). In this case, the vacuum $Z_0(\mathbf{x})$ corresponds to a system with no particles. Higher energy eigenfunctions correspond to statistical systems with a particular number of particles.

These operators can be simply generalized to vector Gibbs systems. For example, in a bipartite system, two creation and two annihilation operators would suffice to generate the set of canonical partition functions. Representing a creation-annihilation algebra using equipartition partition functions (for example) is also possible, but the form of the operators is much more complicated than in the Gibbs case. Indeed, the fact that a creation-annihilation algebra can be inferred from the partition functions is not especially noteworthy. Any set of canonical partition functions represents such an algebra. The interesting aspect is that the operators are both convenient and compact, and therefore can be used as an operator-theoretic method of generating partition functions.

4.1.2 Closed-form solutions and alternate recursive methods

The canonical Gibbs partition functions can be generally computed by recursive methods as explained in section 3.2.1, or by the operator-theoretic method of section 4.1.1, but for some parameter vectors there are either closed-form solutions or simpler recursive or operative methods. These can be useful in extending the range over which the partition functions can practically be computed. Additionally, the existence of simpler methods is a good indication of interesting properties underlying the choice of

parameter vector. This is particularly true of the examples presented here.

Historically, many of these special cases arose mostly from combinatorial identities discovered in symmetric function theory. Percy A. MacMahon's work in this respect is particularly relevant, and the first few examples here are from [201]. Nathan J. Fine [103,104], also has derived a number of interesting partition identities in his work on hypergeometric functions, but they do not seem particularly relevant to physics.[3]

We begin by simply stating some well-known partition identities. The following three partition identities with one free parameter t were known to nineteenth century mathematicians

$$\sum_r \sum_{\pi_r(n)} \prod_{j>0} \frac{t^{\pi_j}}{\pi_j!} = \sum_r \frac{t^r}{n!} \left[\frac{n!}{r!} \binom{n-1}{r-1} \right] = \frac{t}{n} L_{n-1}^{(1)}(-t) \,, \tag{4.8}$$

$$\sum_r \sum_{\pi_r(n)} \prod_{j>0} \frac{1}{\pi_j!} \left(\frac{t}{j} \right)^{\pi_j} = \sum_r \frac{t^r}{n!} \left[{n \atop r} \right] = \binom{t+n-1}{n} \,, \tag{4.9}$$

$$\sum_r \sum_{\pi_r(n)} \prod_{j>0} \frac{1}{\pi_j!} \left(\frac{t}{j!} \right)^{\pi_j} = \sum_r \frac{t^r}{n!} \left\{ {n \atop r} \right\} = \frac{1}{n!} B_n(t) \,, \tag{4.10}$$

where $L_n^{(1)}(t)$ is the 1st associated Laguerre polynomial[4] and $B_n(t)$ is the nth Bell polynomial.[5] In all likelihood Augustin Cauchy discovered the second of these identities (the case $x_k = 1/k$), although the generalized form above is due to James J. Sylvester (according to MacMahon [201]) and C.G.J. Jacobi in 1841 [77].

We also have the following partition identities with two free parameters t, q due to

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[3] Fine's work on partition identities is reviewed in section 5.5 of *Combinatorial identities* by John Riordan [256], a book usually easier to find than the original work.

[4] The numbers $L(n,r) = \frac{n!}{r!}\binom{n-1}{r-1}$ which appear in the series expansion of the 1st associated Laguerre polynomial are also known as the Lah numbers, and appear when computing rising factorials in terms of falling factorials, i.e. $(t)_n = \sum_r L(n,r)[t]_r$.

[5] All three of these identities generate numbers which are special cases of the C-numbers, defined by

$$C(n,r,s) = n! \sum_{\pi_r(n)} \prod_{j>0} \frac{1}{\pi_j!} \binom{s}{j}^{\pi_j}$$

i.e. $C(n,r,-1) = (-1)^n L(n,r)$, $\lim_{s\to 0} s^{-r} C(n,r,s) = (-1)^{n-k} \left[{n \atop r} \right]$, $\lim_{s\to\infty} s^{-n} C(n,r,s) = \left\{ {n \atop r} \right\}$. These numbers satisfy the recurrence $C(n+1,r+1,s) = (sr-n)C(n,r,s) + sC(n,r-1,s)$ and have many other interesting properties, see Charalambides and Singh [57].

P.A. MacMahon [201], Y. Voloshin and I. Tomescu [304,296], and R. Keener, E. Rothman and N. Starr [163], as well as one I have been unable to attribute, but have verified.

$$\binom{t+n-1}{n}_q = \sum_{\pi(n)} \prod_{j>0} \frac{1}{\pi_j!} \left(\frac{1-q^{jt}}{j(1-q^j)} \right)^{\pi_j} , \tag{4.11}$$

$$\binom{tq}{n} = \sum_r \frac{q!}{(q-r)!} \sum_{\pi_r(n)} \prod_{j>0} \frac{1}{\pi_j!} \binom{t}{j}^{\pi_j} , \tag{4.12}$$

$$\binom{tq+n-1}{n} = \sum_r \frac{q!}{(q-r)!} \sum_{\pi(n)} \prod_{j>0} \frac{1}{\pi_j!} \binom{t+j-1}{j}^{\pi_j} , \tag{4.13}$$

$$\frac{t}{t+nq}\binom{t+nq}{n} = \sum_{\pi(n)} \prod_{j>0} \frac{1}{\pi_j!} \left(\frac{t}{qj}\binom{qj}{j} \right)^{\pi_j} , \tag{4.14}$$

where $\binom{n}{k}_q$ is the Gaussian q-polynomial, or q-binomial coefficient[6] MacMahon's identity has several non-trivial limits. Cayley's identity [53] (i.e. equation (2.51)) is obtained by taking $t \to \infty$, and Sylvester's identity is the limit $q \to 1$.

The Keener-Rothman-Starr identity also has several non-trivial limits. Suppose we have q states occupied by n objects, with ν_k the occupancy of the kth state. The multinomial distribution is then defined by

$$\Pr(\boldsymbol{\nu}) = \binom{n+qt-1}{n}^{-1} \prod_{k=1}^{q} \binom{t+\nu_i-1}{nu_i} \tag{4.15}$$

Define the structure of $\boldsymbol{\nu}$ by $\pi_1, \ldots$ where π_k is the number of states occupied by k objects. Then clearly by a counting argument we have

$$\Pr(\boldsymbol{\pi}) = \binom{q}{\pi_1, \ldots, \pi_n} \left(\binom{n+qt-1}{n}^{-1} \prod_{k>0} \binom{t+k-1}{k}^{\pi_k} \right) \tag{4.16}$$

since the rightmost part is the probability of getting a state $\nu_1, \ldots, \nu_q$ with structure $\pi_1, \ldots \pi_n$ and the left part is the number of such states with that structure. This equation is simply the KRS identity rewritten. If $t = 1$, the distribution induced is therefore Bose-Einstein as all states $\boldsymbol{\nu}$ are equiprobable and equal to $\binom{q+n-1}{n}^{-1}$. If $t \to$

---

[6] The Gaussian q-binomial coefficient is defined as

$$\binom{n}{k}_q = \frac{(q)_n}{(q)_k (q)_{n-k}} ,$$

where $(q)_n = (1-q)(1-q^2)\cdots(1-q^n)$. Clearly in the limit $q \to 1$, the coefficient becomes an ordinary binomial coefficient, which explains the nomenclature. See Andrews [11], chapter 3 for a brief introduction to Gaussian polynomials, and Andrews [12] for general results on q-series.

∞, the Maxwell-Boltzmann distribution is obtained since the state $\boldsymbol{\nu}$ has probability $2^{-n}n!/\prod_k \nu_k!$. And if $qt \to \theta$ as $q \to \infty$, $t \to 0$, then the distribution converges to Ewens' sampling formula (section 5.4).

These identities clearly imply closed-form Gibbs models. For example, from equations (4.8), (4.9), (4.10) we can derive the following three partition function identities

$$Z_n(x_k = x) = \frac{x}{n} L^1_{n-1}(-x) = \frac{1}{n!} \sum_{r=1}^{n} \frac{n!}{k!} \binom{n-1}{r-1} x^r \,, \tag{4.17}$$

$$Z_n(x_k = x/k) = \binom{x+n-1}{n} = \frac{1}{n!} \sum_{r=1}^{n} \begin{bmatrix} n \\ r \end{bmatrix} x^r \,, \tag{4.18}$$

$$Z_n(x_k = x/k!) = \frac{1}{n!} B_n(x) = \frac{1}{n!} \sum_{r=1}^{n} \begin{Bmatrix} n \\ r \end{Bmatrix} x^r \,. \tag{4.19}$$

Because of their closed-form solutions, these three models have been analyzed thoroughly in the physics literature as possible models of nuclear fragmentation. The Gibbs model with $x_k = x/k$ was introduced by A.Z. Mekjian [215] and analyzed extensively in the context of nuclear fragmentation in a series of paper by him and S.J. Lee [214,217,216,184,183]. Additionally, it appears in population genetics as Warren J. Ewens' sampling formula [92,93] for the distribution of alleles. The Gibbs model with $x_k = x$, often called the chain model in nuclear physics, was introduced and analyzed by D.H.E. Gross *et al.* [125,126,152] as a model for fragmentation. Finally, the Gibbs model with $x_k = x/k!$ was introduced by A.R. DeAngelis and A.Z. Mekjian [72] (for $x = 1$) and was further analyzed for any x by K.C. Chase and Mekjian [59]. All three of these models also appear in *Reversibility and Stochastic Networks* by Frank P. Kelly [164] and in section 4.2.1 as examples of Markov process models which arise from simple transition rates (e.g. see table 4.2). The clustering behavior of these models, important for judging their applicability to physical systems, is discussed in section 4.2.2.

Two other closed-form canonical Gibbs partition functions can be inferred from the other identities (equations (4.11) and (4.14)), namely

$$Z_n\left(x_k = \frac{1-q^{kx}}{k(1-q^k)}\right) = \binom{x+n-1}{n}_q \,, \tag{4.20}$$

$$Z_n\left(x_k = \frac{x}{qk}\binom{qk}{k}\right) = \frac{x}{x+nq}\binom{x+nq}{n} \,. \tag{4.21}$$

These examples are both generalizations of Ewens' sampling formula (or Sylvester's identity), since when $q \to 1$, they both reduce to that case. The first was examined by Mekjian and Lee [217] in the limit $q \to -1$. In that case only dimers have appreciable probability. The second example is a limiting case of a model introduced in section 6.2.2, and was originally introduced in [58].

Closed-form solutions are not the only expedient we can pursue. Simplified recurrence relations can be applied in some cases. For any choice of x_k, the recursion relation given in equation (3.31) holds. However, for some x_k there are simpler recursion relations. For example, if $Z_n(x)$ is given by an orthogonal polynomial, (e.g., $x_k = x$), then $Z_{n+1}(x) = (a_n + b_n x)Z_n(x) - c_n Z_{n-1}(x)$ (see Abramowitz and Stegun [1]). Table 4.1 lists some models which can be expressed this way. Note that the last choice for x_k in Table 4.1 is related to the Catalan numbers, $C_k = \frac{1}{k+1}\binom{2k}{k}$, specifically, $x_k = xC_{k-1}$. The Catalan numbers have a number of intriguing properties, and are ubiquitous in combinatorics.

Table 4.1: Simplified recursion relations for various Gibbs models.

x_k	Recursion relation	Model
x/k	$nZ_n = (x + n - 1)Z_{n-1}$	Ewens' sampling model
$x/k!$	$nZ_n = (x + x\frac{d}{dx})Z_{n-1}$	
x	$nZ_n = (x + 2n - 2)Z_n - (n-2)Z_{n-1}$	Chain model
$x\delta_{k1}$	$nZ_n = xZ_{n-1}$	Boltzmann gas
$\frac{x}{k}\binom{2(k-1)}{k-1}$	$nZ_n = 2(2n-3)Z_{n-1} + \frac{x^2}{n-1}Z_{n-2}$	

Simplified recurrence relations and closed-forms also occur for the ideal Boltzmann gas. Consider an ideal Boltzmann gas in d dimensions. Its partition function is given by $Z_n(x) = x^n/n! = (x/n)Z_{n-1}(x)$, where $x = V/\lambda_T^d$ and $\lambda_T = h/\sqrt{2\pi m k_B T}$ is the thermal wavelength. This is a canonical Gibbs model with the parameter vector

$$x_k = \frac{V}{\lambda_T^d}\delta_{k1} \ . \tag{4.22}$$

Since $x_k = 0$ for $k \neq 1$, this model only has "fragments" of size one, i.e., there is no clustering. A close relative of the Boltzmann gas, the interacting Boltzmann gas can be described by an interacting Gibbs model. Richard Feynman [102] illustrated that when

the three-body and higher order terms are neglected, the partition function is given by

$$nZ_n(V,T) = \frac{V}{\lambda_T^d}\left(1-\frac{a}{V}\right)^{n-1} Z_{n-1}(V,T)\,, \tag{4.23}$$

where $Z_0(V,T)=1$, $a=\int_0^\infty \left(1-e^{-V(r)/k_BT}\right)4\pi r^2 dr$, and $V(r)$ is the two-body potential. In terms of an interacting Gibbs model, this is specified by the parameter vectors

$$\begin{aligned} x_k &= x\,\delta_{k1} \\ y_{jk} &= 1-\frac{a}{V} \end{aligned} \tag{4.24}$$

So Gibbs models are not unique in having closed-form solutions.

Although we considered only canonical partition functions, similar results apply to microcanonical partitions functions. For example, by identifying the microcanonical partition functions with well known mathematical functions (e.g. the Stirling numbers and Lah numbers if $x_k = x/k, x/k!, x$), we can substitute improved computational algorithms for the generic ones. Conversely, we can use the connection between sums over partitions and these numbers to obtain closed form expressions for some of the functions using equation (3.34). For the Stirling numbers, this leads to the following exact expressions,

$$\begin{bmatrix} n \\ n-2 \end{bmatrix} = 2\binom{n}{3} + 3\binom{n}{4}\,, \tag{4.25}$$

$$\begin{bmatrix} n \\ n-3 \end{bmatrix} = 6\binom{n}{4} + 20\binom{n}{5} + 15\binom{n}{6}\,, \tag{4.26}$$

$$\begin{bmatrix} n \\ n-4 \end{bmatrix} = 24\binom{n}{5} + 130\binom{n}{6} + 210\binom{n}{7} + 105\binom{n}{8}\,, \tag{4.27}$$

and

$$\begin{Bmatrix} n \\ n-2 \end{Bmatrix} = \binom{n}{3} + 3\binom{n}{4}\,, \tag{4.28}$$

$$\begin{Bmatrix} n \\ n-3 \end{Bmatrix} = \binom{n}{4} + 10\binom{n}{5} + 15\binom{n}{6}\,, \tag{4.29}$$

$$\begin{Bmatrix} n \\ n-4 \end{Bmatrix} = \binom{n}{5} + 25\binom{n}{6} + 105\binom{n}{7} + 105\binom{n}{8}\,. \tag{4.30}$$

Similar expressions hold for the Lah numbers.

4.1.3 Vector partition invariants

Vector partition models clearly are computationally more intensive than integer partition models. As a result, any simplification which speeds up the computation without sacrificing accuracy is welcome. This section explores one possible simplification: reducing the partition function to a sum over integer partitions. This clearly reduces the workload if recurrences can be maintained over the integer partitions. Here it is shown to be possible for one type of parameter vector because of a theorem due to Nathan J. Fine. Section 6.2.2 accomplishes a similar reduction for another type of parameter vector.

The following theorem by Nathan J. Fine [103,104] and its vector partition generalization allow us to relate vector and ordinary symmetric functions. In fact, the relations are related to the Cauchy numbers Perm($\boldsymbol{\pi}$), a fact which can be arrived at in many ways.

Theorem 4.1.1 (Fine [103, 104], 1959) *Let* $\psi_j(q) = \sum_{n\geq 0} C_j(n)q^n$, *then*

$$\prod_{j>0} \psi_j(q^j t) \;=\; \sum_{n\geq 0} q^n \sum_{r\geq 0} t^r \sum_{\pi_r(n)} \prod_{j>0} C_j(\pi_j)\,. \tag{4.31}$$

Proof: Since $n = \sum_{j>0} j\pi_j$, $r = \sum_{j>0} \pi_j$ we can identify terms in $\prod_{j>0} \psi_j(q^j t)$ with partitions. The RHS of the equation is then just an accounting of terms on the LHS by partition classes. Remark: Fine restricted his attention to the case $t = 1$.

The vector partition generalization is in the same spirit:

Theorem 4.1.2 *Let* $\psi_{jk}(q) = \sum_{n\geq 0} C_{jk}(n)q^n$, *then*

$$\prod_{jk} \psi_{jk}(x^j y^k t) \;=\; \sum_{mn} x^m y^n \sum_{r} t^r \sum_{\pi_r(m,n)} \prod_{jk} C_{jk}(\pi_{jk})\,. \tag{4.32}$$

Proof: Completely analogous to above proof.

Combining these two theorems gives the following very useful corollary

Corollary 4.1.1 *Given* m, n, r *and* x_j *from* $j = 1, \ldots, m+n$, *then*

$$\binom{m+n}{m} \sum_{\pi_r(m+n)} \prod_{j>0} \frac{x_j^{\pi_j}}{\pi_j!} = \sum_{\pi_r(m,n)} \prod_{jk} \frac{1}{\pi_{jk}!} \left(\binom{j+k}{j} x_{j+k} \right)^{\pi_{jk}}\,. \tag{4.33}$$

Proof: Choose $\psi_{jk}(q) = \exp\left\{tx_{j+k}\binom{j+k}{j}q\right\}$ and $\psi_j(q) = \exp\{tx_jq\}$. If we denote $Z(q,t) = \prod_{j>0}\psi_j(q^jt)$ and $Z(x,y,t) = \prod_{jk}\psi_{jk}(x^jy^kt)$ then it is obvious that $Z(x+y,t) = Z(x,y,t)$. The identity follows by applying the two theorems and expanding both sides in powers of x, y, and t. □

Now if $x_j = s_j/j$ in the above corollary and applying MacMahon's partition identities (section 2.2.2) we can restate this theorem in terms of symmetric functions, which will prove to be very useful when considering isobaric equivalence (see section 6.2.2).

Theorem 4.1.3 *If the elementary bipartite symmetric function is related to the ordinary elementary symmetric function $s_{mn} = s_{m+n}$, then*

$$e_{mn} = \binom{m+n}{m} e_{m+n}\ , \tag{4.34}$$

$$k_{mn} = \binom{m+n}{m} k_{m+n}\ . \tag{4.35}$$

In summary, if $x_{jk} = \binom{j+k}{j}x_{j+k}$, the vector partition functions can be reduced to integer partition functions in a simple way.

4.1.4 Information theory and clustering entropies

The probability distribution associated with the Gibbs model can be analyzed in a purely information theoretic context. Suppose one had to measure the outcome of a continuous fragmentation process acting on 50 objects and record the results for posterity. Every so often you take a look and see a particular pattern, and in your notebook you write down the pattern. The first day your notebook looks something like this: (1) 50 monomers, (2) 50 monomers, (3) 48 monomers, 1 dimer, (4) 50 monomers, (5) 50 monomers, ... In fact, after a while you realize that most of your notebook is filled with events in which you see 50 monomers. The second day your notebook is equally repetitious, but different (1) 1 50-mer, (2) 1 50-mer, (4) 1 49-mer, 1 monomer, (4) 1 50-mer, ... The third day however, your notebook is much more random (1) 20 monomers, 6 dimers, 4 trimers, 1 8-mer, (2) 17 monomers, 8 dimers, 2 trimers, 1 11-mer, ... Clearly the individual observations on the third day contain more information, since it is difficult to predict in advance what they will be. On the first and second

days, however, you could guess with fairly high certainty what your next measurement will be, and therefore each measurement reveals little information.

The informational entropy[7] measures this information capacity and for a probability distribution $\Pr(\boldsymbol{\pi})$ is defined by

$$H = -\langle \ln \Pr \rangle = -\sum_{\pi(n)} \Pr(\boldsymbol{\pi}) \ln \Pr(\boldsymbol{\pi}) \; . \tag{4.36}$$

It is defined so that it is maximal if all events are equally likely, and equal to zero if there is only one possible event. This definition of informational entropy confirms our expectation that a set composed of randomly distributed events contains more information than a set composed of many similar events. So in the above example, the first two days' informational entropy is quite small, whereas the third day there is much more entropy arising from the wider variety of events.

Suppose the distribution of events is given by the canonical Gibbs distribution,

$$\Pr(\boldsymbol{\pi}) = \frac{1}{Z_n(\mathbf{x})} \prod_{k>0} \frac{x_k^{\pi_k}}{\pi_k!} \; . \tag{4.37}$$

The informational entropy is then given by

$$\begin{aligned} H(\mathbf{x}) &= \sum_{\pi(n)} \Pr(\boldsymbol{\pi}) \left(\ln Z_n - \sum_k \pi_k \ln x_k + \ln \pi_k! \right) \\ &= \ln Z_n(\mathbf{x}) - \sum_k \langle \pi_k \rangle_n \ln x_k + \sum_k \langle \ln \pi_k! \rangle_n \; . \end{aligned} \tag{4.38}$$

How can we compute this quantity? The first two terms can be calculated using the methods discussed in section 3.2.1. Computing the last term can be done by computing the probability that $\pi_k = p$, namely

$$\Pr(\pi_k = p) = \frac{x_k^p}{p!} \frac{Z_{n-pk}(x_1, \ldots, x_{k-1}, 0, x_{k+1}, \ldots)}{Z_n(\mathbf{x})} \; , \tag{4.39}$$

and then adding up the contributions from each possible p,

$$\langle \ln \pi_k! \rangle = \sum_{p>1} \Pr(\pi_k = p) \ln p! \; . \tag{4.40}$$

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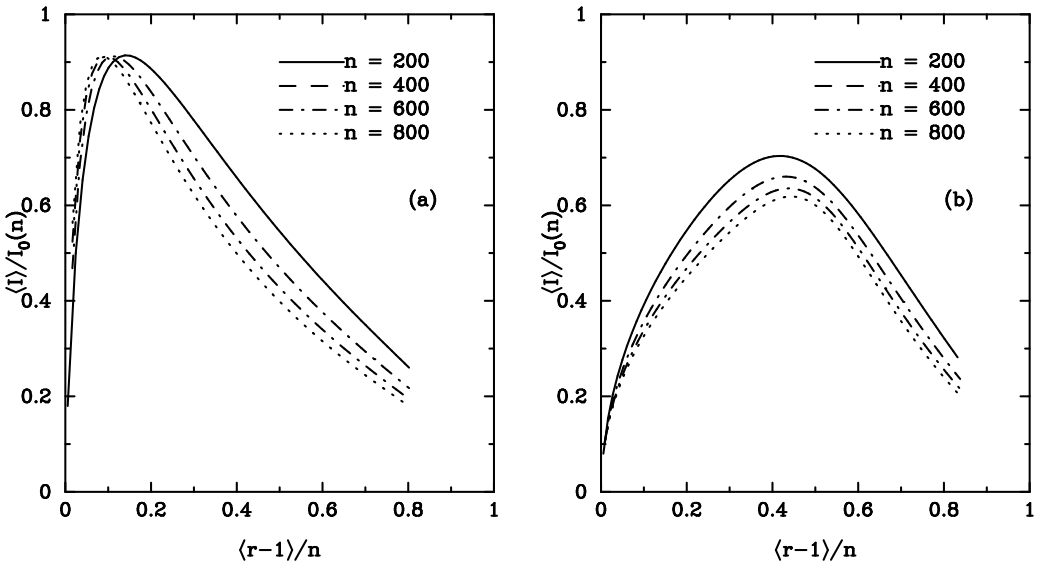
[7] The traditional entropy measure is the thermodynamic entropy, which is the informational entropy of the *microstates* of the system. The partition events here are macrostates of the system, and therefore the two definitions of entropy are different and a distinction between them needs to be made.

This expression for $\Pr(\pi_k = p)$ arises from the fact that $Z_{n-pk}(x_1, \ldots, x_{k-1}, 0, x_{k+1}, \ldots)$ is the Gibbs partition function for $n - pk$ objects subject to the restriction $\pi_k = 0$. Multiplying this by $x_k^p/p!$ therefore yields a Gibbs partition function on n objects with $\pi_k = p$. Dividing this by $Z_n(\mathbf{x})$ then yields the probability that $\pi_k = p$. Figure 4.1 illustrates the behavior of the entropy as a function of $\langle r \rangle$ for $x_k = x/k$ and $x_k = x/k^{5/2}$. The phase transition (see section 4.3) in the second model causes a distinctly different information profile for that model.

Figure 4.1: The informational entropy $\langle H \rangle / \ln p(n)$ for the canonical Gibbs model with (a) $x_k = x/k$ and (b) $x_k = x/k^{5/2}$ plotted against the expected number of parts $(\langle r - 1 \rangle / n)$ for $n = 200, 400, 600, 800$.



4.2 "Physical" properties of canonical Gibbs models

This section deals with two "physical" properties of the Gibbs models. The first, how the model arises from a dynamical competition between an aggregation and fragmentation process, is a possible picture of the underlying physics. It is not unique; for example, sequential (equi)partitioning is a dynamic picture with no aggregation and has been shown to yield the Gibbs model with $x_k = 1/k$ [117]. The second, the mass yield of various models, is a preliminary investigation of the clustering behavior of the Gibbs model. The goal is to identify models (i.e. parameter vectors) with properties

which closely match observed physical systems. Indeed the general behavior of the models investigated will prove to approximate the behavior seen in several physical systems, especially nuclear fragmenting ones.

4.2.1 Markov process dynamics

The Gibbs model has been introduced as an equilibrium distribution to an as yet unspecified physical process. In this section we introduce a Markov process [164] which has the Gibbs ensemble as its canonical equilibrium distribution. This allows for some possible dynamical physical interpretations to be given to the parameter vectors, an alternative to the usual static statistical interpretations.

Suppose we have n indistinguishable objects in some particular partition state. Over time, new partition states form by the underlying physical processes: the joining of two clusters to form a new larger cluster and the splitting of a cluster into two smaller clusters. Notice that these processes conserve particle number but not cluster number, and so the accessible states are defined by the canonical ensemble. Clusters joining and breaking into more than two groups are possible, but we will ignore that for now, assuming that those processes are of lesser importance and will not materially affect the overall equilibrium distribution. We denote these processes by a transition operator T which acts as follows on the partition $\boldsymbol{\pi}$.

$$T^{jk}\boldsymbol{\pi} = \begin{cases} (\ldots, \pi_j - 1, \ldots, \pi_k - 1, \ldots, \pi_{j+k} + 1, \ldots) & j \neq k \\ (\ldots, \pi_j - 2, \ldots, \pi_{2j} + 1, \ldots) & j = k \end{cases} , \tag{4.41}$$

$$T_{jk}\boldsymbol{\pi} = \begin{cases} (\ldots, \pi_j + 1, \ldots, \pi_k + 1, \ldots, \pi_{j+k} - 1, \ldots) & j \neq k \\ (\ldots, \pi_j + 2, \ldots, \pi_{2j} - 1, \ldots) & j = k \end{cases} , \tag{4.42}$$

i.e. $T^{jk}\boldsymbol{\pi}$ combines a j and k sized cluster to form a $j+k$ cluster, and T_{jk} is the inverse operation ($T^{jk}T_{jk} = 1$). Suppose these processes occur at some rate denoted by $q(\boldsymbol{\pi}, \boldsymbol{\pi}')$ for $\boldsymbol{\pi}$ transforms to $\boldsymbol{\pi}'$. For example,

$$\begin{aligned} q(\boldsymbol{\pi}, T^{jk}\boldsymbol{\pi}) &= \lambda_{jk}\pi_j(\pi_k - \delta_{jk}) , \\ q(\boldsymbol{\pi}, T_{jk}\boldsymbol{\pi}) &= \mu_{jk}\pi_{j+k} . \end{aligned} \tag{4.43}$$

This is a very reasonable choice, as the rate is proportional to the number of fragments available for such moves. If there are none, then the transition rate is zero, as needed. These processes when applied repeatedly to a configuration will lead to an equilibrium configuration, at which point the rate at which transitions occur to a new state, weighed to reflect the equilibrium distribution of the original state, is equal to the rate at which transitions occur back to the original state, weighed to reflect the equilibrium distribution of the new state. In other words, if $\Pr(\boldsymbol{\pi})$ is the equilibrium distribution, it must satisfy the detailed balance condition:

$$\Pr(\boldsymbol{\pi})q(\boldsymbol{\pi}, T^{jk}\boldsymbol{\pi}) = \Pr(T^{jk}\boldsymbol{\pi})q(T^{jk}\boldsymbol{\pi}, \boldsymbol{\pi}) \ . \tag{4.44}$$

The equilibrium distribution for the canonical Gibbs ensemble is

$$\Pr(\boldsymbol{\pi}) = \frac{1}{Z_n(\mathbf{x})} \prod_{k \geq 1} \frac{x_k^{\pi_k}}{\pi_k!} \ . \tag{4.45}$$

Using the above transition rates and this equilibrium distribution, detailed balance holds if

$$x_j x_k \lambda_{jk} = x_{j+k} \mu_{jk} \tag{4.46}$$

is met $\forall j, k$. One possible solution to this condition (i.e. not unique) is given by the following choice:

$$\begin{aligned} \lambda_{jk} &= \frac{1}{x_j x_k} \ , \\ \mu_{jk} &= \frac{1}{x_{j+k}} \ , \end{aligned} \tag{4.47}$$

where x_k is any nonnegative function of k. In this case x_j^{-1} is proportional to both the rate at which j clusters break up and combine with other clusters. Notice that if $x_j = 0$ then by the above transition rules, any clusters of size j formed will immediately dissociate, as expected since the equilibrium distribution cannot have any clusters of size j in this case.

So the Gibbs distribution (equation (4.45)) is the equilibrium distribution for a physically simple process. Add to this the simple recursive solution for the canonical Gibbs model and one has a compelling argument for the possible utility of the model.

Table 4.2: Markov processes specified by the transition matrices λ_{jk} and μ_{jk} and their equilibrium Gibbs distribution specified by the parameter vector x_j.

λ_{jk}	μ_{jk}	x_j
α	β	β/α
$\alpha(jk)^\tau$	$\beta(j+k)^\tau$	$(\beta/\alpha)j^{-\tau}$
α	$\beta\binom{j+k}{j}^\tau$	$(\beta/\alpha)j!^{-\tau}$

Indeed we will apply the model in several examples in the next chapter, and more importantly to the case of nuclear fragmentation in chapter six. The motivation for these uses is at least partially explained by this intuitive Markov process.

It is simple to generalize this Markov process to systems with many kinds of distinguishable objects, so that the vector Gibbs model is reproduced in equilibrium. Additionally, if the transition rates are adjusted the equilibrium distribution can reflect models other than the Gibbs model. However the form of these transition rates may be particularly complicated. For example, if we use the transition rate

$$\begin{aligned} q(\boldsymbol{\pi}, T^{jk}\boldsymbol{\pi}) &= \lambda_{jk} \,, \\ q(\boldsymbol{\pi}, T_{jk}\boldsymbol{\pi}) &= \mu_{jk} \,, \end{aligned} \tag{4.48}$$

we will get an equipartition distribution, but it will include states with negative numbers of certain clusters, since the transition rates do not depend on the availability of clusters. Including theta functions in the transition rates so that negative numbers of clusters is forbidden is effective, but unfortunately it then leads to a different distribution than the equipartition distribution.

4.2.2 Expected mass yields

Suppose that each x_k in the parameter vector is proportional to x for all x_k, i.e. $x_k = xb_k$, then the partition function is a polynomial in x of degree n. If b_k is fixed, then all expectation values and related quantities of interest are simply functions of a single parameter x. In this section we consider the general behavior of the expected cluster yields, i.e. $\langle \pi_k \rangle_n$. Specifically, we consider the canonical Gibbs model with $x_k = x/k^\tau$ and $x_k = x/k!$.

The function $f(k) = k\langle\pi_k\rangle_n$ is known as the mass yield distribution, since it measures how many objects (the "yield") appear at a certain fragment size (the "mass"). Because all the models must satisfy $\sum_{k>0} k\langle\pi_k\rangle_n = n$, there are restrictions on the form of the mass yield distribution. If we graph $k\langle\pi_k\rangle_n$ vs. k, then the area under the curve must be equal to n. For different choices of x_k, the area will be distributed differently. This subsection discusses the mass yields in terms of the typical area distributions for these models

These models have simple behaviors at large and small x regardless of b_k which are easy to obtain. For small x, all models will produce $k\langle\pi_k\rangle_n$ with most of the area near $k = n$. This is because for small x, the partition function is given almost entirely by the term proportional to x. This implies that one fragment is the most likely outcome. For $k \neq n$, $k\langle\pi_k\rangle_n$ is proportional to x since

$$\langle\pi_k\rangle_n \approx \frac{x_k x_{n-k}}{x_n} \propto x \ . \tag{4.49}$$

For large x, all models will produce $k\langle\pi_k\rangle_n$ with most of the area near $k = 1$. This is because for large x, the partition function is given almost entirely by the term proportional to x^n. So n fragments is the most likely outcome. For $k \neq 1$, $\langle\pi_k\rangle_n$ and $k\langle\pi_k\rangle_n$ are proportional to x^{1-k} since

$$\langle\pi_k\rangle_n \approx \frac{x_k}{x_1^k}\frac{n!}{(n-k)!} \propto x^{1-k} \ . \tag{4.50}$$

Further refinements to the above arguments can be made by making a high and low temperature expansion of the partition function, For $x_k = x b_k$, $Z_n = \sum_{r=1}^{n} Z_n^{(r)} x^r$. For $x_k = x/k^\tau$ with $\tau > 1$, in the large n limit, the small r coefficients (i.e. low temperature) are given by $Z_n^{(r)} = z_n^{(r)}/n^\tau$ where $z_n^{(r)}$ are only weakly dependent on n for small r. Table 4.3 gives the large n limit for the first few coefficients. Notice that $\lim_{n\to\infty} z_n^{(2)} = \zeta(\tau)$.

The model $x_k = x/k$ was discussed in an earlier set of papers [215, 214, 217, 216, 184, 183]. For small x, most of the area is near $k = n$, as expected. For $x < 1$, $k\langle\pi_k\rangle_n$ is monotonically increasing. At $x = 1$, $k\langle\pi_k\rangle_n = 1$ for all k. For $x > 1$, $k\langle\pi_k\rangle_n$ is monotonically decreasing. At large x, most of the area is near $k = 1$, as expected. This is shown in figure 4.2(a).

Table 4.3: Values of $z^{(r)} = \lim_{n\to\infty} n^\tau Z_n^{(r)}$ in the Gibbs model with $x_k = x/k^\tau$ at $\tau = 3/2, 2, 5/2, 3$.

τ	$z^{(1)}$	$z^{(2)}$	$z^{(3)}$	$z^{(4)}$	$z^{(5)}$
3/2	1.000	2.612	3.412	2.971	1.941
2	1.000	1.645	1.353	0.742	0.305
5/2	1.000	1.342	0.899	0.402	0.135
3	1.000	1.202	0.723	0.289	0.0870

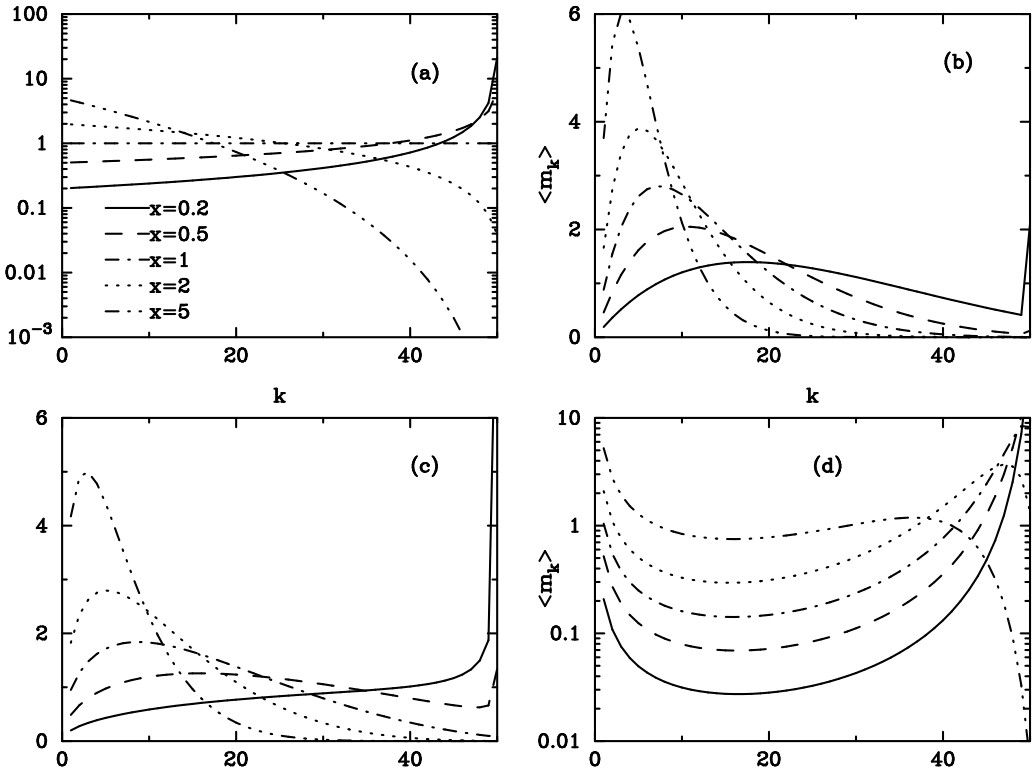
The model with $x_k = x$ for $x \ll 1$ most of the area is below $k = n$. As x increases, some area is distributed along the rest of the graph, mostly around $k = n/2$. As x keeps increasing, the area continues to be redistributed, until most of it is distributed about a point $k < n/2$. At large x it takes on the usual distribution. This is illustrated in figure 4.2(b).

For the model $x_k = x/k^\tau$, with $0 < \tau < 1$, the behavior is very similar to $x_k = x$. For small x, $k\langle\pi_k\rangle_n$ increases monotonically, with most of the area near $k = n$. As x increases, the right-hand side is diminished till the graph attains two turning points, a local minimum near $k = n$, and a local maximum at a point $k < n/2$. The local minimum soon disappears, and the local maximum migrates left till it reaches $k = 1$ at large x. This behavior is illustrated in figure 4.2(c).

The models $x_k = x/k^\tau$, $\tau > 1$ are also all very similar. For small x, $k\langle\pi_k\rangle_n$ starts monotonically decreasing, reaches a minimum, then near $k = n$ rises rapidly. As x is increased, the small k behavior is unchanged, but eventually the large k part turns downward. Thus for a small range of x, the graphs have two turning points. As x continues to increase, the local maximum eventually disappears and the typical large x behavior onsets. This behavior is shown in figure 4.2(d) ($\tau = 2$), and in figure 4.3 ($\tau = 2.5$).

The model $x_k = x/k!$, for $x \ll 1$, $k\langle\pi_k\rangle_n$ is mostly under $k = n$, as expected. From equation (4.49), we see $\langle\pi_k\rangle_n \approx x\binom{n}{k}$ for $k \neq n$, so the remainder of the area is binomially distributed about $k = n/2$. As x increases, the amount of area under $k = n$ diminishes, the balance appearing around $k \approx n/2$ in a binomial or Gaussian distribution. Once most of the area has disappeared from $k = n$, the Gaussian distribution at the center

Figure 4.2: The behavior of $k\langle\pi_k\rangle_n$ vs. k for $n = 50$, $x = 0.2, 0.5, 1, 2, 5$, $x_k = x/k^\tau$, where (a) $\tau = 1$, (b) $\tau = 0$, (c) $\tau = 1/2$, and (d) $\tau = 2$.



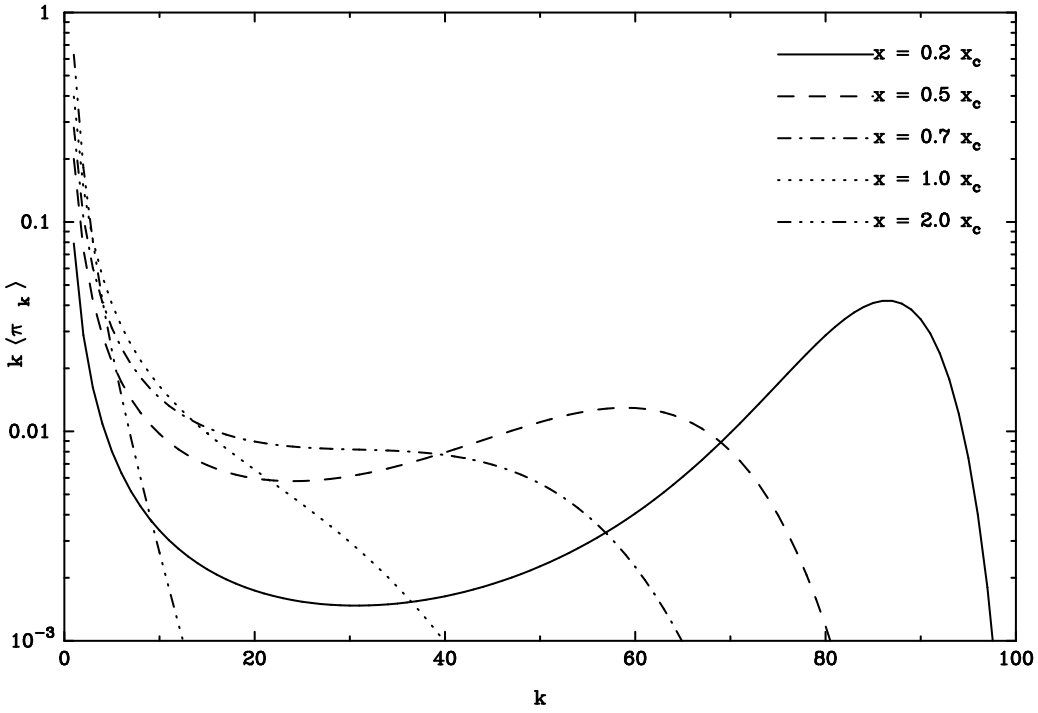
moves to the left as x is increased. For very large x, most of the area is under $k = 1$, as expected.

A simplified description of the $x_k = x/k!$ model can be obtained by making the following approximations. For a given x, the partition function is strongly peaked about a particular number of fragments $m = m_0$, such that $Z_n(x) \approx \{{n \atop m_0}\} x^{m_0}/n!$. To estimate m_0, we use the asymptotic formula for the Stirling numbers of the second kind, $\{{n \atop m}\} \approx m^n/m!$ valid for small m, and maximize $Z_n(x)$. This gives a nonlinear equation for $m_0(n, x)$, namely $m_0 = xe^{n/m_0}$, where we have used Stirling's approximation for $m!$. This implies $\langle\pi_k\rangle_n \approx \binom{n}{k} m_k^{-k} f_n(x)$ where $m_k = m_0(n-k, x)$ and $f_n(x)$ is a normalizing constant. We now make the assumption that $m_k \approx m_0(n - \langle k\rangle_n, x) \equiv \bar{m}$. The value of $f_n(x)$ can now be obtained by imposing the constraint $\sum_{k>0} k\langle\pi_k\rangle_n = n$, which gives

$$\langle\pi_k\rangle_n \approx \binom{n}{k} p^{k-1}(1-p)^{n-k} \ , \tag{4.51}$$

where $p = 1/(\bar{m}+1)$. This distribution is binomial, with $\langle k\rangle_n = pn$. Using this result

Figure 4.3: The behavior of $k\langle\pi_k\rangle_n$ vs. k for $n = 100$, $x_k = x/k^{5/2}$, at various x/x_c.



we arrive at an equation for $\bar{m}$,

$$\bar{m} = x e^{n/(\bar{m}+1)} \ . \tag{4.52}$$

Figure 4.4 compares the exact behavior with this approximation. From the figure we see that $\langle\pi_k\rangle_n$ is reasonably well described by this approximation for $x > 10^{-3}$.

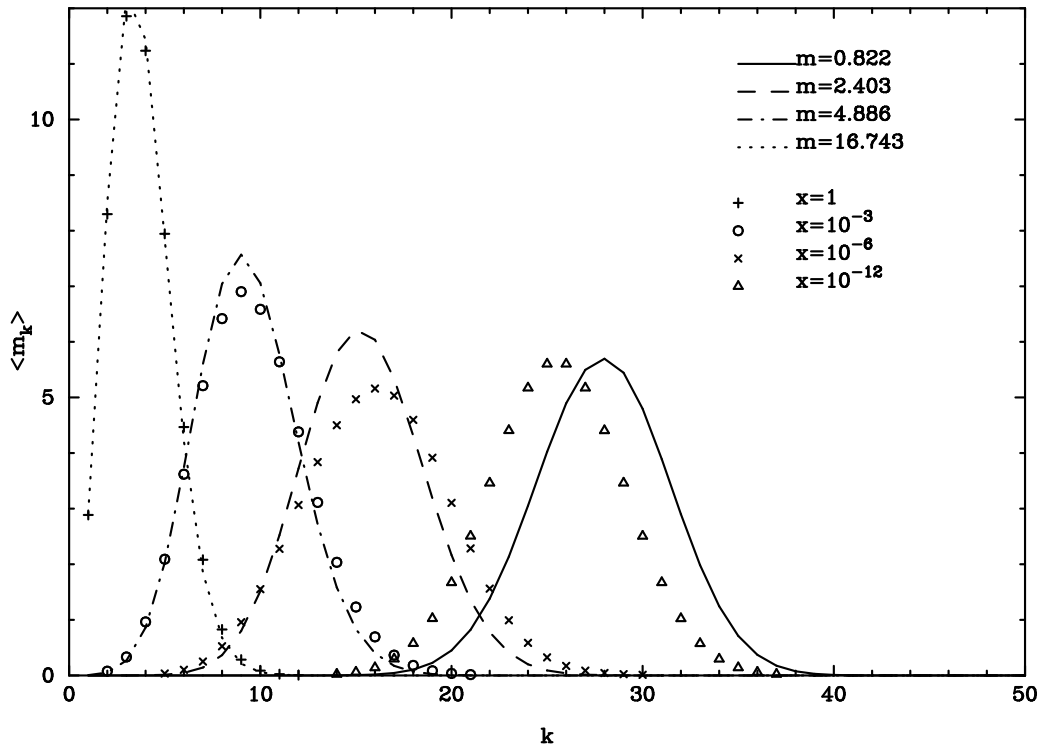
4.2.3 Entropy, Universality and the Gibbs model

The next two chapters principally apply the canonical Gibbs model to systems in physics and mathematics. The question which arises after seeing the Gibbs model appear and reappear in a number of different situations, is why is it so universal in appearance. Why doesn't the equipartition model for instance appear instead?

Part of the answer can be traced back to the Gibbs' paradox. In a microcanonical[8] treatment of the classical ideal Boltzmann gas, the thermodynamic entropy can be computed by taking the logarithm of the volume of the phase space bounded by the

[8]The traditional definition of microcanonical is meant here, meaning energy conserving.

Figure 4.4: The behavior of $k\langle\pi_k\rangle_n$ vs. k for $n = 50$, $x_k = x/k!$, at various x, with a comparison to the approximate model considered in the text. The lines correspond to the approximate model, the points to the exact model.



energy of the system. Suppose we take two ideal gases at the same temperature and density, with n_1 and n_2 particles in volumes V_1, V_2, and we mix them. According to the traditional entropy measure, the entropy would change by

$$\frac{\Delta S}{k_B} = n_1 \ln \frac{V}{V_1} + n_2 \ln \frac{V}{V_2} > 0 \; . \tag{4.53}$$

Unfortunately, this is clearly wrong if the two systems contain the same type of particles, since the entropy shouldn't change, but it is correct if the two systems contain different particles. This is referred to as Gibbs' paradox, after J. Willard Gibbs who first noticed and resolved the problem by assuming an error was made in computing the size of the phase space by a factor of $1/n!$. This doesn't affect the equation of state or other measurable thermodynamic functions of the system, but it does effect the entropy, resulting in the Sackur-Tetrode equation for an ideal gas. With this change, the paradox is resolved, but the reason why this $1/n!$ correction is needed was not known to Gibbs. Quantum mechanics makes the reason plain, since n identical particles are defined by an

n particle wave function for which any permutation of the particles can at most simply change the sign, it seems clear that the $1/n!$ is due to this permutation invariance of the wavefunction.

In the canonical formalism, resolving the Gibbs paradox for an ideal gas is equivalent to replacing the partition function x^n for an ideal gas of particles with $x^n/n!$, where $x = V/\lambda_T^d$ and λ_T is the thermal wavelength (see section 5.1). Suppose we now allow these particles to form clusters, then freeze the configuration. All clusters of a particular size act as an ideal gas of indistinguishable clusters, but each cluster size is distinguishable. So each cluster size should act as a species of indistinguishable particles with partition function $x_k^{\pi_k}$. The Gibbs paradox will still affect us unless we make the Gibbs ansatz and divide these partition functions by $\pi_k!$. So for a particular cluster configuration $W(\boldsymbol{\pi}) = \prod_k x_k^{\pi_k}/\pi_k!$, and the motivation for the Gibbs model becomes apparent.

4.3 Phase transitions in the Gibbs model

Phase transitions in physical systems are characterized by discontinuities in measurable quantities, often thermodynamic ones. For example, in liquid helium, a phase transition (the λ transition) can be identified at the temperature where the specific heat becomes infinite. Clustering and fragmenting systems do not necessarily have thermodynamic degrees of freedom, and so an investigation of their critical properties depends on a cluster based measure of criticality which is independent of thermodynamic or other concerns. Fortunately there is a natural way to identify the critical point in such systems.

Suppose that in a canonical Gibbs model[9] the parameter vector is a function of single variable x (e.g. $x_k = xb_k$). If it is a function of other parameters also, we hold them fixed for the purpose of this investigation. As x is changed, the fragmentation pattern will also change, although predictably. As has already been suggested, for some models the change in fragmentation pattern will be dramatic at one particular value of the parameter x. We will specify this point as the critical point, and say that the

[9]Actually, the discussion here is mostly model independent and applies equally well to any partition based model.

system has changed phase as it crossed it.

What dramatic change to the fragmentation pattern can happen at the critical point? Well, suppose $n \to \infty$ and consider the behavior of the largest cluster as x/n is varied. Since the number of particles is tending to infinity, the grand canonical solution with a fugacity z (i.e. $\langle \pi_k \rangle = z^k x_k$) should be an adequate description of the partition distribution. As such, the canonical constraint $\langle n \rangle = n$, or

$$\lim_{n\to\infty} \sum_{k>0} k \frac{z^k x_k}{n} = 1 \tag{4.54}$$

should hold. If z can be found to satisfy this equation then indeed this is an adequate description of the system. But what if no such z exists? For example, if $x_k = x k^{-\tau}$ with $\tau > 2$ then $\sum_{k>0} k z^k x_k \leq x\zeta(\tau - 1)$ where $\zeta(z)$ is the Riemann zeta function, or is formally infinite (i.e. $z > 1$.) In this case, when $x/n < 1/\zeta(\tau - 1)$ then there is a problem with the grand canonical solution. In fact, all that has happened is that very large clusters have begun to appear in the fragmentation pattern, clusters which the grand canonical solution implicitly assumes occur with negligible probability. The phase transition therefore is a transition from the phase where all the clusters are small to a phase in which there appears large clusters which have a size of some finite fraction of the total mass even as $n \to \infty$. This happens as a very sharp transition in many models, and in this example occurs at

$$x_c = \frac{n}{\zeta(\tau - 1)} \,. \tag{4.55}$$

Below the critical point we can assume enough mass has condensed into large clusters so that the remaining mass can satisfy the mass constraint with $z = 1$.

4.3.1 Reduced moments and critical exponents

Having identified a critical point via the appearance of large clusters, we proceed to characterize the nature of the transition by defining a set of *critical exponents*. To do so, we first introduce the *reduced moments* M_s defined by

$$M_s(\boldsymbol{\pi}) = \sum_{k>0} k^s \pi_k - k_{\max}^s \,, \tag{4.56}$$

where $k_{\max}$ is the largest cluster size in the partition $\boldsymbol{\pi}$. So the term reduced specifically means that the largest cluster has been omitted from the sum. The motivation to do this is manifest from the nature of the critical point. At the critical point, we expect large clusters to begin to form, most probably a single large cluster. As such we want to isolate its effects, and removing it explicitly from the moments is one obvious method.

Consider now the behavior of $\langle M_1 \rangle$. Above the critical point, only small clusters will exist, so removing the largest cluster should have only a small effect on $\langle M_1 \rangle$, and in fact

$$\lim_{n\to\infty} \frac{\langle M_1 \rangle}{n} = 1 \ . \tag{4.57}$$

Below the critical point, a large cluster can exist, and we expect the not too far from the critical point we can say that

$$\lim_{n\to\infty} \langle M_1 \rangle = |1 - x/x_c|^{\beta} \ , \tag{4.58}$$

where β is a critical exponent. Similarly, below the critical point we can study the behavior of other moments such as

$$\langle M_0 \rangle \propto |x - x_c|^{2-\alpha} \ , \tag{4.59}$$

$$\langle M_2 \rangle \propto |x - x_c|^{-\gamma} \ , \tag{4.60}$$

$$\langle M_j \rangle \propto |x - x_c|^{-(1+j-\tau)/\sigma} \ . \tag{4.61}$$

Clearly only three of these exponents are independent: In fact [88]

$$\sigma = \frac{1}{\beta + \gamma} \ , \tag{4.62}$$

$$\tau = 2 + \frac{\beta}{\beta + \gamma} \ . \tag{4.63}$$

In these terms, the critical exponents for the example $x_k = x/k^{5/2}$ are $\alpha = -1$, $\beta = 1$, $\gamma = 1$, $\tau = 5/2$. Other critical exponents can be defined, but α, β, and γ are sufficient to determine the ones of interest to clustering degrees of freedom. From these all the critical exponents can be determined using the various scaling laws for critical exponents 4.4.

How can we compute these moments? Computing the non-reduced part of the moments can be accomplished using the methods discussed in section 3.2.1. The reduced

Table 4.4: Scaling laws for critical exponents.

	Scaling law
Fisher	$\gamma = \nu(2 - \eta)$
Rushbrooke	$\alpha + 2\beta + \gamma = 2$
Widom	$\gamma = \beta(\delta - 1)$
Josephson	$\nu d = 2 - \alpha$

part $\langle k^s_{\max} \rangle$ requires a determination of the probability that $k_{\max}$ is a particular value. That is given by

$$\Pr(k_{\max} = k) = \frac{Z_n(x_1, \ldots, x_k, 0, 0, \ldots) - Z_n(x_1, \ldots x_{k-1}, 0, 0, \ldots)}{Z_n(\mathbf{x})} \,. \tag{4.64}$$

Clearly the numerator includes all the terms in Z_n which have x_k. Furthermore, terms with $x_{k+1}, x_{k+2}, \ldots$ do not appear, and so therefore $k_{\max} = k$ in these terms. Dividing by the overall partition function then obtains the probability the $k_{\max} = k$, as desired. With this results, we can now compute the reduced part

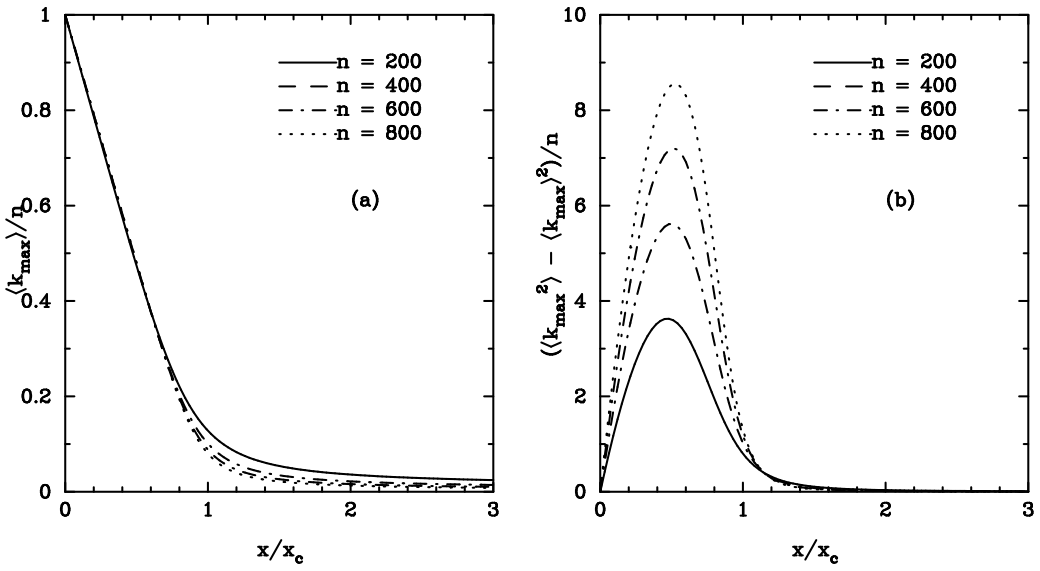
$$\langle k^s_{\max} \rangle = \sum_{k>0} \Pr(k_{\max} = k) k^s \tag{4.65}$$

Figure 4.5 plots the reduced parts for the model $x_k = x/k^{5/2}$.

4.3.2 Fluctuations and cumulant moments

The Gibbs model can be solved effectively in the microcanonical, canonical and grand canonical ensembles. Of the three solutions, however, the grand canonical has a particular advantage over the other two due to the closed form expression for its partition function. Similarly, the canonical partition function takes less time and less storage space to compute than an average microcanonical partition function. This knowledge suggests it may sometimes be helpful to abandon one strict ensemble (e.g. microcanonical) for a less strict one (e.g. grand canonical), at least from a computational point of view. From a modeling point of view, this at first appears to be terrible, since the other ensembles permit states that are impossible to occur in the "correct" ensemble. However, by careful adjusting of parameters, we can have the most probable configurations be the allowed configurations. The forbidden configurations will then occur

Figure 4.5: The mean and variance of the maximum cluster size (a) $\langle k_{\max}\rangle$ and (b) $\langle k_{\max}^2\rangle - \langle k_{\max}\rangle^2$ for the canonical Gibbs model with $x_k = x/k^{5/2}$ plotted against x/x_c for $n = 200, 400, 600, 800$.



with a smaller probability, and the hope is that they will not affect the predictions of the theory very much. In other words, even though particle number may be conserved, the grand canonical assumption can sometimes be made without the results being measurably affected. Similarly, the canonical ensemble can often be substituted in a microcanonical model.

Of course, such substitutions can't always be made, or there would be no need for more than one ensemble. All calculations could be done in the grand canonical ensemble, and physics would be greatly simplified. Consider then the fluctuations of the conserved quantities. To be precise, in a less strict ensemble, the conserved quantities will no longer be conserved over the entire ensemble, but they will be conserved "on average". Since the conserved quantities aren't strictly conserved, we expect there to be a measurable fluctuation in these ensembles. For example, in the grand canonical ensemble, we can adjust parameters so that $\langle n\rangle = n$, but the fluctuation $\langle n^2\rangle - \langle n\rangle^2 > 0$, whereas in the canonical ensemble this fluctuation would be identically zero. This suggests that the fluctuation of the conserved quantities are useful in estimating when other ensembles can be substituted. If the fluctuation of a conserved quantity is small

compared to the quantity conserved, the predictions of the two ensembles shouldn't be altogether that much different, and either ensemble can be used. If the fluctuations are large, the strict ensemble must be used. In short, a careful consideration of fluctuations should be made in these models both for their inherent interest and for identifying regions where calculations can be simplified.

Although these considerations are correct in any statistical model, here we restrict attention to the Gibbs model. The behavior of the Gibbs model is determined by the parameter vector $\mathbf{x}$. Consider $x_k = xz^k b_k$. The weight then is given by (equation (3.25))

$$W(\boldsymbol{\pi}) = \prod_{k>0} \frac{x_k^{\pi_k}}{\pi_k!} = x^r z^n \prod_{k>0} \frac{b_k^{\pi_k}}{\pi_k!} \,, \tag{4.66}$$

where $r = \sum_{k>0} \pi_k$, $n = \sum_{k>0} k\pi_k$, i.e. r is the number of clusters and n is the number of particles. So in a microcanonical ensemble, each weight is multiplied by the same constant factor $x^r z^n$. Ensemble averages are therefore unaffected by these variables. Similarly, in a canonical ensemble, changing z does not affect ensemble averages. These variables then are the adjustable parameters which determine the expected cluster and particle number in the canonical and grand canonical ensembles, i.e. adjusting x and z will effect $\langle r\rangle_n$, $\langle r\rangle$, $\langle n\rangle$. Specifically, in the grand canonical model

$$\langle n\rangle = z\frac{\partial}{\partial z}\ln \mathcal{Z} = x\sum_{k>0} kz^k b_k = \sum_{k>0} k\langle \pi_k\rangle \,, \tag{4.67}$$

$$\langle n^2\rangle - \langle n\rangle^2 = \left(z\frac{\partial}{\partial z}\right)^2 \ln \mathcal{Z} = x\sum_{k>0} k^2 z^k b_k = \sum_{k>0} k^2\langle \pi_k\rangle \,, \tag{4.68}$$

and

$$\langle r\rangle = x\frac{\partial}{\partial x}\ln \mathcal{Z} = x\sum_{k>0} z^k b_k \,, \tag{4.69}$$

$$\langle r^2\rangle - \langle r\rangle^2 = \left(x\frac{\partial}{\partial x}\right)^2 \ln \mathcal{Z} = x\sum_{k>0} z^k b_k = \langle r\rangle \,. \tag{4.70}$$

Notice that the variance in $\langle r\rangle$ is equal to $\langle r\rangle$ independent of b_k. In the canonical model, there is no fluctuation in n and the fluctuation in r is given by

$$\langle r\rangle_n = x\frac{\partial}{\partial x}\ln Z_n \,, \tag{4.71}$$

$$\langle r^2\rangle_n - \langle r\rangle_n^2 = \left(x\frac{\partial}{\partial x}\right)^2 \ln Z_n \,. \tag{4.72}$$

The variance is only the first of a whole family of moments which are critical to the understanding of these models. Let m be an observable, and $\langle\bullet\rangle$ denote an expectation value for functions of that variable. The *central* and *factorial moments* are defined by the following expressions:

$$\mu_k(m) := \langle (m - \langle m\rangle)^k\rangle \ , \tag{4.73}$$

$$\xi_k(m) := \langle [m]_k\rangle = \langle m(m-1)\cdots(m-k+1)\rangle \ . \tag{4.74}$$

A quick calculation shows that $\mu_2(m) = \mathrm{Var}(m)$. Additionally, the standard statistical functions of skewness and kurtosis, are defined by

$$\sqrt{\beta_1(m)} = \frac{\mu_3(m)}{\mu_2^{3/2}(m)} \ , \tag{4.75}$$

$$\beta_2(m) = \frac{\mu_4(m)}{\mu_2^2(m)} \ . \tag{4.76}$$

and generalize somewhat the notion of variance.

From these moments $(\langle m^k\rangle, \mu_k(m), \xi_k(m))$, one can construct the *cumulant moments* in a systematic fashion by taking the logarithm of their exponential generating functions, i.e. for power moments, the exponential generating function is

$$\left\langle e^{-\lambda m}\right\rangle = \sum_{n\geq 0} \frac{(-\lambda)^n}{n!}\langle m^n\rangle \ . \tag{4.77}$$

The exponential generating function for the cumulant power moment is then simply the natural logarithm of the above expression, i.e.

$$\ln\left\langle e^{-\lambda m}\right\rangle = \sum_{n\geq 0} \frac{(-\lambda)^n}{n!}\kappa_n(m) \ , \tag{4.78}$$

where $\kappa_n(m)$ is the nth power cumulant moment. The first few are given by

$$\begin{aligned}
\kappa_1(m) &= \langle m\rangle \ , \\
\kappa_2(m) &= \mu_2(m) = \langle m^2\rangle - \langle m\rangle^2 \ , \\
\kappa_3(m) &= \mu_3(m) = \langle m^3\rangle - 3\langle m\rangle\langle m^2\rangle + 2\langle m\rangle^3 \ , \\
\kappa_4(m) &= \mu_4(m) - 3\mu_2^2(m) = \langle m^4\rangle - 4\langle m\rangle\langle m^3\rangle + 12\langle m^2\rangle\langle m\rangle^2 - 3\langle m^2\rangle^2 - 6\langle m\rangle^4 \ .
\end{aligned} \tag{4.79}$$

in general $\kappa_n(m)$ is a symmetric function, related to the $\langle m^k \rangle$ as shown by Ronald A. Fisher [108]

$$\langle m^n \rangle = n! \sum_{\pi(n)} \prod_{j>0} \frac{1}{\pi_j!} \left(\frac{\kappa_j(m)}{j!} \right)^{\pi_j} , \tag{4.80}$$

$$\kappa_n(m) = n! \sum_r (-1)^{r-1} (r-1)! \sum_{\pi_r(n)} \prod_{j>0} \frac{1}{\pi_j!} \left(\frac{\langle m^j \rangle}{j!} \right)^{\pi_j} . \tag{4.81}$$

i.e. in terms of the elementary symmetric functions (section 2.2.2),

$$k_n(m) = \frac{\langle m^n \rangle}{n!} , \tag{4.82}$$

$$s_n(m) = \frac{\kappa_n(m)}{(n-1)!} . \tag{4.83}$$

Similar definitions hold for the central and factorial cumulants.

In statistics cumulants simplify many problems, and our motivation for introducing them is their natural appearance in various thermodynamic functions of the Gibbs model. Specifically, suppose that the weight is given by the Gibbs model with $x_k = xb_k$, i.e. $W(\boldsymbol{\pi}) \propto x^r$ where r is the number of clusters. Suppose the number of parts r is the observable and we wish to determine cumulant moments of r. Then we will prove that

$$\left(x \frac{\partial}{\partial x} \right)^k \ln Z = \kappa_k(r) , \tag{4.84}$$

where Z is the appropriate partition function for the ensemble.

To prove this, we will first prove some preliminary lemmas.

Lemma 4.3.1 *For the Gibbs model with* $x_k = xb_k$,

$$x \frac{\partial}{\partial x} \langle [r]_k \rangle = \langle r[r]_k \rangle - \langle r \rangle \langle [r]_k \rangle . \tag{4.85}$$

Proof: Let Z be the partition function, then

$$\begin{aligned} x \frac{\partial}{\partial x} \langle [r]_k \rangle &= x \frac{\partial}{\partial x} \frac{x^k}{Z} \frac{\partial^k Z}{\partial x^k} = \frac{x^{k+1}}{Z} \frac{\partial^{k+1} Z}{\partial x^{k+1}} + \frac{k x^k}{Z} \frac{\partial^k Z}{\partial x^k} - \frac{x^{k+1}}{Z^2} \frac{\partial Z}{\partial x} \frac{\partial^k Z}{\partial x^k} \\ &= \langle [r]_{k+1} \rangle + k \langle [r]_k \rangle - \langle r \rangle \langle [r]_k \rangle = \langle r[r]_k \rangle - \langle r \rangle \langle [r]_k \rangle \end{aligned} \tag{4.86}$$

Lemma 4.3.2 *For the Gibbs model with* $x_k = xb_k$,

$$x \frac{\partial}{\partial x} \langle r^k \rangle = \langle r^{k+1} \rangle - \langle r \rangle \langle r^k \rangle . \tag{4.87}$$

Proof:

$$\begin{aligned} x\frac{\partial}{\partial x}\langle r^k\rangle &= x\frac{\partial}{\partial x}\sum_{j=0}^{k}\left\{{k \atop j}\right\}\langle [r]_j\rangle = \sum_{j=0}^{k}\left\{{k \atop j}\right\}(\langle r[r]_j\rangle - \langle r\rangle\langle [r]_j\rangle) \\ &= \sum_{j=0}^{k}\left\{{k \atop j}\right\}\sum_{i=0}^{j}(-1)^{j-i}\left[{j \atop i}\right](\langle r^{i+1}\rangle - \langle r\rangle\langle r^i\rangle) = \langle r^{k+1}\rangle - \langle r\rangle\langle r^k\rangle \quad (4.88) \end{aligned}$$

by applying the previous lemma and since $\sum_{j=0}^{k}\left\{{k \atop j}\right\}(-1)^{j-i}\left[{j \atop i}\right] = \delta_{ki}$.

Theorem 4.3.1 *For the Gibbs model with* $x_k = xb_k$,

$$x\frac{\partial}{\partial x}\kappa_n(r) = \kappa_{n+1}(r)\ . \tag{4.89}$$

Proof: Since $\kappa_n(r)$ and $\langle r^j\rangle$ are related to symmetric functions by equations (4.82) and (4.83), we have the following recursive identity for $\kappa_n(r)$ using equation (2.62)

$$\kappa_n(r) = \langle r^n\rangle - \sum_{j=1}^{n-1}\binom{n-1}{j-1}\kappa_j(r)\langle r^{n-j}\rangle\ . \tag{4.90}$$

So we will proceed with an inductive proof. Clearly the identity holds for $n = 1$. Assume it is true up to $n-1$. Then we have

$$\begin{aligned} x\frac{\partial}{\partial x}\kappa_n(r) &= \langle r^{n+1}\rangle - \langle r\rangle\langle r^n\rangle \\ &\quad - \sum_{j=1}^{n-1}\binom{n-1}{j-1}\left[\kappa_{j+1}(r)\langle r^{n-j}\rangle + \kappa_j(r)\langle r^{n+1-j}\rangle - \kappa_j(r)\langle r\rangle\langle r^{n-j}\rangle\right] \\ &= \langle r^{n+1}\rangle - \sum_{j=1}^{n-1}\binom{n-1}{j-1}\left[\kappa_{j+1}(r)\langle r^{n-j}\rangle + \kappa_j(r)\langle r^{n+1-j}\rangle\right] \\ &\quad + \langle r\rangle\left[\langle r^n\rangle - \sum_{j=1}^{n-1}\binom{n-1}{j-1}\kappa_j(r)\langle r^{n-j}\rangle\right] \\ &= \langle r^{n+1}\rangle - \sum_{j=2}^{n-1}\binom{n}{j-1}\kappa_j(r)\langle r^{n+1-j}\rangle \\ &\quad - \binom{n-1}{n-2}\kappa_n(r)\langle r\rangle - \binom{n-1}{0}\kappa_1(r)\langle r^n\rangle - \langle r\rangle\kappa_n(r) \\ &= \langle r^{n+1}\rangle - \sum_{j=1}^{n}\binom{n}{j-1}\kappa_j(r)\langle r^{n+1-j}\rangle = \kappa_{n+1}(r) \end{aligned} \tag{4.91}$$

from the recursion relation and since $\binom{n-1}{j-1} + \binom{n-1}{j-2} = \binom{n}{j-1}$.

Corollary 4.3.1 *For the Gibbs model with* $x_k = xb_k$,

$$\left(x\frac{\partial}{\partial x}\right)\ln Z = \kappa_n(r)\ . \tag{4.92}$$

Proof: $x\frac{\partial}{\partial x}\ln Z = \kappa_1(r)$, and apply the above theorem.

The following theorem can also be quite useful in doing some calculations

Theorem 4.3.2 *For the Gibbs model with* $x_k = xb_k$,

$$x\frac{\partial}{\partial x}\mu_k(r) = \mu_{k+1}(r) - k\mu_2(r)\mu_{k-1}(r)\ . \tag{4.93}$$

Proof:

$$\begin{aligned}
x\frac{\partial}{\partial x}\langle(r-\langle r\rangle)^k\rangle &= x\frac{\partial}{\partial x}\sum_{j=0}^{k}\binom{k}{j}(-1)^{k-j}\langle r^j\rangle\langle r\rangle^{k-j} \\
&= \sum_{j=0}^{k}\binom{k}{j}(-1)^{k-j}\langle r^j\rangle(k-j)\langle r\rangle^{k-j-1}\mu_2(r) \\
&\quad + \sum_{j=0}^{k}\binom{k}{j}(-1)^{k-j}(\langle r^{j+1}\rangle - \langle r\rangle\langle r^j\rangle\langle r\rangle^{k-j}) \\
&= \sum_{j=0}^{k-1}\binom{k-1}{j}(-1)^{k-1-j}(-k)\langle r^j\rangle\langle r\rangle^{k-1-j}\mu_2(r) \\
&\quad + \sum_{j=0}^{k+1}\left\{\binom{k}{j-1} + \binom{k}{j}\right\}(-1)^{k+1-j}\langle r^j\rangle\langle r\rangle^{k+1-j} \\
&= -k\mu_{k-1}(r)\mu_2(r) + \mu_{k+1}(r)
\end{aligned} \tag{4.94}$$

by the lemma 4.3.2 and since $\binom{k}{j-1} + \binom{k}{j} = \binom{k+1}{j}$.

We are principally concerned with the canonical ensemble, so it would be helpful if we could use the exact solutions of the grand canonical model to determine the behavior in the canonical ensemble. The principle objection to the grand canonical ensemble is its particle number fluctuations. The canonical ensemble has none, and in fact, if we vary z in the canonical ensemble it has no effect on the observables, since it just multiplies the partition function by a constant factor. So let us take the grand canonical solution for $\langle r\rangle/\langle n\rangle$ as being appropriate for the canonical model, but let us try to remove the effects of particle number fluctuations from higher order moments. Consider the case $x_k = xk^{-\tau}$. From our previous considerations it is easy to see that the number of objects $\langle n\rangle$ above the critical point satisfies

$$\langle n\rangle = n = xg_{\tau-1}(z(x)) \tag{4.95}$$

where $g_\tau(z) = \sum_{k>0} z^k k^{-\tau}$. To eliminate particle number fluctuations, this must define a relation between z and x (i.e. they are no longer independent) such that $x\frac{d}{dx}\langle n\rangle = 0$. So above the critical point

$$x\frac{d}{dx}\langle n\rangle = x g_{\tau-2}(z(x)) + x^2\frac{dz}{dx} g_{tau-1}(z(x)) \tag{4.96}$$

where we have used the fact that $dg_\tau/dz = g_{\tau-1}(z)$. Setting this equal to zero determines the dz/dx,

$$\frac{dz}{dx} = -\frac{1}{x}\frac{g_{\tau-1}(z)}{g_{\tau-2}(z)}\,. \tag{4.97}$$

So from the behavior of the multiplicity $\langle r\rangle = \sum_k \pi_k$ in the grand canonical ensemble

$$\langle r\rangle \quad = \quad \begin{cases} 1 + x g_\tau(1) & x < x_c \\ x g_\tau(z(x)) & x > x_c \end{cases} \tag{4.98}$$

we can determine the behavior of the higher moments by replacing the partial derivatives with total derivatives, yielding the following expressions for the second, third and fourth order cumulants.

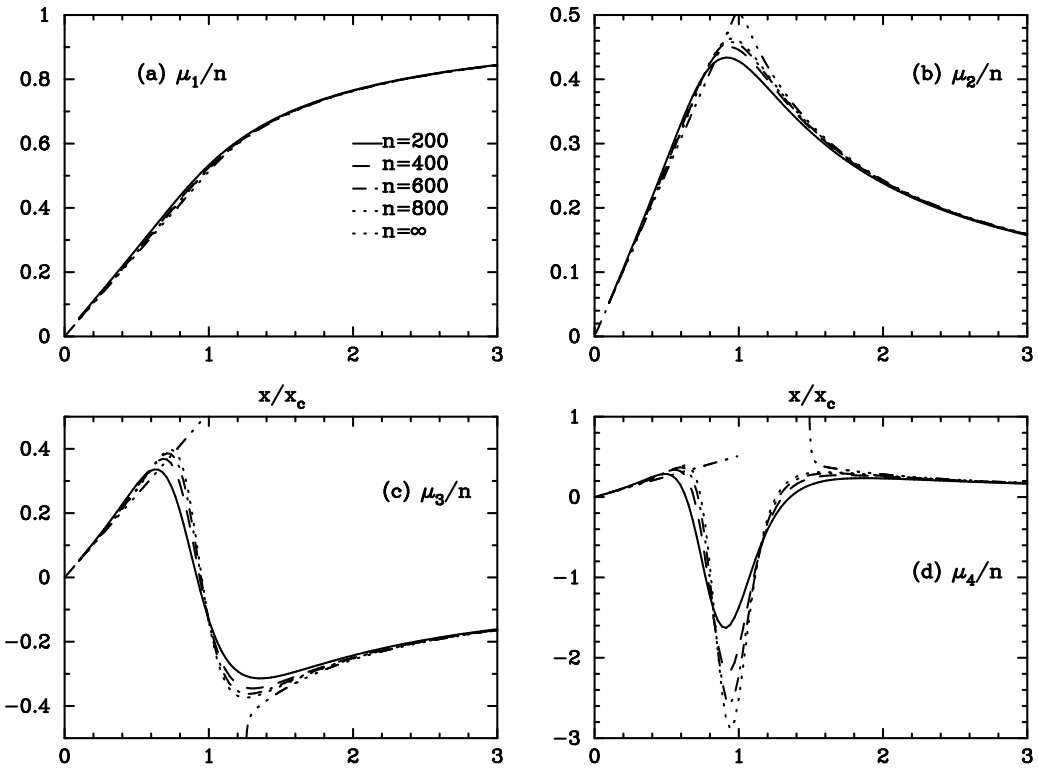
$$\mu_2(r) \quad = \quad \begin{cases} x g_\tau(1) & x < x_c \\ x g_\tau(z) - x\frac{g_{\tau-1}(z)^2}{g_{\tau-2}(z)} & x > x_c \end{cases} \tag{4.99}$$

$$\kappa_3(r) \quad = \quad \begin{cases} x g_\tau(1) & x < x_c \\ x g_\tau(z) - x\left(\frac{g_{\tau-1}(z)}{g_{\tau-2}(z)}\right)^3 g_{\tau-3}(z) & x > x_c \end{cases} \tag{4.100}$$

$$\kappa_4(r) \quad = \quad \begin{cases} x g_\tau(1) & x < x_c \\ x g_\tau(z) - x\frac{g_{tau-1}(z)^2}{g_{\tau-2}(z)} + 2x\left(\frac{g_{\tau-1}(z)}{g_{\tau-2}(z)}\right)^3 2g_{\tau-3}(z) & \\ \quad -3x\left(\frac{g_{\tau-1}(z)}{g_{\tau-2}(z)}\right)^4\frac{g_{\tau-3}(z)^2}{g_{\tau-2}(z)} + x\left(\frac{g_{\tau-1}(z)}{g_{\tau-2}(z)}\right)^4 g_{\tau-4}(z) & x > x_c \end{cases} \tag{4.101}$$

Figure 4.6 plots these moments $\kappa_1, \ldots, \kappa_4$ in the canonical models and the grand canonical estimates. The agreement is quite good, except around the critical points in the higher cumulants, but that is to be expected. Figure 4.7 plots the variance of the multiplicity versus the multiplicity, showing that on both sides of the critical points the variance is essentially a straight line. The important thing to note from both figures is that the finite size effects are most pronounced near the critical point. Canonical partition evaluations are quite crucial there, and the grand canonical solutions are not entirely reliable in that region.

Figure 4.6: The first four cumulant moments for the canonical Gibbs model with $x_k = x/k^{5/2}$, $n = 200, 400, 600, 800$ and the infinite n limit.

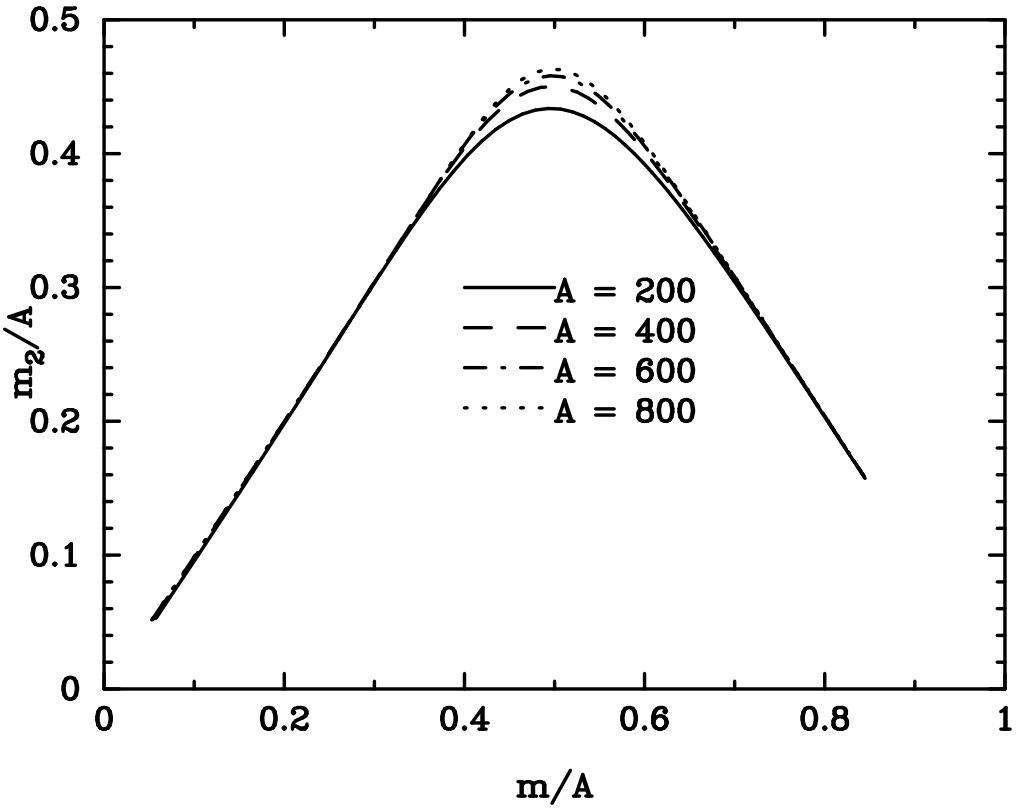


4.3.3 Zeros of the partition function

The methods of Lee and Yang in describing phase transitions affords us yet another method of exploring phase transitions: the behavior of the zeros of the partition function. For $x_k = xb_k$, the canonical partition function $Z_n(x)$ is a polynomial of order n in x with positive coefficients, the coefficients being the microcanonical partition functions. For example, for $x_k = x/k$, $Z_n(x) = x(x+1)\cdots(x+n-1)/n!$. By a theorem of Gauss, a polynomial of order n has n roots or zeros in the complex plane. For positive coefficients, no real roots are on the positive real axis, which is also the physical meaningful axis. The above example has its roots at the $x = 0$ and the negative integers $x = -1, -2, \ldots, -n+1$.

Complex roots correspond to an extension of the real domain into the complex plane. Lee and Yang, in their discussion of phase transitions, showed that such transitions manifest themselves as zeros of the partition function approach the physical axis, which

Figure 4.7: Var(m) vs. $\langle m \rangle$ for the canonical Gibbs model with $x_k = x/k^{5/2}$, $n = 200, 400, 600, 800$.



in this case is the real positive axis, as the thermodynamic limit $n \to \infty$ is approached. Taking the logarithm of the partition function to obtain the free energy can then lead to a singularity.

To illustrate the above remarks, we consider the example of the 2D Ising model on an $m \times n$ lattice. Bruria Kauffman [161,162] while simplifying Lars Onsager's original solution of the model [234] showed that the partition function for this model is given by

$$Z_{mn} = \prod_{r=1}^{m} \prod_{s=1}^{n} \left\{ \left(\frac{1+v^2}{1-v^2} \right)^2 - \frac{2v f_{rs}}{1-v^2} \right\} , \tag{4.102}$$

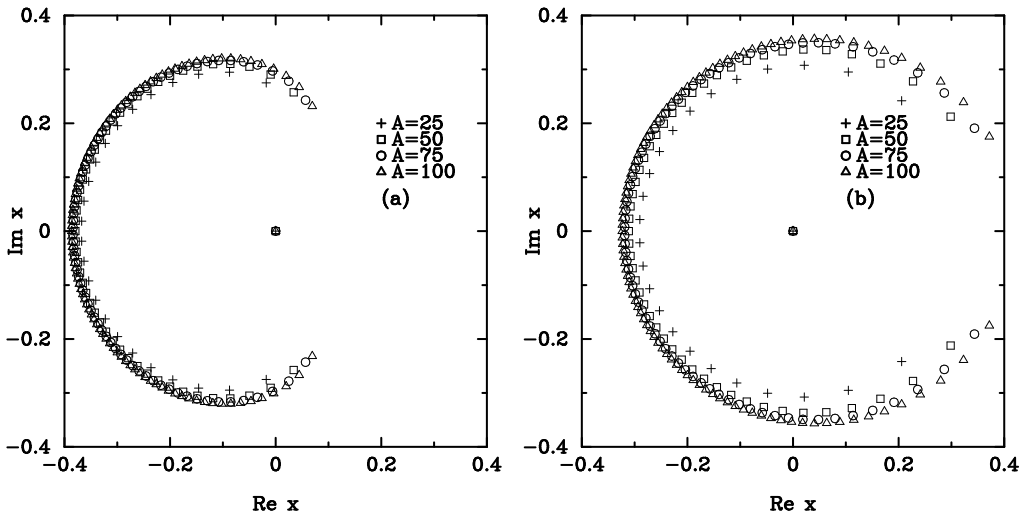
where $f_{rs} = \cos(2\pi r/m) + \cos(2\pi s/n)$, $v = \tanh(J/k_B T)$. In this case the zeros of the partition function are located on two circles in the complex v plane, namely $v = \pm 1 + \sqrt{2} e^{i\theta}$. The physically meaningful domain of the v plane is the part of the real line

$v \in (0,1)$ (assuming $J > 0$). The zeros of the partition function approach this domain at one point, $v = -1 + \sqrt{2}$. This implies there should be a phase transition when

$$k_B T_c = \frac{J}{\tanh^{-1}(-1+\sqrt{2})} = \frac{2J}{\ln(1+\sqrt{2})}\,, \tag{4.103}$$

which is the commonly known value for the critical temperature.

Figure 4.8: Zeros of the partition function $Z_A(x)$ for the choice (a) $x_k = x/k^2$ and (b) $x_k = x/k^3$ scaled by $1/A$ (i.e. root x is plotted at x/A). The cases $A = 25, 50, 75, 100$ are shown.



Now consider the zeros of the Gibbs model partition function with $x_k = xb_k$ in the complex x plane. The physically meaningful domain of x, the part with positive temperature, is the positive real axis. So for a phase transition to manifest itself in the infinite particle limit, the zeros of the partition function must approach the positive real axis. The $x_k = x/k$ model therefore has no phase transition, for in the infinite particle limit, the roots of the partition function are zero and the negative integers, which never approach the real temperature domain. Similarly, $x_k = x/k!$ has roots only on the negative real axis (cf. Wilf [310], pg. 129 for a proof)[10], and therefore has no phase transition. Another example we consider is $x_k = x/k^\tau$ for the cases $\tau = 2, 3$.

[10]Curiously, the fact that the roots are all on the negative axis implies the microcanonical partition functions in this case are unimodal, that is they rise, reach a peak or plateau, and then fall. Having negative real roots implies unimodality, but not vice versa, cf. Wilf [310].

For this model we will show the critical point is at $x/n = 1/\zeta(\tau - 1)$. This essentially[11] corresponds to an ideal Bose gas in two and four dimensions (see section 5.1). So we expect that the zeros should approach the physically meaningful domain for large n for the case $\tau = 3$, but not for the case $\tau = 2$ (since $\zeta(1) = \infty$, $\zeta(2) = \pi^2/6$). Figure 4.8 illustrates the zeros for these two models for $n = 25, 50, 75, 100$. These graphs suggest that for both models, the roots lie on simple curves. Whether these curves close on the positive real axis is not clear from these small n results. The roots near the negative real axis scale with n, which suggests that the crossing point on the positive real axis should scale with n as well, which agrees with the known critical point. The fact that the curve will not close for $d = 2$ is not evident from the graph, however.

[11] See section 5.1 for a discussion of the limitation of this identification.

Chapter 5

Application to physical and mathematical systems

The previous chapters introduced and analyzed statistical models over partitions without showing that the models were applicable to actual physical systems. A "leap of faith" was required on the part of the reader to believe not only that the models would prove to be useful, but to be essential to our attempts at modeling real physical systems. In other words, the effort made in solving the statistical models of the previous chapters could be for naught if no physical system was found to which the models applied. Fortunately, the Markov process which generated the canonical Gibbs model (section 4.2.1) and the discussion of ideal Boltzmann gas entropies (section 4.2.3) suggest strongly that physical systems can be described by Gibbs models, and in fact this chapter produces a number of examples from physics, mathematics and biology which apply that and other models to systems of interest.

The first four sections discuss applications of the Gibbs model. Section 5.1 discusses the ideal Bose gas, which is probably the earliest model in physics from which a non-trivial Gibbs model emerged. The cluster expansion method of Mayer for non-ideal gases makes this connection with the Gibbs model explicit. Section 5.2 discusses polymer theory and gelation from the point of view of Stockmayer, who adapted Mayer's cluster expansion method in real-space, supplementing results derived earlier by Flory. Section 5.3 discusses the Feynman model for the λ transition in liquid helium, a model introduced in the 1950s to attempt to explain some of the unusual properties of liquid ^{4}He at low temperatures. Section 5.4 is an example from population genetics. Gene samples from a population are shown to have a distribution determined by a canonical Gibbs model, known as Ewens' sampling formula. Section 5.5 illustrates that the Gibbs

model might also have applications to problems in sociology. Whereas the above sections all apply the Gibbs model to historical problems, the following sections show that the equipartition, separable and interacting Gibbs models are also useful. Section 5.6 discusses an early treatment of nuclear fragmentation using the equipartition model. Section 5.7 introduces a separable model which interpolates between the Gibbs and equipartition models, a fact which is intimately related to the model's relation to the problem of enumerating the number of involutions or Young tableaux. Section 5.8 notes some graph enumeration problems which are equivalent to interacting Gibbs models.

5.1 Ideal Bose-Einstein gas, condensation, and the Mayer cluster expansion

The following model of an ideal gas of indistinguishable particles was introduced in the 1924 by Albert Einstein [86,87] based on Satyendra Nath Bose's [39] work on Planck's radiation formula. Einstein realized that Bose's statistical treatment of photons might also apply to massive particles, and worked out the statistical physics of an ideal gas of "bosons." At the time he was uncertain whether such particles actually existed, but considered the model of sufficient theoretical interest to proceed. This model reduces to a Gibbs canonical model, but was originally solved in the grand canonical ensemble. This should not be too surprising, since the recursive treatment is usually impractical to implement for all but small systems, but in retrospect it is curious that the exact solution of the canonical Bose gas is rarely if ever mentioned considering the large number of textbook derivations.[1] Especially since some calculations (such as its virial expansion) can be computed more simply in the canonical ensemble. Possibly this is the case because the connection between the model and symmetric functions, where the recursive solution naturally appears, may have been overlooked. Although this example is analyzed thoroughly in the literature, it is instructive to follow how the Gibbs model arises from such a simple system as well as to explore the utility of the

[1] I am unaware of any statistical mechanics textbook which draws attention to this fact. All the ones I am familiar with work entirely in the grand canonical limit, and have no advice for Bose systems with small numbers of particles.

canonical approach.[2]

An ideal Bose gas is a system of identical, indistinguishable particles. The canonical partition function is given by

$$Z_n = \sum_{\{n_{\mathbf{p}}:\sum_{\mathbf{p}} n_{\mathbf{p}}=n\}} e^{-\sum_{\mathbf{p}} n_{\mathbf{p}}\varepsilon_{\mathbf{p}}/k_BT} , \tag{5.1}$$

where $n_{\mathbf{p}}$ is the number of particles with momentum $\mathbf{p}$ and energy $\varepsilon_{\mathbf{p}} = p^2/2m$ in the non-relativistic limit. The grand canonical partition function, the sum of canonical partition functions, is given by

$$\begin{aligned} \mathcal{Z} &= \sum_{n\geq 0} z^n Z_n = \sum_{n_{\mathbf{p}}} \prod_{\mathbf{p}} (z e^{-\varepsilon_{\mathbf{p}}/k_BT})^{n_{\mathbf{p}}} \\ &= \prod_{\mathbf{p}} \frac{1}{1 - z e^{-\varepsilon_{\mathbf{p}}/k_BT}} . \end{aligned} \tag{5.2}$$

with $z = \exp\{-\mu/k_BT\}$ the fugacity. Now if we take a logarithm of both sides and convert the sum over $\mathbf{p}$ into an integral (adding the zero momentum mode in explicitly rather than in the integral[3]), we can evaluate this grand canonical partition function explicitly

$$\begin{aligned} \ln \mathcal{Z} &= -\sum_{\mathbf{p}} \ln(1 - z e^{-\varepsilon_{\mathbf{p}}/k_BT}) = -\frac{V}{h^d} \int d^d\mathbf{p} \ln(1 - z e^{-p^2/2mk_BT}) - \ln(1-z) \\ &= -\frac{V}{h^d} \int_0^\infty dp \frac{d\Omega_p}{dp} \ln(1 - z e^{-p^2/2mk_BT}) - \ln(1-z) \\ &= -\frac{V}{h^d} \frac{2\pi^{d/2}}{\Gamma(d/2)} (2mk_BT)^{d/2} \int_0^\infty dx\ x^{d-1} \ln(1 - z e^{-x^2}) - \ln(1-z) \\ &= \frac{V}{\lambda_T^d} \sum_{k>0} \frac{z^k}{k^{1+d/2}} - \ln(1-z) = \sum_{k>0} z^k \left(\frac{V}{\lambda_T^d} \frac{1}{k^{1+d/2}} + \frac{1}{k} \right) , \end{aligned} \tag{5.3}$$

where $\lambda_T = h/\sqrt{2\pi m k_B T}$ is the thermal wavelength (essentially the de Broglie wavelength except for a constant factor, i.e. $\lambda_{dB} = \lambda_T \sqrt{2\pi/3}$) and we have expanded $-\ln(1-z) = \sum_k z^k/k$. So the grand canonical partition function is given by

$$\mathcal{Z} = \exp\left\{ \sum_{k>0} z^k \left(\frac{V}{\lambda_T^d} \frac{1}{k^{1+d/2}} + \frac{1}{k} \right) \right\} . \tag{5.4}$$

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[2] V.S. Nanda [227] in 1953, extending work of H.N.V. Temperley [293] attacked the problem in a different way which attracts our attention as it also tried to connect the problem to an underlying partitioning problem. Later [229] he attempted a similar analysis for polymer models.

[3] In transforming the sum to an integral, the zero momentum mode is lost since it has zero volume in phase space and must be therefore added back in. Since the zero momentum mode $\langle n_0 \rangle / V$ is the only mode to persist when $V \to \infty$, we don't have to explicitly add every momentum mode in this fashion.

Notice that this is the exact form of a Gibbs model (cf. equation (3.26)) with parameter vector

$$x_k = \frac{V}{\lambda_T^d} \frac{1}{k^{1+d/2}} + \frac{1}{k} \; , \tag{5.5}$$

so the canonical partition function is given by

$$Z_n = \sum_{\pi(n)} \prod_{k \geq 1} \frac{1}{\pi_k!} \left(\frac{V}{\lambda_T^d} \frac{1}{k^{1+d/2}} + \frac{1}{k} \right)^{\pi_k} \; . \tag{5.6}$$

This is equivalent to equation (5.1), except the the physical states $\{n_{\mathbf{p}}\}$ have been repartitioned into integer partitions, but not in any physically meaningful way. The configuration vector $\boldsymbol{\pi}$ does not reflect the formation of actual clusters in real or momentum space, nevertheless, we can describe "states" of the gas by such partitions, i.e. we can consider the partitions to represent actual states of a physical system which when statistically averaged reproduce the results for an ideal Bose gas.

The first application of this canonical solution is for the determination of thermodynamic functions. From the above parameter vector, we see that all the thermodynamic variables are contained in the single parameter

$$x \;\; = \;\; \frac{V}{\lambda_T^d} \; , \tag{5.7}$$

and that the canonical partition function therefore can be written as

$$Z_n = \sum_{m=0}^{n} Z_n(m) x^m \; . \tag{5.8}$$

These coefficients $Z_n(m)$ are obtained from recursion relation

$$n Z_n(m) = \sum_{k=1}^{n} \frac{Z_{n-k}(m-1)}{k^{3/2}} + Z_{n-k}(m) \; , \tag{5.9}$$

with $Z_0(m) = \delta_{m0}$. This is arrived at by identifying like powers of x in $nZ_n = \sum_{k>0} k x_k Z_{n-k}$. The usual thermodynamic functions are then given by

$$PV \;\; = \;\; m_1 k_B T \; , \tag{5.10}$$

$$U \;\; = \;\; \frac{d}{2} m_1 k_B T \; , \tag{5.11}$$

$$\frac{C_V}{k_B} \;\; = \;\; \frac{d}{2} m_1 + \frac{d^2}{4} m_2 \; , \tag{5.12}$$

$$\frac{S}{k_B} \;\; = \;\; \ln Z_n + \frac{d}{2} m_1 \; , \tag{5.13}$$

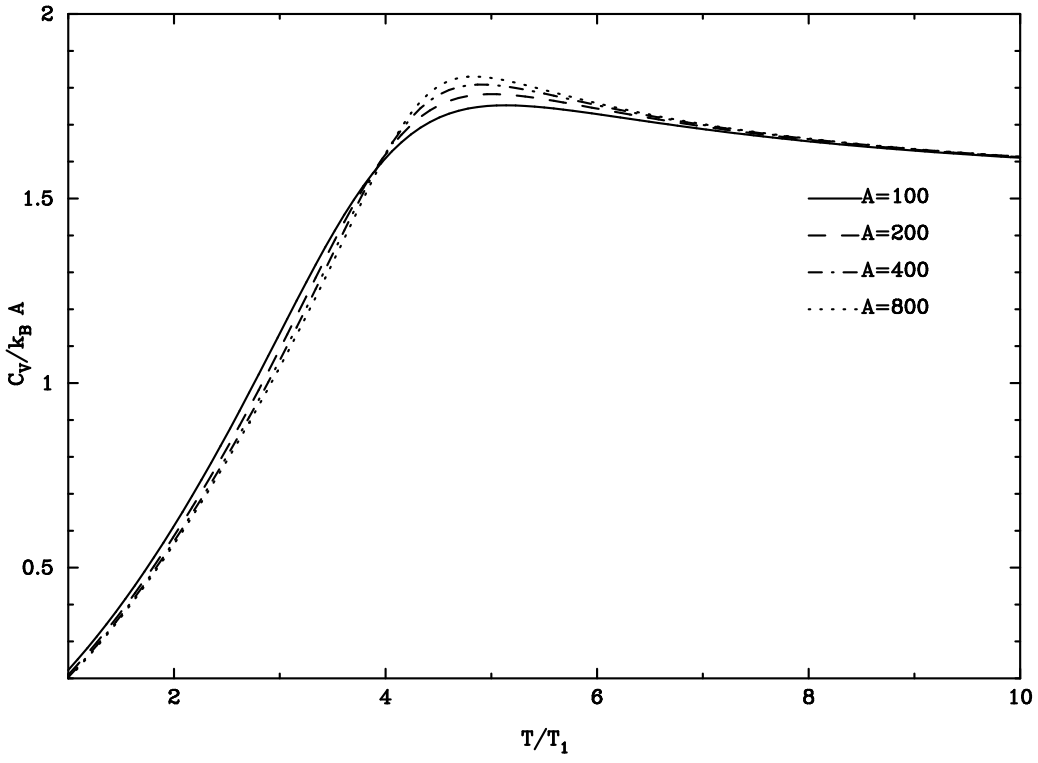
where

$$m_k = \left(x \frac{\partial}{\partial x} \right)^k \ln Z_n \ . \tag{5.14}$$

From this we can immediately derive the virial expansion for the equation of state, which describes the high temperature/low density behavior. In this limit, we can ignore the effect of the second term in x_k. Then $x_k = x b_k$, and the high temperature expansion for $\ln Z_n$ given in equation (3.35) can be applied, since $m_1 \to x \frac{\partial}{\partial x} \ln Z_n$, which gives us the following expansion

$$\begin{aligned} \frac{PV}{nk_BT} &= 1 - \lambda_T^d \frac{n-1}{V} \frac{1}{2^\tau} - \lambda_T^{2d} \frac{n-1}{V^2} \left(\frac{2(n-2)}{3^\tau} + \frac{2(2n-3)}{4^\tau} \right) \\ &\quad - \lambda_T^{3d} \frac{n-1}{V^3} \left(\frac{3(n-2)(n-3)}{4^\tau} - \frac{3(n-2)^2}{6^\tau} + \frac{4(5n^2-17n+15)}{8^\tau} \right) \\ &\quad + \ldots \ . \end{aligned} \tag{5.15}$$

Figure 5.1: Specific heat C_V of an ideal Bose-Einstein gas.



The virial expansion introduced above was first computed by a different method known as a Mayer cluster expansion. It essentially is a mathematical trick of some

ingenuity which makes computing each term in the series an accounting problem. Suppose we are interested in computing the equation of state from the canonical partition function

$$Z_n = \frac{1}{\lambda_T^{dn} n!} \int d^{dn} r \exp\left\{ -\sum_{i<j} v_{ij}/k_B T \right\} . \tag{5.16}$$

Let f_{ij} be defined by

$$\exp\{-v_{ij}/k_B T\} = 1 + f_{ij} \tag{5.17}$$

so that the partition function becomes

$$Z_n = \frac{1}{\lambda_T^{dn} n!} \int d^{dn} r [1 + (f_{12} + f_{13} + \ldots) + (f_{12} f_{13} + f_{12} f_{14} + \ldots) + \ldots] . \tag{5.18}$$

Each term in this series expansion can be identified with a graph by associating each f_{ij} in the term with an edge connecting the vertex i to j (i.e. if $i \sim j$). We now define the k-cluster integral b_k by

$$b_k = \frac{1}{k! \lambda_T^{3k-3} V} \int d^d r_1 \cdots d^d r_k \sum_{\substack{\text{connected} \\ k-\text{graphs}}} \prod_{i \sim j} f_{ij} . \tag{5.19}$$

Mayer [207–209, 144] showed that the grand canonical equation of state is given by

$$\ln \mathcal{Z} = \frac{PV}{k_B T} = x \sum_{k=1}^{\infty} b_k z^k , \tag{5.20}$$

$$n = x \sum_{k=1}^{\infty} k b_k z^k . \tag{5.21}$$

By combining these equations z can be eliminated term by term arriving at the virial expansion.

$$\frac{PV}{n k_B T} = \sum_{k=1}^{\infty} a_k \left(\frac{n}{x} \right)^{k-1} \tag{5.22}$$

with

$$\begin{aligned} a_1 &= b_1 = 1 , \\ a_2 &= -b_2 , \\ a_3 &= 4b_2^2 - 2b_3 , \end{aligned} \tag{5.23}$$

etc.

Historically[4], Mayer's theory was motivated by limitations of the van der Waals theory of non-ideal gases presented in his 1873 dissertation [301]. Shortcomings of this theory led Heike Kamerlingh Onnes[5] in 1901 to suggest that certain unphysical aspects of the van der Waal's equation of state might be removed if a complete expansion of PV/nk_BT in ascending powers of ρ were made. This is the virial expansion for a non-ideal gas, but no practical method for theoretically computing the expansion was then known. H.D. Ursell [300], in 1927 suggested how to go about about calculating the coefficients systematically, and J. Yvon [316] in 1935 and Joseph Mayer [207–209, 144] in 1937-38 introduced the above described cluster expansion method to implement such a systematic evaluation.

There are three interesting comments that should be made. First, this was the first successful attempt to improve upon the van der Waal's equation of state since its introduction fifty years earlier. Second, this work represents the first graphical perturbation series, a decade or so before Richard P. Feynman [98] made such approaches popular in the context of quantum electrodynamics (QED), a noteworthy fact which is often overlooked today. Mayer realized that the virial equation of state was a perturbation expansion in the f_{ij}'s, and invented some of the apparatus that was to find much wider application in QED later. For example, the reduction an expansion over all graphs to the exponential of an expansion over only the connected ones, a general phenomenon known as the *linked cluster theorem*, is due to Mayer, but is equally applicable to quantum field theory. Third, the Mayer cluster expansion, although introduced for a classical system, can be extended to intrinsically quantum systems. B. Kahn and G.E. Uhlenbeck [157] generalized this work to quantum mechanical systems, and showed that the expansions are usually impossible to solve exactly, in contrast to the classical case. T.D. Lee and C.N. Yang [68] generalized it to systems obeying Bose-Einstein and Fermi-Dirac statistics.

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[4]This historical interlude draws substantially from George E. Uhlenbeck's *Lectures in Statistical Physics* [299].

[5]Onnes is famous for liquefying helium in 1908.

For the purpose it was invented for, the Mayer cluster expansion is ideal, but a significant simplification can be made using some results from canonical Gibbs models. In terms of Gibbs models, Mayer showed that the canonical partition function in the region where the virial expansion is valid is a Gibbs partition function with x_k given by

$$x_k = x b_k \; . \tag{5.24}$$

For example, the Bose-Einstein gas in d dimensions has $b_k = k^{-1-d/2}$ and $x = V/\lambda_T^d$ in the large x limit. Using the large x expansion for $\ln Z_n$ given by equation (3.35) and the list of microcanonical partition functions $Z_n^{(n-r)}$ given by equation (3.34), the grand canonical ensemble can be avoided, and the term by term inversion eliminated in finding a_k.

Comparing equation to equation (5.24) to equation (5.5) in three dimensions for example shows the virial expansion can't be valid at small x. At some x therefore the predictions of the virial expansion must become incorrect. Although this transition could happen smoothly, the breakdown of the virial expansion instead happens in a rather spectacular fashion. As is well known, an ideal Bose-Einstein gas condenses suddenly as the temperature is dropped (or the density increases) in $d > 2$ dimensions, a phase transition in which the zero momentum mode or ground state is populated with a finite fraction of the particles of the system. Bose-Einstein condensation is of much recent interest due to its experimental observation in ultra-low temperature solids (July 14th 1995, Science). It also figures prominently in descriptions of low temperature ^{4}He and its λ phase transition. In an ideal Bose gas, such condensation can occur when the thermodynamic parameter x drops below a certain value, at which point the zero momentum state, or "condensed" state becomes partially populated and the gas is said to undergo a phase transition. This happens at $x = x_c = n/\zeta(d/2)$.[6] In terms of V, T, this defines a critical temperature and volume (or density) by,

$$k_B T_c(V) = \frac{h^2}{2\pi m}\left(\frac{n}{V\zeta(d/2)}\right)^{2/d} , \tag{5.25}$$

$$V_c(T) = \frac{n\lambda_T^d}{\zeta(d/2)} \; . \tag{5.26}$$

[6] See Huang [149], page 286 for a derivation of this fact.

When $d \leq 2$, $x_c = 0$ and no phase transition is observed. This phase transition is first order because there is a latent heat

$$L = \frac{5}{2}\frac{\zeta(1+d/2)}{\zeta(d/2)}k_B T \tag{5.27}$$

associated with removing a particle from the condensed phase. Theoretically, it can be seen as a cusp in the specific heat in the thermodynamic limit ($n, V \to \infty, n/V$ finite), i.e.

$$C_V \quad \sim \quad |T - T_c|^{-\alpha} \ , \tag{5.28}$$

The specific heat at both finite and infinite n is illustrated in figure 5.1. Gunton and Buckingham [131] have computed the critical exponents for this phase transition from the thermodynamic point of view, three of which are $\alpha = 2 - d$, $\beta = 1/2$, $\gamma = d - 1/2$, From the point of view of section 4.3, these exponents are defined differently, giving $\alpha = 1 - 2/(d-2)$, $\beta = 1$, $\gamma = 2/(d-2) - 1$.

5.2 Polymers and gelation

Polymers represent one of the earliest applications of the Gibbs model. The ideal Bose-Einstein gas theory was presented earlier, and Mayer's cluster expansion made its relation to clustering apparent, but Walter H. Stockmayer [283,284] appears to be the first to apply the model to an actual system (polymers in solution) that aggregates and fragments. His model is entirely analogous to the Mayer cluster expansion, which he credited, except that the clustering in his model is more than a helpful mathematical device, it is the essential physics. In his seminal paper, he also realized the need to introduce vector partitions when considering systems with more than one type of indistinguishable particle, and results for one, two and three kinds of objects (functional units in his language) are included. Stockmayer used the maximal entropy approach to "solve" the Gibbs model, specifying that the equilibrium distribution is given by the states with the largest entropy, which is equivalent to applying the grand canonical ensemble. He seemed to be unaware that recursive solutions to the problem existed, but since computing machines were not available at the time, it is understandable why this

is the case. However, unlike the case of the ideal Bose-Einstein gas, the exact recursive solutions for polymers have not been entirely ignored. R. Botet[7] and R. Jullien [40] recognized and used the microcanonical solutions in 1984, and Frank P. Kelly [164] used the canonical model in 1979.

Polymers are long chains of organic molecules connected by bonds formed between the functional units that comprise the chain. The number of functional units is kept fixed, as is the total number of polymers, since each polymer of size k has $k-1$ bonds (intramolecular reactions are excluded) which implies the energy of the system is given by

$$\sum_k \varepsilon(k-1)\pi_k = \varepsilon(n-r)\ , \tag{5.29}$$

which should be constant. Since n is already fixed, r must be fixed and the ensemble should therefore be microcanonical. Typically the number of functional units is sufficiently large that a grand canonical ensemble or canonical ensemble can be used with chemical potentials chosen so that n and r produce the microcanonical values in ensemble averages.[8]

One way to model polymers is to assume a Markov process, as shown by Frank P. Kelly [164] (chapter 8). There, Kelly assumed that the molecules combine to form polymers by forming bonds between molecules, up to a maximum of f bonds on a single molecule. He also assumed that the shape of the polymers are distinguishable, so the fundamental configurations are more complicated than just partitions. However, these final configurations can be mapped onto partitions just as permutations and set partitions could be mapped onto partitions (section 2.1.2). If existing bonds between functional units break at a rate κ and new bonds form at rate proportional to the number of sites available for new bonds, Kelly showed that the equilibrium polymer distribution for polymers divided into partition classes is given by the canonical Gibbs ensemble with parameter vector given by

$$x_k = \kappa \frac{f^k(fk-k)!}{k!(fk-2k+2)!}\ , \tag{5.30}$$

[7] R. Botet who began his work in polymers is now active in nuclear fragmentation modeling [41].

[8] See section 4.3.2 for a discussion of the limitations of this approach.

a result originally due to Stockmayer who argued from a combinatorial point of view, which we will discuss below. This is known today as the RA_f model, for f-functional random polycondensation. If f tends to infinity then we have the RA_∞ model, given by (ignoring the f^k term which does not affect the canonical distribution).

$$x_k = \kappa \frac{k^{k-2}}{k!} \sim \frac{\kappa}{\sqrt{2\pi}} e^k k^{-5/2} \ . \tag{5.31}$$

Notice that asymptotically, this is the same x_k as in the high temperature ideal Bose gas in three dimensions (the e^k term does not affect the canonical distribution). Typical polymer yields of the RA_f model are given in figure 5.2. More general models are known as $\mathrm{A}_g\mathrm{RB}_{f-g}$ for models with g functional groups of type A, $f-g$ of type B. For ARB_{f-1} we have

$$x_k = \kappa \frac{(fk-k)!}{k!(fk-2k+1)!} \ , \tag{5.32}$$

and for ARB_∞ we have

$$x_k = \kappa \frac{k^{k-1}}{k!} \ . \sim \frac{\kappa}{\sqrt{2\pi}} e^k k^{-3/2} \ . \tag{5.33}$$

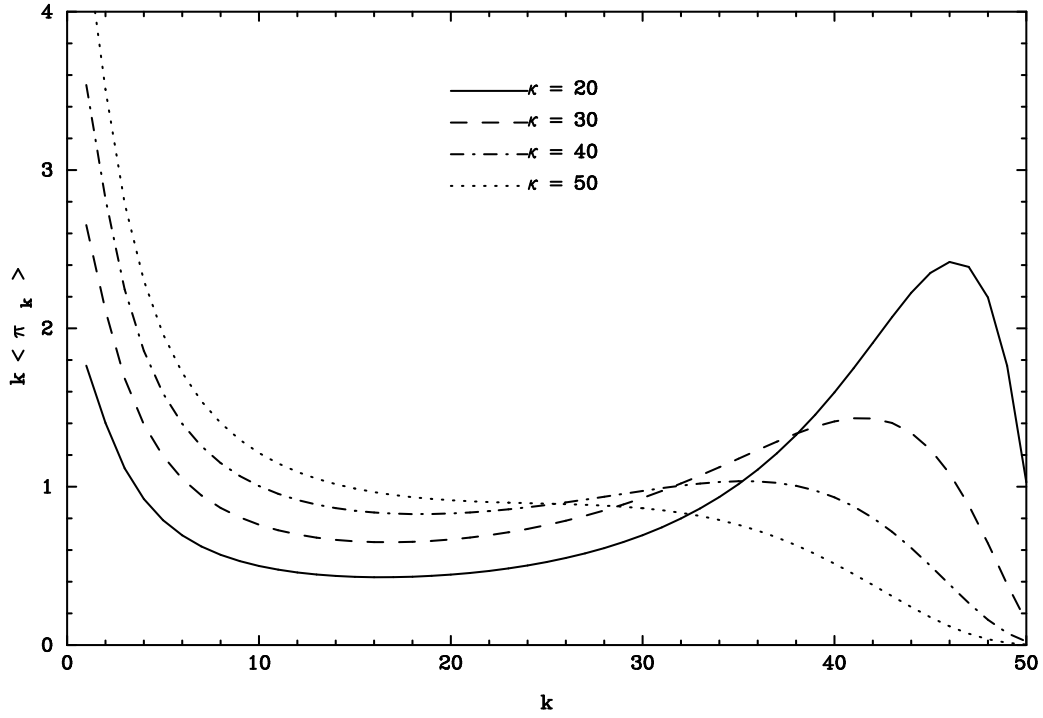
These models are typically derived from the *kinetic kernel* method, introduced by John Spouge [278] as a complement to the combinatorial method of Stockmayer. In this method, one assumes $w_k = x_k k!$ is the number of ways of forming a k-mer from k distinguishable functional units, and a_{ij} is the number of different bonds that may be formed between an i-mer and a j-mer. This combinatorial object must satisfy

$$2(k-1)w_k = \sum_j \binom{k}{j} a_{j,k-j} w_j w_{k-j} \ , \tag{5.34}$$

since the LHS is the number of ways of assembling a k-mer, choosing one of its $k-1$ bonds and one of the polymers induced by cutting the bond, while the RHS is the number of ways of taking k units, forming two clusters one of size j and one of size $k-j$, and then choosing a bond to combine them to form a k-mer. So a_{ij} determines x_k from the above relation. It can be shown that all the above models are examples of $a_{ij} = A + B(i+j) + Cij$. For example, the RA_f model is given by

$$a_{ij} = (2 + (f-2)i)(2 + (f-2)j) \ . \tag{5.35}$$

Figure 5.2: Expected mass yield $k\langle\pi_k\rangle_n$ of polymers for the RA_f model. Here $n = 50$, $f = 3$ and κ ranges from 20 to 50. Compare this behavior with figure 4.2(d).



This approach simplifies the determination of w_k and the partition functions when compared to Stockmayer's original derivations or Kelly's canonical method.

To solve this model, we will apply the maximal entropy approach. We assume the equilibrium distribution is given by the most probable configuration $\langle\boldsymbol{\pi}\rangle_{\max S}$. Lagrange multipliers μ, ν are introduced to maintain conservation of n, r, and so the most probable configuration is given by the maximum of $\ln W(\boldsymbol{\pi}) - \mu n - \nu r$, i.e.[9]

$$\max_{\pi(n)} \left(\ln \prod_j \frac{x_j^{\pi_j}}{\pi_j!} - \mu \sum_j j\pi_j - \nu \sum_j \pi_j \right) , \tag{5.36}$$

which is specified by

$$\langle\pi_j\rangle_{\max S} = x_j e^{-\mu j - \nu} , \tag{5.37}$$

which is the same answer that the grand canonical approach would have given with $x_k = (w_k/k!)e^{-\mu k - \nu}$, i.e. the Lagrange multipliers are the chemical potentials which

[9]The maximum of $\ln f(x)$ and $f(x)$ are the same since $\ln f$ is a monotonic function of f, so we can maximize over $\ln f$ or f. Taking the natural logarithm in this case simplifies the computation significantly.

regulate $\langle n \rangle$, $\langle r \rangle$ in the grand canonical ensemble. Denote by $z = e^{-\mu}$, $x = e^{-\nu}$ the fugacities and by $F = -\ln \mathcal{Z} = -\sum_j (w_j/j!) e^{-\mu j - \nu}$ the "free energy". Let η denote r/n and α the extent of reaction,

$$\eta := \left\langle \frac{r}{n} \right\rangle , \tag{5.38}$$

$$\alpha := \left\langle \frac{2(n-r)}{fn} \right\rangle = \frac{2}{f}(1-\eta) . \tag{5.39}$$

Thus

$$F = -\langle r \rangle , \tag{5.40}$$

$$zF' = z\frac{\partial}{\partial z}F = -\langle n \rangle , \tag{5.41}$$

which implies that the first derivative of F is given by

$$F' = F\frac{1}{\eta z} . \tag{5.42}$$

Let us rewrite equation (5.34) for the bilinear case $\alpha_{ij} = A + B(i+j) + Cij$,

$$2(k-1)\frac{w_k}{k!} = \sum_{i+j=k} \frac{w_i}{j!}\frac{w_j}{j!}(A + B(i+j) + Cij) . \tag{5.43}$$

Multiplying both sides by $e^{-\mu k - \nu}$ and summing over k yields

$$-2zF' + 2F = \left(AF^2 + 2BFzF' + C(zF')^2\right)/x , \tag{5.44}$$

which gives an exact expression for $F(x,z)$, namely:

$$F = \frac{-2x\eta(1-\eta)}{A\eta^2 + 2B\eta + C} \tag{5.45}$$

Differentiating equation (5.44) yields an expression for the second derivative of F,

$$-2zxF'' = 2AFF' + 2B(FF' + z(F')^2 + zFF'') + 2C(zF')(zF'' + F') \tag{5.46}$$

which after some manipulation yields an exact expression for the second derivative of $F(x,z)$

$$F'' = \frac{4(1-\eta)^2((A+B)\eta + B + C)x}{(A\eta^2 + 2B\eta + C)^2((A+2B)\eta^2 + 2C\eta - C)} \tag{5.47}$$

As in an ideal Bose-Einstein gas, there is a phase transition *gelation* which occurs with the formation of very long polymers. Gelation is a phenomenon in which part of the solution solidifies, forming a colloidal suspension (or jelly) in the liquid, and occurs suddenly in materials in which the formation of branched-chain polymers is allowed. Stockmayer summarized the understanding of the phenomenon succinctly,

> Reactions which can lead only to unbranched linear chains yield products which are always soluble in suitable media, regardless of the extent of the reaction, and as the reaction proceeds the change from a fluid to a plastic material is gradual. On the other hand, if frequent branching of chains is structurally permissible, as for example in the glycerol-phthalic anhydride reaction, the material gels suddenly at a certain critical extent of reaction which appears to depend on the composition of the reacting mixture but not on the temperature at which the reaction is carried out.[10]

The sudden change in properties of the material suggest a phase transition. Consider Stockmayer's RA_f model. The free energy and its first derivative specified by equations (5.45) and (5.42) are free from singularities in the physically meaningful range of parameters ($\eta = 1 - f/2 < 0$ is an unphysical singularity), but its second derivative does have an additional singularity at $\eta_c = (f-2)/2(f-1) < 1/2$ for $f > 2$. This implies a phase transition if $f > 2$ at the critical extent

$$\alpha_c = \frac{1}{f-1} \,. \tag{5.48}$$

This is similar to the Bose requirement that $d > 2$ for a phase transition to occur, and agrees with Flory's earlier work [109,112], which treated the problem in an intuitive percolative approach.

Since asymptotically the theory is identical to an ideal Bose gas in three dimensions, its critical exponents should be the same, and indeed, $\alpha = -1$, $\beta = 1$, $\gamma = 1$ $\sigma = 1/2$, $\tau = 5/2$ (cf. Stauffer [280]).

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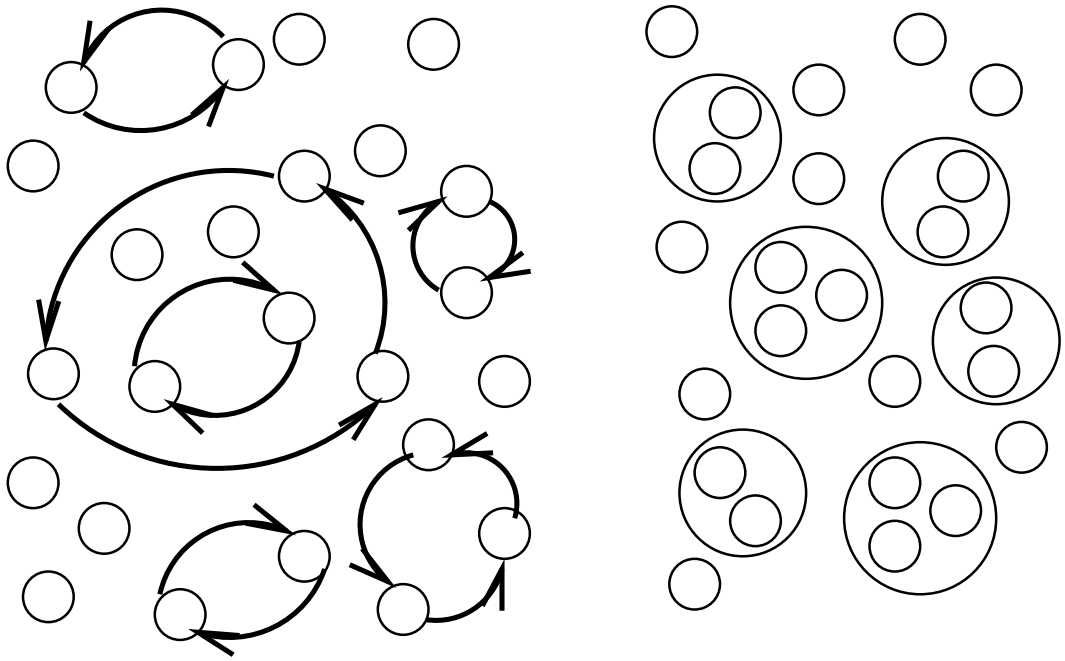
[10] [283], page 45.

5.3 Liquid ^{4}He and the λ transition

Figure 5.3: Permutations among objects. Left-hand side of graph shows a group of particles and a permutation operator as it would act on the particles. Right-hand side gives cluster interpretation of the same permutation.



In 1908, Heike Kamerlingh Onnes liquified helium, a technical achievement which was to lead to the discovery of superconductors a few years later. It was not until 1938 however, that liquid helium itself became of interest with the discovery of the "superfluidic" properties of the liquid during attempts to measure its viscosity by P.L. Kapitza [158] and J.F. Allen and Misener [10].[11] They discovered that at 2.17K liquid ^{4}He undergoes a phase transition in which part of the fluid apparently moves with zero viscosity. Named for the shape of the experimental specific heat curve for this transition, the λ transition has interested physicists since its discovery. At that time a number of theories were proposed, from the phenomenological two-fluid model due to L. Tisza [294] to the more detailed models of Fritz London [190–192], Oliver Penrose and Lars Onsager [237], and Lev Landau [178,179]. In this section we give some of the results of Richard Feynman's later theory [100, 99, 101, 102] for the λ transition from the 1950s, which we shall see

[11] See Donnelly [78] for a historical review of the discovery of superfluidity

reduces to a Gibbs model.[12] It should be noted that Feynman's model as presented here is inadequate in explaining the phenomena. This is due to the approximations made to "solve" the model, and if these approximations are done more carefully, a more robust theory results. Kikuchi *et al.* [165,166] has done such an analysis, and more recently Ceperley and Pollock [56] have done an exact evaluation.

The starting point is the partition function obtained by a path integral [98], given by equation 11.52 in [102]

$$\begin{aligned} e^{-F/k_BT} &= \frac{1}{n!}\left(\frac{2\pi m' k_B T}{h^2}\right)^{3n/2} \\ &\quad \times \sum_{P\in S_n} \int d^3\mathbf{R}_1 \cdots d^3\mathbf{R}_n \rho(\mathbf{R}_1, \ldots, \mathbf{R}_n) \\ &\quad \times \exp\left\{-\frac{m' k_B T}{2\hbar^2} \sum_i (\mathbf{R}_i - P(\mathbf{R})_i)^2\right\} , \end{aligned} \tag{5.49}$$

where n is the total number of helium atoms, m' is the effective mass, $\mathbf{R_i}$ the coordinate of the ith helium atom, $\rho(\mathbf{R}_1, \ldots, \mathbf{R}_n)$ is the potential contribution and P is the permutation operator. A given permutation among the particles is illustrated in figure 5.3, and can be visualized as the atoms being connected by a set of edges, the edges forming polygons (cycles) of various sizes (cycle lengths). After some algebra and approximations, Feynman reduces the partition function to

$$e^{-F/k_BT} = \sum_{\pi(n)} \prod_{k=1}^{n} \frac{x_k^{\pi_k}}{\pi_k!} , \tag{5.50}$$

where

$$x_k = \begin{cases} n & k = 1 , \\ y^k \left(\frac{nc}{k^{5/2}} + \frac{1}{k}\right) & k > 1 , \end{cases} \tag{5.51}$$

and $y = l \exp\{-m' d^2 k_B T/(2\hbar^2)\}$, l is the number of nearest neighbors per lattice site for a particular choice of spatial discretization, and c is a proportionality constant close to one dependent on the discretization. This result can be partially understood as follows. Only permutations which permute local atoms contribute significantly to the partition function. We can consider one k-cycle of such a permutation as a random walk from

[12] Feynman's work in condensed matter physics, especially his contributions to the theory of liquid helium, is discussed in an excellent article by David Pines [238].

one atom back to itself. Starting at a given atom, there are l^k random walks in k steps, and the fraction of these that return to their starting point is inversely proportional to the volume in which the random walk is likely to end, or $k^{-3/2}$. We have overcounted, since any point on the cycle could have been the starting point, so the number of walks is proportional to $k^{-5/2}$. This random walk result is then corrected for the very large polygons that encompass a large fraction of the sites. This determines the form for x_k, as given above.

This model is a Gibbs type model and was arrived at essentially because of the connection between permutations and integer partitions as shown in section 2.1.2 and some properties of random walks in three dimensions. Interestingly, comparing the results of this section with those of section 5.1, we see a strong parallel between Bose condensation and this model for the λ transition. If $y \equiv 1$, $c = 1$ the forms for x_k in the two models would be exact except for x_1. But Feynman did not start out trying to model liquid helium as a gas, and the closeness of the two models is therefore more surprising than might otherwise be thought. As a result even with y different this model has the same specific heat curve as an ideal Bose gas, with its characteristic cusp. The discontinuity seen in "real" liquid helium is due to the interactions which in this treatment have been grossly approximated. Later we will see that the model is also fairly close to a model for nuclear fragmentation proposed.

5.4 The frequency of alleles and Ewens' sampling formula

Our next example is from population genetics [93]. We begin by supposing we have an infinite number of allelic types $A_1, A_2, \ldots$ which may occur on a gene at a locus A. We assume a mutation rate u to new allelic types (not previously seen) and that all allelic types are selectively equivalent. Suppose at time t, alleles $A_1, A_2, \ldots$ appear $n_{t1}, n_{t2}, \ldots$ at the locus., then the probability that they will appear at time $t+1$ with numbers $n_{t+1,1}, n_{t+1,2}, \ldots$ with $n_{t+1,0}$ new mutant genes is

$$M! \frac{u^{n_{t+1,0}}}{n_{t+1,0}!} \prod_{j \geq 1} \frac{(n_{t,j}(1-u)/M)^{n_{t+1,j}}}{n_{t+1,j}!} , \tag{5.52}$$

with $M = \sum_j n_{t,j}$. Eventually, any specific allele will disappear, but allelic patterns may persist. In other words, the state at time t can be described by the partition $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_M)$ where π_j is the number of allelic types which are each represented by exactly j genes. This model is referred to as the Wright-Fisher model.

A lot of population genetics can be inferred from the above model, but we immediately move to a sampling formula based on the above process. Suppose a sample of n genes is taken at random from this population. What is the probability a particular partition will be seen? Warren Ewens, in a classic paper [92], conjectured that

$$\Pr(\boldsymbol{\pi}) = \binom{\theta + n - 1}{n}^{-1} \prod_{j \geq 1} \frac{1}{\pi_j!} \left(\frac{\theta}{j}\right)^{\pi_j} . \tag{5.53}$$

where $\theta = 2Mu$. S. Karlin and J. McGregor [160] proved the correctness of this result, and readers interested in the proof should refer to the original papers. For our purpose, it is enough to note that this is equivalent to a Gibbs weight with $x_k = \theta/k$.

The story could well end there in this chapter of applications of the Gibbs model, but the Ewens' sampling formula has many properties which suggest it is much more important than an isolated example of a canonical Gibbs ensemble model. First of all, several other models from population genetics when sampled reduce to this distribution, although θ may be redefined. This is not surprising in view of later research. Indeed, J.F.C. Kingman a few years after the discovery of Ewens' formula observed that it is in some sense unavoidable. He argued as follows. A sample of n genes could have come from a sample of $n+1$ genes in which one of the genes was lost. Clearly the $n+1$ sample should have the same distribution as the n sample, so if $\boldsymbol{\pi}$ is a partition of n and $\Pr(\boldsymbol{\pi})$ is the partition probability, then

$$\Pr(\boldsymbol{\pi}) = \frac{\pi_1 + 1}{n+1} \Pr(\pi_1 + 1, \pi_2, \ldots) + \sum_{r=2}^{n+1} \frac{r(\pi_r + 1)}{n+1} \Pr(\ldots, \pi_{r-1} - 1, \pi_r + 1, \ldots) . \tag{5.54}$$

Ewens' formula does satisfy this, but so do other formulae. Kingman then argued that there should exist a "non-interference" condition, defined by the requirement that if a gene is taken at random from the sample, and all r genes of its allelic type removed, the probability distribution of the remaining $n - r$ genes should be that of an original sample of $n - r$ genes. Put another way, suppose we can't see a particular gene, because

our sampling technique is insensitive to those genes. Then non-interference says that our inability to detect that gene shouldn't affect the distribution we see of the other genes. Mathematically, this requires

$$\frac{r\pi_r}{n}\Pr(\boldsymbol{\pi}) = C(n,r)\Pr(\ldots,\pi_r-1,\ldots)\,, \tag{5.55}$$

where $C(n,r)$ is independent of $\boldsymbol{\pi}$. Kingman showed that the only *representable*[13] partition distribution which satisfies both these conditions is Ewens' sampling formula. In population genetics it seems, all roads lead to Ewens' sampling formula. We shall return to this fact in our discussion of isobaric and isotopic equivalences in nuclear models (section 6.2.2).

5.5 Social group dynamics

On entering a large hall filled with people (say for a high school reunion), one is struck with a variety of choices to make. Instinctively one tends to seek out an existing group of people (perhaps old friends) who are amicably chatting and laughing, and after some introductions settle in to the conversation at hand. After time you may leave the group to join another, or perhaps retire to a reclusive corner for a time to reflect on some thoughts in private (gee, I never expected him to become a doctor, etc.).

A physicist with sociological ambitions[14] might try to understand the politics and dynamics of group formation in this high school reunion with a simple model. Except at the beginning and end of the event, the number of people is more or less fixed, and at any time there are π_1 people alone, π_2 people in groups of two, etc. A Markov process then determines the dynamical formation and dissolution of groups. Let's assume that at any point in time only one thing can happen: a person can leave one group and join another group, i.e. there is a transition operator

$$T^{jk}\boldsymbol{\pi} = (\ldots,\pi_{j-1}+1,\pi_j-1,\ldots,\pi_{k-1}-1,\pi_k+1,\ldots)\,, \tag{5.56}$$

[13]This is a highly technical condition. Physicists and biologists may substitute the word "reasonable" without loss of meaning. Mathematicians are advised to review Kingman's original papers.

[14]Not necessarily to be confused with the author.

where T^{jk} specifies that a person leaves a group of size j and joins a group of size $k-1$ (T^{kj} is its inverse). Suppose these events happen at a rate

$$q(\boldsymbol{\pi}, T^{jk}\boldsymbol{\pi}) = \begin{cases} \pi_j \pi_{k-1} \lambda_{jk} & k > 1 \ , \\ \pi_j \lambda_{j1} & k = 1 \ , \end{cases} \tag{5.57}$$

i.e. the rate is proportional to the number of existing groups size, times some (to be determined) parameters. Now assume that the equilibrium distribution is specified by a Gibbs model and that detailed balance holds (i.e. equations (4.45) and (4.44) hold), then it is a short computation to show that

$$x_j x_{k-1} \lambda_{jk} = x_k x_{j-1} \lambda_{kj} \ , \tag{5.58}$$

with $x_0 = 1$. So what choices of λ_{jk} satisfy this requirement. Clearly $\lambda_{jk} = x_k x_{j-1}$, $\lambda_{jk} = (x_j x_{k-1})^{-1}$, $\lambda_{jk} = \frac{x_{j-1}}{x_j}$, and $\lambda_{jk} = \frac{x_k}{x_{k-1}}$ are possible solutions. The last two of these are interesting, since they imply that there exist solutions in which the transition rates are independent of the size of the group someone is either joining or leaving. A reasonable approximation might be to expect people to join groups independent of the size of the group they were just in, which suggests the last of the four solutions is a candidate for a model of social dynamics. For example, suppose after leaving the group, the person is equally likely to join any existing group, or start a new group. Then $\lambda_{jk} = 1.0$ and $x_k = 1.0$. The distribution of group sizes is easy to calculate in this case. Another interesting solution is $\lambda_{jk} = k$ which suggests people are more likely to join larger groups. In this case, $x_k = k!$ determines the equilibrium solution.

There are many more aspects which drive social dynamics than just group size, one of which might be the gender mix of existing groups. Perhaps social dynamics tries to distribute men and women equally among the groups, or alternately in some circumstances, tends to segregate the men and women into separate groups. In this formalism, such dynamics can be explored by using a bipartite Gibbs model where one component is women and the other is men. Such models would not differ markedly from the one above. Other distinctions between the members of the groups can be explored likewise.

In conclusion, it may be reasonable to assume that the underlying social dynamic

driving group formation can be encapsulated in a canonical Gibbs model. Expected group sizes and compositions could be made from such a model and the results should be of at least theoretical value to sociologists interested in groups and group formation. Much more needs to be done however before this can be anything more than a toy model.

5.6 Minimal information and statistical shattering

The next chapter discusses the fragmentation of nuclei in detail, but the following historical model of nuclear fragmentation is of interest since it reduces to an equipartitioning model. This model was introduced to describe the shattering of nuclei in analogy with the shattering of glass spheres. The shattering of glass is poorly understood, but empirically it is known that the distribution of fragments is approximately a power law in the fragment size. Since early nuclear fragmentation data also showed this power law behavior, J. Aichelin and J. Hüfner [5] proposed to reproduce this behavior by applying a maximum likelihood or minimum bias principle. In other words, they assumed that the fragmentation pattern defined by the probability of observing a particular fragmentation event $\Pr(\boldsymbol{\pi})$ tended to minimize the information content[15] I defined by

$$I = \sum_{\pi(n)} \Pr(\boldsymbol{\pi}) \ln \Pr(\boldsymbol{\pi}) \; . \tag{5.59}$$

Clearly this minimum occurs when all the probabilities are equal, which implies an equipartitioning model (section 3.2.2) with $x_j = 1$[16].

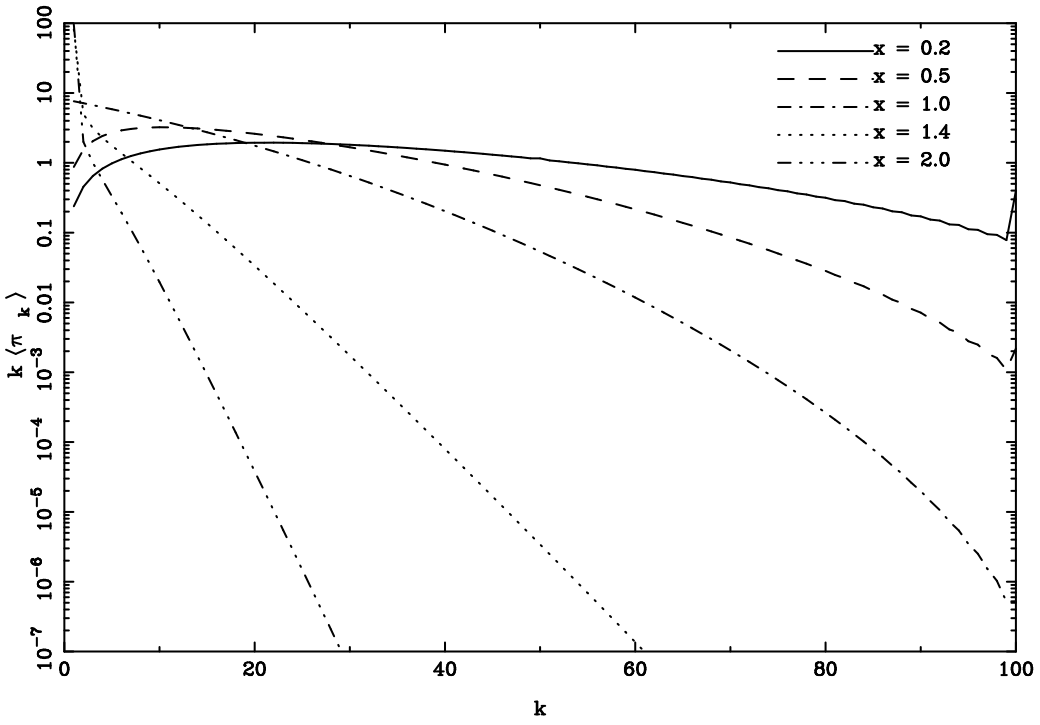
Aichelin and Hüfner only allowed states which satisfied charge conservation, but other modifications are no more difficult to impose. Y. Shibata and T. Fujita [270] additionally imposed energy conservation and G. Fái and A.Z. Mekjian [95] tried to impose the principle on microstates which included the momentum and position of the fragments as well. Kim Sneppen and R. Donangelo [275] explored the general problem

[15]The information I is the negative of the informational entropy, so a minimal information principle is equivalent to a maximal entropy principle.

[16]This was deduced originally from the asymptotic behavior, see Aichelin and Hüfner [6] and L.G. Sobotka and L.G. Moretto [276].

implicit in these generalizations: How is the probability of macrostates (e.g. $\Pr(\boldsymbol{\pi})$) affected by a minimal bias principle applied to the microstates? They concluded that "coarse graining" of the microstates leads to macrostates with probabilities equivalent to the Copenhagen model [37, 38] with some reasonable additional restrictions. As such, interest in strictly information-theoretic models of nuclear fragmentation has faded, although Sneppen applied the idea to vector partitions [274] and R. Englman [89, 90] has surveyed the usefulness of the method in many other areas in physics. The more general equipartition model with $x_j = x$ (i.e. a non-minimal distribution when $x \neq 1$) has also been explored by Chase and Mekjian [59]. It's characteristic distribution of cluster sizes is shown in figure 5.4 for various x.

Figure 5.4: Expected mass yield $k\langle\pi_k\rangle_n$ in for the equipartition $x_k = x$ model at $n = 100$ and $x = 0.2, 0.5, 1.0, 1.4, 2.0$.



Without particular assumptions about coarse graining, the minimal bias principle leads to models which fail to approximate the actual data from nuclear fragmentation experiments, so recent models of nuclear fragmentation make different assumptions, resulting in models closer in spirit to the Gibbs model. But equipartitioning models

Table 5.1: Number of involutions or Young tableaux t_n for $n = 1(1)10$.

n	1	2	3	4	5	6	7	8	9	10	11	12
t_n	1	2	4	10	26	76	232	764	2620	9496	35696	140152

sometimes do appear in physics, for example in energy level density calculations [263, 127]. Nevertheless, information theoretic concepts may still have some utility in nuclear fragmentation. For example, section 4.1.4 evaluates the information content for a Gibbs model which suggests the appearance of critical phenomenon may be signaled by a maximization of the informational entropy.

5.7 Involutions, Young tableaux, and Gibbs-equipartition interpolations

Involutions are permutations which are their own inverses. The number of involutions on n elements t_n is also the number of distinct Young tableaux on n elements [272], and so this number is of some interest to both physicists and mathematicians. The number is specified by the following exponential generating function

$$\sum_{n\geq 0} \frac{t_n q^n}{n!} = \exp\left\{ q + \frac{q^2}{2} \right\} , \tag{5.60}$$

and table 5.1 list first few such numbers. Although much more could be said about these objects, it will suffice to point out that they arise in a particular separable model which tries to interpolate between the Gibbs and equipartition models.

Recall that for the Gibbs model, the partition function satisfies $\frac{\partial Z_n}{\partial x_k} = Z_{n-k}$ and for the equipartition model, $\frac{\partial Z_n}{\partial x_k} = \sum_{s\geq 1} x_k^{s-1} Z_{n-ks}$. Suppose, we want the following derivative rule to hold for a model,

$$\frac{\partial Z_n}{\partial x_k} = Z_{n-k}(\mathbf{x}) + x_k Z_{n-2k}(\mathbf{x}) . \tag{5.61}$$

This is like the equipartition rule, only cutoff after two terms. The Gibbs derivative rule could be said to be the equipartition rule, except only cutoff after the first term. In this sense, such a model could be said to interpolate between the Gibbs and equipartition models, and in fact it is for that reason that the rule was proposed. Reviewing the

formalism of the separable model (section 3.2.3) we see that this derivative rule is true for a separable model specified by

$$g_k(n) = \begin{cases} 1 & n = 0, 1 \\ 0 & \text{otherwise} \end{cases} . \tag{5.62}$$

Using $G_j(x) = \sum_n g_j(n)x^n = \frac{\partial}{\partial x} \ln F_j(x)$, this can be true if $F_j(x) = \sum_n f_j(n)x^n = \exp\{x + x^2/2\}$, i. e. if $f_j(n)/n!$ is the number of involutions on n objects. So a weight given by

$$W(\boldsymbol{\pi}) = \prod_j \frac{t_{\pi_j} x_j^{\pi_j}}{\pi_j!} \tag{5.63}$$

lies somewhere between the two models (since $1 \leq t_n \leq n!$) and satisfies equation (5.61). The usefulness of this model as more than a mathematical curiosity is however debatable.

5.8 Counting classes of graphs and digraphs

We have already seen a simple example of the interacting Gibbs model used to describe an ideal interacting Boltzmann gas in section 4.1.2. Here we show an example from pure mathematics that also uses this model. Proofs are not given, but can be found in Tomescu [295] and are in fact simple applications of Burnside's lemma (see page 35).

A *graph* $G = (V, E)$ is a set of vertices V with edges E connecting the vertices. In an *oriented graph* (or *digraph*) the edges have a direction from one vertex to the second (called arcs). A *loop-free* graph is a graph in which there is not more than one path from any vertex to any other vertex. With these definitions we can now introduce the two results.

Theorem 5.8.1 *The number of non-isomorphic loop-free digraphs with n nodes is given by*

$$D_n^{LF} = \sum_{\pi(n)} \left(\prod_{j \geq 1} \frac{1}{(2j)^{\pi_j} \pi_j!} \right) 2^{\sum_{jk} \pi_j \pi_k \gcd(j,k)} . \tag{5.64}$$

Theorem 5.8.2 *The number of non-isomorphic loop-free graphs with n nodes is given by*

$$G_n^{LF} = \sum_{\pi(n)} \left(\prod_{j \geq 1} \frac{1}{j^{\pi_j} \pi_j!} \right) 2^{\frac{1}{2}(\sum_{jk} \pi_j \pi_k \gcd(j,k) - \sum_{j \ odd} \pi_j)} . \tag{5.65}$$

Obviously these are examples of the interacting Gibbs model (section 3.2.4). For loop-free digraphs, the parameters are given by

$$x_j = \frac{2^j}{2j} , \tag{5.66}$$

$$y_{jk} = 4^{\gcd(j,k)} , \tag{5.67}$$

and for loop-free graphs, the parameters are given by

$$x_j = \begin{cases} \frac{2^{(j-1)/2}}{j} & j \text{ odd} \\ \frac{2^{j/2}}{j} & j \text{ even} \end{cases} , \tag{5.68}$$

$$y_{jk} = 2^{\gcd(j,k)} . \tag{5.69}$$

Table 5.2 lists these numbers for $n \leq 12$, which were obtained by direct evaluation of the above identities. Since no method better than direct enumeration is known for interacting models, we do not pursue these models further.

Table 5.2: The number of non-isomorphic loop free graphs and digraphs for $n = 1(1)12$.

n	G_n^{LF}	D_n^{LF}
1	1	1
2	2	3
3	4	16
4	11	218
5	34	9608
6	156	15 40944
7	1044	8820 33440
8	12346	179 33591 92848
9	2 74669	13 02795 68243 99552
10	120 05168	3 41260 43195 29725 80352
11	10189 97866	3 25229 09385 05588 61111 97440
12	16 50911 72592	11 36674 54308 25400 57443 38940 04224

Chapter 6

Thermodynamics of nuclear fragmentation

Under excitation from sufficiently energetic heavy-ion or proton collisions, nuclei fragment into a collection of isotopes which are not directly related to the parent nuclei. Unlike the usual picture of direct reactions of nuclei fissioning into products with strict branching ratios for the expected products, an increase in beam energy causes the products to be a mixed collection of seemingly unpredictable isotopes, known as complex fragments. Experimentally, these events were observed in the 1950s [116], but there was little interest in these now termed intermediate energy events until the early 1980s when the availability of higher energy beams and better detectors sparked a renaissance in experimental work [105,221]. Today, a number of experimental groups routinely collect fragmentation data using sophisticated 4 π detectors[1] which allow much of the fragmentation event to be reconstructed, such as ALADIN [150,241] and FOPI [9,145] at GSI, MINIBALL [236] at Michigan State, AMPHORA [76] at Grenoble, INDRA [43,265] at GANIL, and FOBOS at Dubna.

The improved experimental situation has encouraged substantial theoretical research, and a number of theoretical models have competed to explain the experiments. These models can roughly be grouped into two categories, namely statistical and dynamical. Statistical theories attempt to explain the outcome as the statistical equilibrium or steady-state of some process which itself might not be specified. For example, many models assign probabilities for the emission of fragments based on thermodynamic arguments. Dynamical theories attempt to model the outcome by directly simulating the dynamics of colliding nuclei, i.e. by simulating the process itself. The nucleons

[1] 4 π corresponds to the surface angle covered, i.e. fragments emitted at all angles are detected in a 4 π detector.

are assumed to obey some particular transport theory, such as the Boltzmann-Uehling-Uhlenbeck equation.

This chapter explores the statistical point of view for this phenomenon.[2] After the collision the excited hadronic matter expands until the fragments "freeze-out" from the heated matter. It is assumed that the final configuration of the nucleons is due to a statistical fragmentation process occurring at or near the freeze-out density and temperature. Certainly the validity of this assumption is questionable[3], since there is little time for an equilibrium to be established, but the results of the analysis are sufficiently good to suggest that the statistical approach is not without merit, and it is possible to assume that the distribution of fragments due to another non-equilibrium process may be similar. In other words, this chapter treats the detailed mechanism of the disassembly of nuclear matter as perhaps inaccessible, but assumes it can be approximated by some equilibrium process.

Section 6.1 discusses early attempts to model nuclear fragmentation using statistical models dating back to the early 1980s. Although some of these models were abandoned, key concepts were introduced which continue to be relevant today. Section 6.2 discusses mass (6.2.1) and isotopic yields (6.2.2) from nuclear fragmentation experiments and theories. Relatively simple vector Gibbs models are shown to be able to explain the general features of the experimental yield curves. Furthermore, the models can often be reduced to the simpler integer partition models. This simplification, though not strictly needed, simplifies future discussions about phase transitions and thermodynamic properties, and connects this theory to sampling theories from population genetics. Section 6.3 discusses the thermodynamic aspects of one class of models, determining explicit formulas for the thermodynamic functions, such as the internal energy and specific heat (6.3.1), the pressure and compressibility (6.3.2) and the entropy and thermodynamic potentials (6.3.3). Section 6.4 explores the various phase-transitional regions of the model, distinguishing the liquid-gas transition (6.4.1) from Bose-Einstein condensation

[2]For some dynamical points of view, see J. Aichelin [2] and S.R. Souza, *et al.* [277].

[3]Indeed, some researchers claim that there is significant evidence for "multifragmentation", the non-binary simultaneous fragmentation of nuclei. The assumption of thermalization still has many adherents though, see S.J. Yennello *et al.* [315] for example, for experimental evidence.

(6.4.2) and percolative transitions (6.4.3). Section 6.4.3 in fact compares this Gibbs approach with results from three dimensional bond percolation theories, which is a popular model used to explain current experimental data. Remarkably, the Gibbs model reproduces some of the best features of the percolation theories, and arguably can reproduce mass yield data better. Section 6.5 sketches how to apply fragmentation concepts to the higher energy states in which particle production becomes an issue. Although there is an explosion in the number of possible final states, many of the methods used in fragmentation theory can be applied to this case.

6.1 A short history of statistical nuclear fragmentation

Statistical approaches to nuclear physics have a long history with the compound nucleus model of Niels Bohr (1936) [30], the evaporation model of Victor F. Weisskopf (1937) [307], the multiparticle production models of Enrico Fermi (1950) [97] and Lev Landau (1953) [180] and the statistical fission model of Peter Fong (1956) [113–115] all having substantial statistical foundations. Thermodynamic approaches have also enjoyed some early success, such as the phenomenological liquid-drop approach to excitation energies of W. Stocker and J. Burzlaff(1974) [282], the quasiparticle approach of W.A. Küpper, G. Wegemann and E.R. Hilf (1974) [177] and the Hartree-Fock approach of G. Sauer, H. Chandra and U. Mosel(1976) [267]. The application of statistical and thermodynamic concepts to nuclear fragmentation, the central phenomenon of interest in this dissertation, is more recent. Aram Mekjian in 1977 introduced the first statistical model for high-energy collisions [210, 211, 213, 70] which is principally applicable at small excitation energies where the law of mass action can be reasonably applied. It's principal feature was the assumption that for central collisions the nucleus should be sufficiently excited to make a statistical and thermodynamic approach to the phenomenon reasonable.

Mekjian's model suggested the essential features of nuclear collisions can be successfully contained in a statistical framework, and other physicists soon proposed similar models. G. Röpke, L. Münchow and H. Schulz proposed a similar approach in 1982 [261, 268] including effects due to the Mott transition where the bound states

of nuclei disappear. Jørgen Randrup and Steve Koonin [248,174] in 1981 expanded on Mekjian's model, introducing a grand canonical model of infinite nuclear matter relevant at somewhat higher excitation energies, and G. Fái and J. Randrup [96,247] refined and extended this model.

The fact that nuclear matter is finite however was not addressed in these early models. G. Fái, J. Randrup and J.A. Lopez [193,194] incorporated such restrictions into the earlier models, and two other competing models of similar sophistication and intent were introduced in 1982-83 and refined in later years, one by the Copenhagen group[4] [36–38,17] of J.P. Bondorf and collaborators, the other by the Berlin group[5] [129, 130,317,318] of D.H.E. Gross and collaborators. These models incorporate as much of the detailed physics about nuclei as possible, and require Monte Carlo sampling to analyze. They are in many ways the direct descendents of Fong's fission model, and are quite successful in predicting many features of nuclear fragmentation.

Around 1984, these existing models were supplemented by a new approach based on dynamical transport theories. These are mean field theories which vary in particular assumptions, but all try to simulate the collisions and learn details about some of the their dynamical features, especially the type of momentum flow. They are identified by the specific transport model they are based on, such as the Boltzmann-Uehling-Uhlenbeck (BUU) equation [297] proposed for nuclear fragmentation by G.F. Bertsch, S. Das Gupta and H. Kruse [27] and investigated by them and others [3,118,121,19, 188]. Other schemes include the the Vlasov-Uehling-Uhlenbeck (VUU) approach of H. Kruse, B.V. Jacak and H. Stöcker [176,303], the Landau-Vlasov (LV) approach of B. Rémaud *et al.* [253,124], the Boltzmann-Langevin (BL) approach of S. Ayik and C. Grégoire [15,16] which includes the effects of fluctuations [249,246,45,44,64,285, 319] and the Boltzmann-Nordheim-Vlasov (BNV) equation [233] of A. Bonasera and F. Gulminelli [31,32]. Quantum molecular dynamics (QMD) proposed by J. Aichelin *et al.* is a related dynamical theory [262,8,7,4,2] that has also received significant attention.

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[4]Niels Bohr Institute in Copenhagen.

[5]Hahn-Meitner Institute in Berlin

The minimal information approach, introduced by J. Aichelin and J. Hüfner [5, 151], in 1984 is another approach which tried to simplify some of the features of the existing models. It was shown by them [6] and independently by L.G. Sobotka and L.G. Moretto [276] to be equivalent to an equipartition model. It was motivated by a belief that some aspects of the physics could be understood by a relatively simple model, which directly contrasts the approaches taken before then. They assumed that the final state had a minimal information or equivalently a maximal entropy content. Further details can be found in section 5.6. Kim Sneppen [274] extended this approach to account for the distinguishability of protons and neutrons, and interest in this model has never entirely disappeared [95,275]. These models are interesting but unfortunately do not explain the experimental data very well. However, the idea of modeling the process statistically with a simplified weight scheme determined by some physical or mathematical argument is an appealing one, and is partly adopted here.

Another minimalist approach, percolation theory, was introduced in 1985 by Xavier Campi and J. Desbois [49, 46, 75, 74] and W. Bauer *et al.* [21, 22, 20] and is still used today in analyzing experimental data [120]. In this approach the fragmentation of nuclei occurs on a 3D lattice. Each bond connecting adjacent lattice sites is broken with probability p and the resulting connected groups of nucleons form the final clusters. Although exceedingly simple, this model agrees substantially with experimental data and contains several features which appeal to nuclear physicists, for example a power law in the fragment distribution appearing at a critical point p_c. Furthermore, the model has been studied extensively by statistical physicists as it is a close cousin to the Ising model and is one of the simplest systems which exhibits critical behavior.

The approach adopted here is to apply the canonical Gibbs model to nuclear fragmentation. This is principally minimalist, but closer in spirit to the equipartition model of Aichelin and Hüfner than to the percolation model of Campi, Desbois and Bauer. However, the model can be expanded to include the same detailed physical assumptions of the Copenhagen and Berlin models, and still remain exactly solvable.[6] A.J.

[6]Some aspects of these models break the simple solvable methods discussed in chapter three. Instead, the models need to be decomposed into well behaved partition classes, solved there, and then the

Cole *et al.* [66,65] in 1989 introduced the Gibbs model in the context of nuclear fragmentation. They discovered it could explain all the current experimental data on mass yields if one chose the parameter vector x_k a posteori. This however is not surprising, since there are $A-1$ independent parameters and $A-1$ independent yield points. A.Z. Mekjian [215] independently introduced a Gibbs model of nuclei in 1990 with the a priori chosen parameter vector $x_k = x/k$, arguing it has the qualitatively correct behavior with x a single parameter describing the degree of fragmentation. This model was motivated additionally by its "critical" point[7] $x_c = 1$ at which the cluster size distribution is a perfect power law, $\langle \pi_k \rangle_A = 1/k$. Early fragmentation experiments showed power-law distributions, and such distributions were argued to evidence a phase transition in nuclear matter. This model was extensively developed and analyzed by him and S.J. Lee in a series of papers [214,217,216,182,184,183] which explored various properties and remarked on the models' appearance also in population genetics (cf. section 5.4). Later papers by them have specialized on scaling laws and self-similarity [218,185,186].

Detailed quantitative predictions of this model are at a variance with current experiments, and as such the more general canonical Gibbs model with $x_k = x/k^\tau$ and $\tau \approx 2.5$ has been investigated [59,61] in an effort to improve on the quantitative predictions and introduce a true phase transition into the model. It is this model that is explored in this chapter, with particular attention to the thermodynamic dependence of the the parameters.

6.2 Charge, mass and isotopic fragmentation yields

This section explores the simplest aspect of nuclear fragmentation processes, namely the charge, mass and isotopic yields. These were the first quantities to be studied

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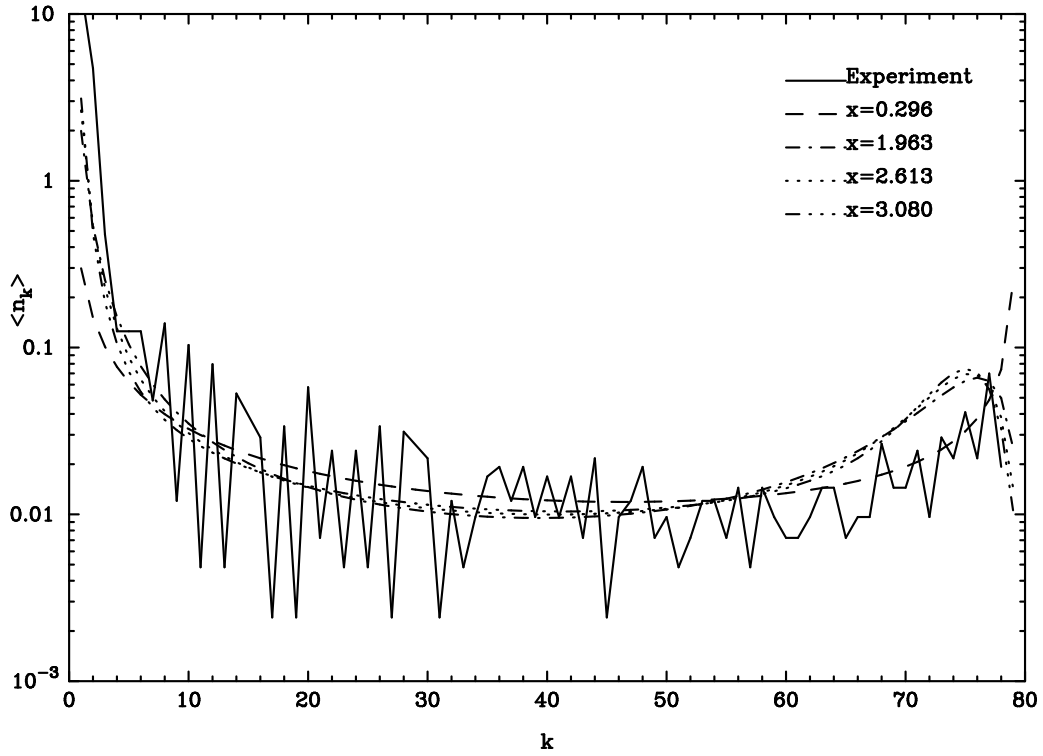
solutions need to be convolved together. Nonetheless, this can still be done without any approximations being made in the canonical ensemble.

[7] This model has no zeroes of its partition function encroaching the positive x axis in the large A limit, and therefore can have no real critical point or associated phase transition. However, oftentimes in the literature the appearance of a power-law behavior in the cluster size distribution is termed a "critical" point, but this should not be confused with the critical point of a phase transition.

6.2.1 Charge yields in theory and experiment

Figure 6.1: Experimental and theoretical predictions for mass yields $\langle \pi_k \rangle_Z$ vs. k for various Gibbs models for the fragmentation of $^{192}_{79}$Au nuclei at 0.99 GeV/nucleon. Table 6.1 has detailed information on the parameter vectors used.



Nuclear fragmentation has a characteristic mass yield distribution which is met generically by only a few of the above models. For the experiment we will analyze, $k\langle \pi_k \rangle_Z$ drops, then rises. This suggests models with $x_k = x/k^\tau$ with $\tau > 1$ might be satisfactory if one x is used. Models with two or more x's are considered in [182,184,183]. The large k behavior is somewhat indeterminate. It could be rising or falling; there are not enough events to determine the behavior accurately.

This parameter vector with another choice for x could also be used as a model for fragmentation, suggesting a parallel between fragmentation and Bose-Einstein condensation. In Bose systems, however, the "clustering" occurs in momentum space, not in real space. For example, the formation of the large $k = n$ cluster in a fragmentation process has its analog in the Bose condensation into the ground state in momentum space.

Table 6.1: Fits of experimental data for the fragmentation of $^{192}_{79}$Au nuclei at 0.99 GeV/nucleon to various Gibbs models

x_k	x	a	τ	σ^2
x/k	0.296	n/a	n/a	78.58
x/k^τ	1.895	n/a	1.817	63.10
$x(a/k+(1-a)/k^\tau)$	0.93745	0	1.5	65.61
$x(a/k+(1-a)/k^\tau)$	1.96263	0.0587	2	62.34
$x(a/k+(1-a)/k^\tau)$	2.61313	0.0747	2.5	61.55
$x(a/k+(1-a)/k^\tau)$	3.0803	0.0732	3	62.20

Fits were made to $\ln\langle\pi_k\rangle_Z$, dropping from the experimental distribution any $\langle\pi_k\rangle_Z$ that were zero due to insufficient statistics. A previous paper [217] showed that for $x = 0.3$, the $x_k = x/k$ model gives a fairly good fit. Here, we consider the models which parallel models in other areas of physics. Specifically, $x_k = x/k^\tau$ is considered in analogy with the Bose gas in $d = 2(\tau - 1)$ dimensions as well as in analogy with various Markov process models. Also, $x_k = x(a/k + (1-a)/k^\tau)$, with various τ is considered in analogy with Feynman's model for the λ transition in liquid helium [100, 102]. The results are shown in Table 6.1, and in figure 6.1. For some choice of τ, x, and a, each of these models produced reasonable fits of the data, and appear to be better than the simple $x_k = x/k$ model, which predicts too small a number of light fragments.

How well these proposed models actually fit some experimental data obtained from heavy ion collider experiments [305]? Data obtained from emulsion experiments for $^{197}_{79}$Au at 0.99 GeV/nucleon. 415 events were recorded and identified by the charges of the fragments, i.e. each event is represented by $\mathbf{n} = (n_1, \ldots, n_{79})$ where n_z represents the number of fragments with charge z in a given event. Ensemble averages were obtained by averaging over all events.

Since the experimental method measured only the electric charge of fragments leaving the collision, there is some question about how applicable are models developed considering only nucleons with no separation into protons and neutrons. Since the nuclear force treats protons and neutrons nearly identically, and the models proposed derived from a combinatorial viewpoint, the models should be identical whether one includes the neutrons or not. In fact, it can be shown (next section) that for the simple

$x_k = x/k$ model, the results are the same whether one considers Z nucleons coming out, or whether one considers A nucleons coming out, but only the Z protons can be followed, such that one must sum over the possible neutron configurations to obtain the expectation values.

6.2.2 Isotopic and isobaric yields and equivalences

Nuclear matter fragmenting due to a collision can be considered to be a system with two varieties of indistinguishable particles (protons and neutrons) which forms clusters of arbitrary content and number from the original protons and neutrons. The states are therefore described by vector partitions according to the discussion in section 2.1.1. The number of accessible states for a typical nuclear fragmenting system is extremely large as can be seen from table 6.2. Since it is impractical to construct all the partitions, we should restrict our attention if possible to models which are exactly solvable. Fortunately, as we have seen there are several such models.

Table 6.2: Representative values for $p(Z+N)$ and $p(Z,N)$ for nuclear systems.

Z	N	$p(Z+N)$	$p(Z,N)$
10	10	627	59521
20	20	37338	3026 73029
30	35	20 12558	231 50477 43167
40	50	566 34173	6 00944 62493 61633
50	70	18443 49560	26953 04447 12166 28606

The historical evidence presented in the last chapter strongly suggests a statistical Gibbs model as a candidate for describing such excited nuclear matter, i.e. assume each possible fragmentation outcome has the statistical weight

$$W(\boldsymbol{\pi}) = \prod_{jk} \frac{x_{jk}^{\pi_{jk}}}{\pi_{jk}!} \; . \tag{6.1}$$

Section 3.2.1 detailed the solution of this model which originally appeared in [58]. Since there is a Markov process (see section 4.2.1) that yields this weight which is a possible picture of the dynamics of nuclear fragmentation, we can be confident that this weight is not unreasonable, and at least represents an approximation to the actual physics.

In principle, if nuclear systems were governed exactly by the above model, a series of experiments could be done to determine the parameters x_{jk}. However, current experiments are sensitive to only some of the parameters. Each fragmentation event is often not fully reconstructed since experimental detectors are often insensitive to some of the degrees of freedom. For example, many experiments detect only the charge, not the mass of the final fragments. In this case, the isotopic degrees of freedom are averaged over by the experiments[8], and the final states appear as integer partitions of Z, the total charge of the system. Typically, it is assumed that in this process the structure of the weight is not affected even though isotopic information has been lost. That is, the Gibbs structure we expect for the isotopic states is maintained for the averaged states. This is a precarious assumption and one which is indeed invalid for a number of choices of x_{jk}. However, we shall see that this assumption can be justified in a number of cases we will be interested in.

As mentioned in section 2.1.2, two-component models are sometimes equivalent to one-component models. A two-component model is said to be *isotopically equivalent* to a one-component model if for every function $f(\boldsymbol{\pi})$, the one-component ensemble average

$$\langle f \rangle_Z = \sum_{\pi(Z)} f(\boldsymbol{\pi}) P_Z(\boldsymbol{\pi}) \tag{6.2}$$

is equal to the two-component ensemble average

$$\langle f \rangle_{ZN} = \sum_{\pi' \in \pi(Z,N)} f(\boldsymbol{\pi}(\boldsymbol{\pi}')) P'_{ZN}(\boldsymbol{\pi}') \ , \tag{6.3}$$

where $\pi_j(\boldsymbol{\pi}') = \sum_{k=0}^{N} \pi'_{jk}$. For example, $\langle \pi_j \rangle_Z = \sum_{k=0}^{N} \langle \pi_{jk} \rangle_{ZN}$ must hold if two models are considered to be isotopically equivalent. This is true if and only if

$$P_Z(\boldsymbol{\pi}) = \sum_{\boldsymbol{\pi}' \to \boldsymbol{\pi}} P'_{ZN}(\boldsymbol{\pi}') \ , \tag{6.4}$$

where $\boldsymbol{\pi}' \to \boldsymbol{\pi}$ denotes all partition vectors $\boldsymbol{\pi}' \in \pi(Z,N)$ such that $\pi_j = \sum_{k=0}^{N} \pi'_{jk}$.

If we consider deriving the models over the permutation group, we can define the notion of *permutation equivalence* of $P'_{Z'N'}(p')$ to $P_{ZN}(p)$ by the condition

$$P_{ZN}(p) = \sum_{p' \in S_{Z'+N'}(p)} P'_{Z'N'}(p') \ , \tag{6.5}$$

[8]Sometimes this is termed "coarse graining" in the literature.

where $Z' \geq Z$, $N' \geq N$ and $S_{Z'+N'}(p)$ is the set of all permutations $p' \in S_{Z'+N'}$ which give p by the following construction. Decompose p' into its cycle representation. Eliminate the numbers $Z+1, \ldots, Z'$ and $Z'+N+1, \ldots, Z'+N'$ from the cycles. Renumber the elements $Z'+1, \ldots, Z'+N$ as $Z+1, \ldots, Z+N$ to recover the permutation in S_{Z+N}. In other words, if k is an element to eliminate, find j such that $p_j = k$, and modify the permutation vector so that $p_j = p_k$. This removes the element from the permutation. Do this for all the numbers to eliminate, resulting in a new permutation isomorphic to a permutation in S_{Z+N}. For example, $p' = (1,5)(3)(4,6,2) \in S_6$ becomes $(1,5)(4,2)$ by eliminating $3,6$. After renumbering this becomes $p = (1,4)(2,3) \in S_4$.

Permutation equivalence of the weights $P'_{ZN}(p')$ to $P_{Z0}(p)$ implies isotopic equivalence of the weights $\mathrm{Perm}(\boldsymbol{\pi}'(p'))P'_{ZN}(\boldsymbol{\pi}'(p'))$ to $\mathrm{Perm}(\boldsymbol{\pi}(p))P_{Z0}(\boldsymbol{\pi}(p))$, assuming the permutation weights are only functions of $\pi(p)$, i.e. all permutations which have the same partition configuration or cycle decomposition have the same weight. One particular permutation weight which satisfies this condition is the unnormalized weight $W_{ZN}(p, \mathbf{z}) = \prod_{jk} z_{jk}^{\pi_{jk}(p)}$. We will now show that this weight with $A = Z+N$ is permutationally equivalent to the $Z, N+1$ weight with the same z_{jk} if $z_{jk} = z_j$. This implies by induction that the $Z0$ model is permutationally equivalent to the ZN model, and therefore the two weights corrected by the Cauchy factor are isotopically equivalent.

For any permutation $p \in S_A$, there are $A+1$ permutations in $S_{A+1}(p)$. One of these permutations has the element $A+1$ in its own cycle. It has weight $W_{Z,N+1}(p', \mathbf{z}) = W_{ZN}(p, \mathbf{z}) z_{01}$. A of the permutations are hybrids, with the extra element combined with a cycle from p. Suppose the element is in a cycle of j neutrons, k protons. The weight of that cycle is $W_{Z,N+1}(p', \mathbf{z}) = W_{ZN}(p, \mathbf{z}) z_{j,k+1}/z_{jk}$, since the introduction of the additional element has reduced π_{jk} by one, but increased $\pi_{j,k+1}$ by one. There are $j+k$ possible places for the element to be inserted into that cycle, and there are π_{jk} cycles of that type it can combine with. So the following is true

$$\sum_{p' \in S_{A+1}(p)} \frac{W_{Z,N+1}(p')}{W_{ZN}(p)} = z_{01} + \sum_{jk} f_{jk} \pi_{jk} \ , \tag{6.6}$$

where $f_{jk} = (j+k) z_{j,k+1}/z_{jk}$. If z_{jk} is independent of k, this reduces to $z_{01} + N + Z$. In this case, we can multiply both sides of the equation by $W_{ZN}(p)$ and sum over $\forall p \in S_A$

to arrive at

$$Z_{Z,N+1}(\mathbf{z}) = Z_{ZN}(\mathbf{z})(z_{01} + Z + N) \; . \tag{6.7}$$

This implies equation (6.5) when substituted back into equation (6.6). So under these conditions, P_{ZN} is equivalent to $P_{Z,N+1}$. Therefore, P_{Z0} is equivalent to P_{ZN} by induction and transitivity, and the one component weight is equivalent to the two component weight for x_{jk} given by

$$x_{jk} = x_j \binom{j+k-1}{k} \; . \tag{6.8}$$

The partition function for this two-component model is

$$Z_{ZN}(\mathbf{x}) = \frac{\Gamma(z_{01} + Z + N)}{\Gamma(z_{01} + Z)} Z_Z(\mathbf{x}) \; . \tag{6.9}$$

Notice that at no point was it asserted that these are the only two-component models that are isotopically equivalent to the one-component models. In the previous discussion, the key property was the independence of $\sum_{jk} f_{jk}\pi_{jk}$ from $\boldsymbol{\pi}$. Perhaps we could satisfy this with choices other than $f_{jk} = j + k$. In fact, it can be proven that this condition is satisfied only by $f_{jk} = \alpha Aj/Z + (1-\alpha)Ak/N$ where α is arbitrary. However, $\alpha \in [0,1]$ to guarantee non-negative probabilities in the statistical model. Given z_{j0}, we could then construct permutationally equivalent two-component models specified by α and the recursion relation

$$z_{j,k+1} = z_{jk} \frac{A}{j+k} \left(\alpha \frac{j}{Z} + (1-\alpha)\frac{k}{N} \right) \tag{6.10}$$

and evaluate the equivalent partition weights using equations (6.1) and (2.38).

If we require that the models be isotopically equivalent for any choice of N, these are the only models given by equations (3.25) and (6.1) that are isotopically equivalent. This is true because isotopic equivalence for any N implies permutation equivalence of N to $N+1$. Permutation equivalence requires $\sum_{jk} f_{jk}\pi_{jk}$ to be independent of $\boldsymbol{\pi}$, which can be shown to be true only if z_{jk} is of the form given above. Notice that this condition is very similar to Kingman's non-interference condition on one-component partition weights [169, 170]. We require that the neutrons do not "interfere" with the

overall proton distribution, just as in one-component models Kingman required that the removal of one gene type does not interfere with the probability structure of the original set of objects.

This technique can be generalized to construct an $s+1$-component model that is equivalent to an s-component model. For example, if the s-component weight is given by equation (3.37), then an equivalent $s+1$-component model is given by the parameter vector defined by

$$x_{k_1 \ldots k_{s+1}} = x_{k_1 \ldots k_s} \binom{\sum_{j=1}^{s+1} k_j - 1}{k_{s+1}} . \tag{6.11}$$

These results provide a simple way of constructing two-component models from the one-component models explored in earlier papers. For example, one could apply equations (6.8) and (6.9) to the chain model, $x_j = x$, to construct a two-component extension of the chain model as developed by D.H.E. Gross *et al.* [125].

Above, a set of conditions for isotopic equivalence was derived. Under these conditions, a two-component model reduces to a one-component model with a similar structure when a summation over isotopes is performed. The complementary notion of isobaric equivalence is treated now, in which a summation over isotopes is replaced with a summation over isobars (fragments of the same mass).

A two-component model is said to be *isobarically equivalent* to a one-component model if for every function $f(\boldsymbol{\pi})$, the one-component ensemble average

$$\langle f \rangle_{Z+N} = \sum_{\pi(Z+N)} f(\boldsymbol{\pi}) P_{Z+N}(\boldsymbol{\pi}) \tag{6.12}$$

is equal to the two-component ensemble average

$$\langle f \rangle_{ZN} = \sum_{\pi' \in \pi(Z,N)} f(\boldsymbol{\pi}(\boldsymbol{\pi}')) P'_{Z,N}(\boldsymbol{\pi}') , \tag{6.13}$$

where $\pi_i = \sum_{i=j+k} \pi'_{jk}$. For example, $\langle \pi_i \rangle_{Z+N} = \sum_{i=j+k} \langle \pi_{jk} \rangle_{ZN}$ must hold if two models are considered to be isobarically equivalent. This is true if and only if

$$P_{Z+N}(\boldsymbol{\pi}) = \sum_{\boldsymbol{\pi}' \to \boldsymbol{\pi}} P'_{ZN}(\boldsymbol{\pi}') , \tag{6.14}$$

where $\boldsymbol{\pi}' \to \boldsymbol{\pi}$ denotes all partition vectors $\boldsymbol{\pi}' \in \pi(Z,N)$ such that $\pi_j = \sum_{k=0}^{Z} \pi'_{k,j-k}$.

Let the unnormalized one-component and two-component weights be Gibbs weights specified by x_j and x_{jk}, i.e. $W_{Z+N}(\boldsymbol{\pi}) = \prod_j x_j^{\pi_j}/\pi_j!$, $W'_{ZN}(\boldsymbol{\pi}) = \prod_{jk} x_{j,k}^{\pi_{jk}}/\pi_{jk}!$, and let Z_{Z+N}, Z_{ZN} denote their partition functions. Suppose that the parameters are given by

$$x_{jk} = \binom{j+k}{j} x_{j+k} \ . \tag{6.15}$$

Evaluating the RHS of equation (6.14) in this case is relatively uncomplicated.

$$\begin{aligned}
\sum_{\pi' \to \pi} P'_{ZN}(\boldsymbol{\pi}') &= \sum_{\pi' \to \pi} \mathrm{Perm}(\boldsymbol{\pi}')^{-1} \sum_{p \to \pi'} P'_{ZN}(\boldsymbol{\pi}'(p)) \\
&= \frac{1}{Z!N!Z_{ZN}} \sum_{\pi' \to \pi} \sum_{p \to \pi'} \prod_{jk} ((j+k)x_{j+k})^{\pi'_{jk}} \\
&= \frac{1}{Z!N!Z_{ZN}} \sum_{\pi' \to \pi} \sum_{p \to \pi'} \prod_{j} (jx_j)^{\sum_k \pi'_{k,j-k}} \\
&= \frac{1}{Z!N!Z_{ZN}} \sum_{p \to \pi} \prod_{j} (jx_j)^{\pi_j} = \frac{1}{Z!N!Z_{ZN}} \mathrm{Perm}(\boldsymbol{\pi}) \prod_j (jx_j)^{\pi_j} \\
&= \binom{Z+N}{Z} \frac{1}{Z_{ZN}} \prod_j \frac{x_j^{\pi_j}}{\pi_j!} = \binom{Z+N}{Z} \frac{Z_{Z+N}}{Z_{ZN}} P_{Z+N}(\boldsymbol{\pi}) \ .
\end{aligned} \tag{6.16}$$

Theorem 4.1.3 applied to this case shows that

$$Z_{ZN} = \binom{Z+N}{Z} Z_{Z+N} \ . \tag{6.17}$$

so equation (6.14) holds.

Notice that applying this identity to $x_k = x/k$ gives the same result as the two-component generalization based on isotopic equivalence. In other words, this particular bipartite model is both isobarically and isotopically equivalent to the same integer partition model. This property is probably unique to this model, and as such, recalls work by J.F.C. Kingman [167–172] on the integer partition model, who showed that it is the unique weight satisfying two conditions, a non-interference condition and a sampling condition.

The two-component analogs of one-component models given by equation (6.10) could be taken as the starting point for a fully isotopic model of fragmentation. These models would contain no surprises in their one-component expectation values, and would provide predictions for the isotopic behavior.

This is perhaps too strong a requirement. Equation (6.10) constrains the set of possible partition weights, forbidding a number of physically interesting choices for x_{jk}.

For example, if the symmetric term $\exp\{-\alpha_s(j-k)^2/(j+k)\}$ appeared in the parameter z_{jk}, the resulting parameter vector could never satisfy equation (6.10). Since such a symmetry term should appear due to the symmetry term in the binding energy of nuclei, we should not expect realistic models to be isotopically equivalent to the models considered in earlier papers.

With that in mind, we start with a simplified model of nuclear fragmentation specified by the following choice for x_{jk}

$$x_{jk} = \frac{x}{(j+k)^\tau}\binom{j+k}{j}\exp\left\{-\frac{\alpha_s(j-k)^2}{j+k}\right\} . \tag{6.18}$$

We will find it appropriate sometimes to modify this when $j+k=1$, i.e. to avoid the exponential suppression factor $e^{-\alpha_s}$ for monomers. Let us specialize to the case $\tau = 1$ and consider the limiting cases. When $\alpha_s \to 0$, the model becomes the two-component analog of the model $x_k = x/k$, which has a closed-form solution.

$$Z_A(x) = \binom{x+A-1}{A} . \tag{6.19}$$

When $\alpha_s \to \infty$, x_{jk} is proportional to a Kronecker delta function and the model reduces explicitly to the one-component model specified by parameters

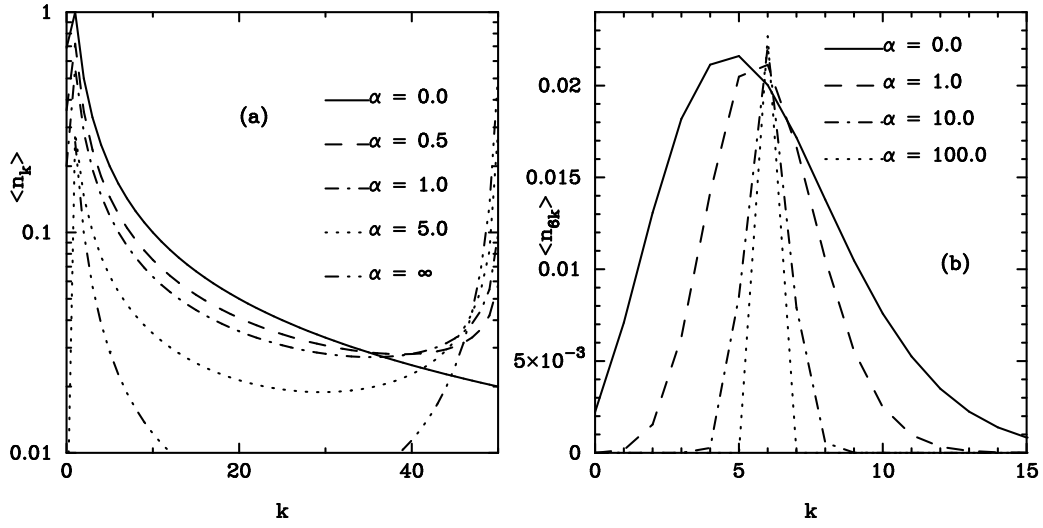
$$x_k = \frac{x}{2k}\binom{2k}{k} , \tag{6.20}$$

where k indexes both proton and neutron number, since only symmetric fragments with $j = k$ are allowed. In this case, the partition function also has a closed-form solution (see equation (4.14))

$$Z_A(x) = \frac{x}{x+2A}\binom{x+2A}{A} . \tag{6.21}$$

Models with intermediate values for α_s are not as simple as these two limits, but can still be computed easily. Figures 6.2, 6.3 show the prediction of this model at $x = 1$ and various α_s for a symmetric case $Z = N = 50$ as well as an asymmetric case $Z = 50$, $N = 75$. These figures display the total charge distribution $\langle \pi_j \rangle_Z = \sum_{k=0}^{N} \langle \pi_{jk} \rangle_{ZN}$, as well as the distribution of isotopes for a particular charge, specifically carbon, i.e. $\langle \pi_{jk} \rangle_{ZN}$ for $j = 6$.

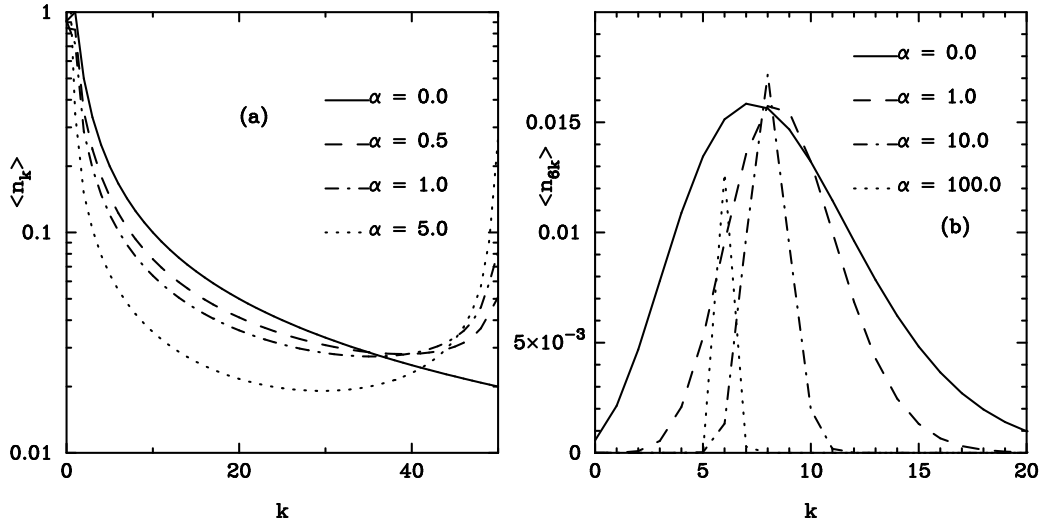
Figure 6.2: Overall (a) and Isotopic (b) distribution of fragments for the Gibbs model specified by equation (6.18) at $Z = 50$, $N = 50$, $x = 1$, $\tau = 1$, and various α_s. Isotopic distribution is for carbon, $Z = 6$.



The total charge distribution figures indicate that increasing α_s increases the number of large fragments. This is due to the exponential suppression of asymmetric fragments, which make up a large fraction of the partition space, especially for smaller fragments. The isotopic distribution figures reveal that the distribution of isotopes is essentially Gaussian. As seen earlier [274,18], an initial asymmetry in the relative numbers of protons and neutrons yields a similar asymmetry in the distribution of fragments. This asymmetry can be diminished by increasing α_s and removing the exponential suppression from monomer parameters (x_{01}, x_{10}), as was done in the figures. Indeed, as $\alpha_s \to \infty$, such a model would allow only symmetric fragments and monomers.

To this simple model, we can add other effects, eventually including all the terms in the semi-empirical mass-formula. For example, nucleon pairing interactions can be added using the term $\exp\{\alpha_p p_{jk}/(j+k)\}$ where p_{jk} is 0 for even-odd nuclei, -1 for odd-odd nuclei, and $+1$ for even-even nuclei. This can be done for all intrafragment interactions. Interfragment interactions do not fit the form of equation (6.1) and must be handled in some kind of mean-field manner in this approach. Coulomb interactions are the only persistent long-range interactions in the thermalized phase. Suppose each fragment interacts with all the others via the Coulomb interaction. This contributes

Figure 6.3: Overall (a) and Isotopic (b) distribution of fragments for the Gibbs model specified by equation (6.18) at $Z = 50$, $N = 75$, $x = 1$, $\tau = 1$ and various α_s. Isotopic distribution is for carbon, $Z = 6$.



an interaction energy given by

$$E_I = \frac{1}{2}\sum_{jklm} \pi_{jk}(\pi_{lm} - \delta_{jl}\delta_{km})E^I_{jklm} \ . \tag{6.22}$$

If we choose $E^I_{jklm} = jre^2/\bar{r}$ for the Coulomb interaction, then

$$E_I = \frac{e^2}{2\bar{r}}(Z^2 - \sum_{jk} j^2\pi_{jk}) \ , \tag{6.23}$$

which suggests we include interfragment Coulomb interactions by appending the term $\exp(\alpha_c j^2)$ to x_{jk}. We can estimate α_c by assuming $\bar{r} \approx V^{1/3} \approx r_0 A^{1/3}$.

6.3 Thermodynamics of fragmenting nuclei

Two fundamental issues are of interest in nuclear fragmentation. At the simplest level, the observed distribution of fragments needs to be explained and related to the beam energy and the size of the initial nuclei. Aspects of this problem were discussed in the previous section. A more fundamental question addressed in this section concerns the thermodynamic aspects of fragmentation. If the process is indeed statistical then nuclear matter is heated by the collision and fragments. The hadronic equation of state (EOS) encapsulates this information, and an understanding of this equation over a range

of temperatures and densities is the aim of much current research in nuclear physics. The current generation of detectors and colliders have provided a wealth of data about the EOS and the next generation, such as the relativistic heavy-ion collider (RHIC) being built at Brookhaven, should introduce even higher densities and temperatures, and potentially new physics such as the hypothesized quark-gluon plasma.

If the statistical models defined in the previous chapter have parameters which depend on thermodynamic variables such as volume and temperature, then there is a range of thermodynamic functions and properties which these models capture. Analyzing these functions is crucial to extend our understanding of the physical properties these models predict. Moreover, the thermodynamic functions are oftentimes the only accessible variables, partition vectors far too often being unavailable in large systems.

Consider the case of a Gibbs model on indistinguishable particles, with parameter vector defined by

$$x_k = x(V,T)y(V,T)^{k-1}b_k \; . \tag{6.24}$$

In this case, the canonical partition function is given by

$$Z_A \;\; = \;\; \sum_{m=0}^{A} Z_A^{(m)}(\mathbf{b})x^m y^{A-m} = y^A \sum_{m=0}^{A} Z_A^{(m)}(\mathbf{b})(x/y)^m \; , \tag{6.25}$$

where $Z_A^{(m)}$ is a function only of the vector $\mathbf{b}$, not of the thermodynamic variables. This specialization of the form of the weight is not completely arbitrary but is motivated by the form of the weight in the cases of a fragmenting nuclear system. Namely, x is determined by kinetic factors, whereas y contains information about the internal excitations. Additionally, the two limiting cases of $x/y \ll 1$ and $x/y \gg 1$ can be analyzed for this form by expanding $\ln Z_A$ in x/y using the various microcanonical partition functions. In the low temperature region, equation (3.36) when corrected for the overall y^A factor in the partition function determines the behavior ($t \to x/y$). In the high temperature region, the high temperature expansion (equation (3.35)) can be similarly used to evaluate thermodynamic functions such as the virial expansion of the equation of state.

Given the partition function, various logarithmic derivatives determine the thermodynamic functions, e.g. $P = -k_B T \frac{\partial}{\partial V} \ln Z_A$. As a result, logarithmic derivatives of

the partition function with respect to the thermodynamic parameters x, y are of great interest. In section 4.3.2 we evaluated such derivatives and showed that

$$x\frac{\partial}{\partial x}\ln Z_A = \langle m\rangle_A \tag{6.26}$$

$$\left(x\frac{\partial}{\partial x}\right)^2 \ln Z_A = \mu_2(m)_A \tag{6.27}$$

where $\mu_k = \langle(m - \langle m\rangle_A)^k\rangle_A$ is the kth central moment of $m = \sum_j \pi_j$. In general, $(x\frac{\partial}{\partial x})^k \ln Z_A(x)$ is the kth cumulant moment of m. The relations for derivatives with respect to y are similar

$$y\frac{\partial}{\partial y}\ln Z_A = A - \langle m\rangle_A \tag{6.28}$$

$$\left(y\frac{\partial}{\partial y}\right)^2 \ln Z_A = \mu_2(m)_A \tag{6.29}$$

$$\left(y\frac{\partial}{\partial y}\right)^3 \ln Z_A = -\mu_3(m)_A\ . \tag{6.30}$$

and in general $(y\frac{\partial}{\partial y})^k \ln Z_A(y)$ is the kth cumulant moment of m times $(-1)^k$.

The choice of x, y and b_k is determined by the physics of the situation. The assumptions we make to determine them are the following:

- The term x^m in the weight comes from phase space factors and translational considerations. Since the partition function of a gas of nucleons is given by $x^A/A!$, with

  $$x = V\left(\frac{2\pi m k_B T}{h^2}\right)^{d/2}\ , \tag{6.31}$$

  (cf. section 5.1), λ_T the thermal wavelength of a nucleon and d the dimensionality of the system ($d = 3$ typically), the equivalent partition function for a gas of nuclear clusters should be proportional to x^m, times some cluster size dependent parameters which can be incorporated into b_k. Since we are interested in the properties of nuclei in their rest frame, not in the lab frame, we want to replace x^m by x^{m-1} since the overall center of mass motion shouldn't contribute to the thermodynamics. In other words, unlike the case of a gas in a container of a particular volume, we can arbitrarily factor out one fragments motion.[9]

[9]Removing the motion of one of the fragments is actually quite necessary for otherwise the model would violate the third law of thermodynamics. Intuitively it is reasonable since the rest frame of the nucleons is the natural frame in which to consider its thermodynamics.

- The term y^{A-m} is due to cluster binding and internal excitations. Suppose the binding energy per nucleon is a_V. Then each cluster of size k requires $a_V(k-1)$ in binding energy. The Boltzmann weight associated with such a binding would then be $e^{E_B/k_BT} = y^{A-m}$ where $y = \exp(a_V/k_BT)$. Internal excitations are expected to modify this binding energy per nucleon, which we model by assuming assuming the nuclear level density given by the Bethe level density formula

$$\rho_A(E) = \frac{\pi^{1/2}}{12E^{5/4}a^{1/4}} \exp(2\sqrt{aE}) \; . \tag{6.32}$$

where a is such that $a\pi^2/6$ is the single particle level density on the Fermi surface. If we integrate this times e^{-E/k_BT} we will get the contribution of these internal excitations to the bulk free energy,

$$F_{\rm int}/A = -W_0 - \frac{(k_BT)^2}{\varepsilon_0} \tag{6.33}$$

where $\varepsilon_0 = (4/\pi^2)\varepsilon_F$ for an ideal Fermi gas. This form for the free energy is known to be good only at low temperatures. S.E. Koonin and J. Randrup [174] have argued that a reasonable correction is to cutoff the Bethe density at high energies, since these high-energy states are of such short lived nature that they shouldn't contribute to the internal partition function. Introducing an exponential cutoff e^{-E/k_BT_0} yields an effective temperature for the internal partition function of $T_{\rm eff}^{-1} = T^{-1} + T_0^{-1}$, where T_0 is the cutoff temperature. Thus T_0 can be interpreted as the maximum temperature attainable by nuclear fragments. Theoretical predictions indicate T_0 should be around 7–12 MeV [34,35,187,226], and we have used the standard value 12 MeV throughout this work. Replacing k_BT with $k_BT_{\rm eff}$ for the internal excitations yields the following form for y.

$$y = \exp\left\{\frac{a_V}{k_BT} + \frac{k_BT}{\varepsilon_0}\frac{T_0}{T+T_0}\right\} \; , \tag{6.34}$$

- The only remaining parameter to set in this model is b_k. We can determine it by requiring that the mass yield distribution at and below criticality be a power law, as is observed in many nuclear fragmentation experiments, cf. J.E. Finn *et al.* [105] and M.L. Gilkes *et al.* [120,88] and is known to happen theoretically in a droplet

model, see Michael E. Fisher [106]. This phenomenological approach suggests $b_k = k^{-\tau}$, with $\tau \approx 2.2$, since it is known that for such a b_k, $\langle \pi_k \rangle \propto b_k$. Such a choice of τ is also suggested by analogy with the ideal Bose gas. If the weight $W(\boldsymbol{\pi})$ from equation (3.25) was for an ideal Bose gas, then [149] $x_k = x/k^\tau + 1/k$, with $\tau = 1 + d/2$. The $1/k$ term arises from the zero momentum states of the Bose condensate, and is irrelevant at high temperatures, but of some importance below the critical point. Since the low temperature behavior we want is essentially Fermi gas like, we can ignore the zero momentum term, which suggests we use $b_k = k^{-1-d/2}$. We choose $\tau = 5/2$ to match the exponent of a Bose gas in three dimensions, but we are free to adjust τ in this model if it is required, unlike in the Bose gas where it is determined by the dimensionality of the system.

Notice the similarity between this model for nuclear fragmentation and the Feynman model for the λ transition (section 5.3). First, the exponent of equation (5.50) is identical to that internal excitation factor y for nuclear fragmentation, up to a numerical constant, if we neglect the cutoff temperature factor ($T_0 \to \infty$) and make substitutions for the density ($A/V \to d^{-3}$) and the thermal wavelength ($\lambda_T \to d$). Second, the overall x_k is the same except for the $1/k$ term which is negligible at large enough x/y. In fact, the modification Feynman makes to x_k might well be motivated in the case of nuclear fragmentation, and we will consider the case $x_k = a/k + (1-a)/k^\tau$ in section 6.2.1.

The general form of the model is exactly as sketched above, but the fact that the parameters a_V and ε_0 are density dependent requires the introduction of some additional physics. We assume that the binding energy per nucleon can be approximated using a Skyrme [273, 302] parameterization, such that $a_V(\rho)$ is given by

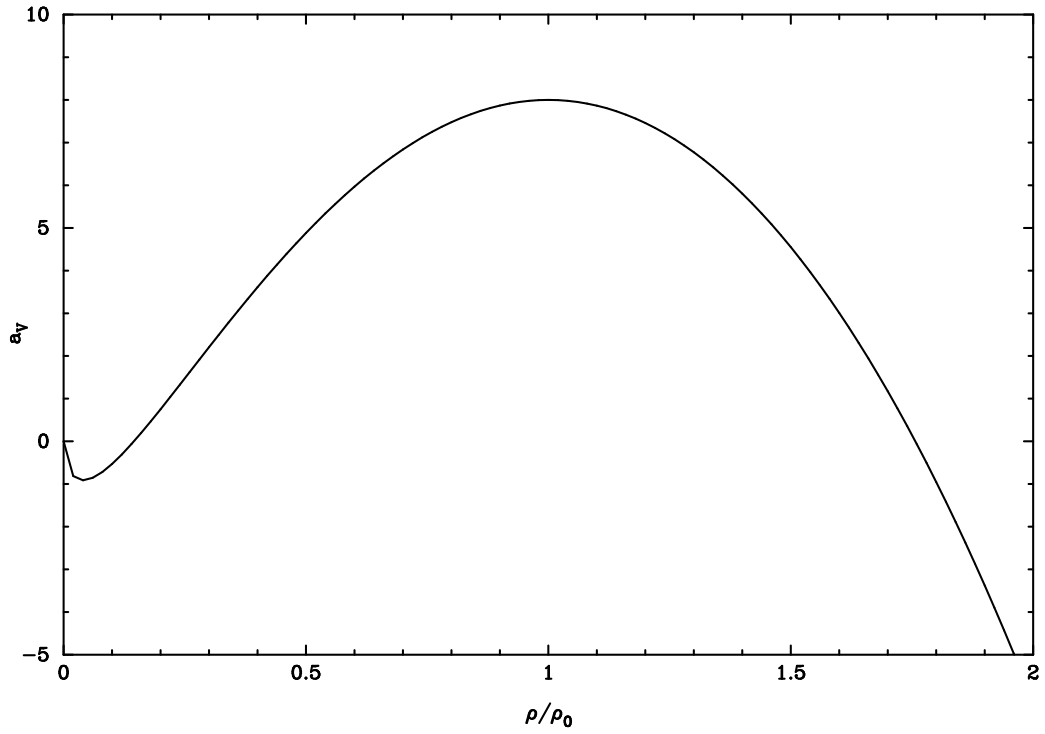
$$a_V(\rho) = -a_D \left(\frac{\rho}{\rho_0}\right)^{2/3} + a_0 \left(\frac{\rho}{\rho_0}\right) - a_3 \left(\frac{\rho}{\rho_0}\right)^{1+\sigma} . \tag{6.35}$$

Similarly, we assume that the level spacing parameter ε_0 varies with the density in proportion to the Fermi energy from which it was originally determined, i.e. for a Fermi gas/liquid, $\varepsilon_0(\rho) = (4/\pi^2)\varepsilon_F(\rho)$ where

$$\varepsilon_F(\rho) = \frac{\hbar^2}{2m}((4\pi)^{d/2}\Gamma(1+d/2)\rho)^{2/d} \tag{6.36}$$

is the Fermi energy for a noninteracting gas. Using $a_D = 3\varepsilon_F(\rho_0)/5$, the Skyrme parameters a_0, a_3 can be determined by requiring that the binding energy per nucleon is a maximum at $\rho = \rho_0$ with the observed value of 8.0 MeV. For $\sigma = 1$, this gives $a_0 = 48.0$ MeV and $a_3 = 16.0$ MeV. Figure 6.4 sketches the density dependence of a_V in this approximation.

Figure 6.4: Binding energy per particle $a_V(\rho)$ in the Skyrme model, with $\sigma = 1$, $a_D = 24$ MeV, $a_0 = 48$ MeV and $a_3 = 16$ MeV.



Given x, y and b_k we have completely specified the model, although various derivatives of x, y will also be needed in determining the thermodynamic behavior. For our purposes, only the first two derivatives are needed, and a quick calculation shows that

$$\frac{T}{x}\frac{\partial x}{\partial T} = \frac{d}{2}\,, \tag{6.37}$$

$$\frac{T^2}{x}\frac{\partial^2 x}{\partial T^2} = \frac{d}{2}\left(\frac{d}{2}-1\right)\,, \tag{6.38}$$

$$\frac{V}{x}\frac{\partial x}{\partial V} = 1\,, \tag{6.39}$$

$$\frac{V^2}{x}\frac{\partial^2 x}{\partial V^2} = 0\,, \tag{6.40}$$

and

$$\frac{T}{y}\frac{\partial y}{\partial T} = -\frac{a_V}{k_B T} + \frac{k_B T}{\varepsilon_0}\left(\frac{T_0}{T+T_0}\right)^2 , \tag{6.41}$$

$$\frac{T^2}{y}\frac{\partial^2 y}{\partial T^2} = \frac{2a_V}{k_B T} - \frac{2k_B T}{\varepsilon_0}\frac{TT_0^2}{(T+T_0)^3} + \left(\frac{T}{y}\frac{\partial y}{\partial T}\right)^2 , \tag{6.42}$$

$$\begin{aligned}\frac{V}{y}\frac{\partial y}{\partial V} &= \frac{2}{3}\frac{a_D}{k_B T}\left(\frac{\rho}{\rho_0}\right)^{2/3} - \frac{a_0}{k_B T}\left(\frac{\rho}{\rho_0}\right) + (1+\sigma)\frac{a_3}{k_B T}\left(\frac{\rho}{\rho_0}\right)^{1+\sigma} \\ &\quad + \frac{2}{3}\frac{k_B T}{\varepsilon_0}\left(\frac{T_0}{T+T_0}\right) ,\end{aligned} \tag{6.43}$$

$$\begin{aligned}\frac{V^2}{y}\frac{\partial^2 y}{\partial V^2} &= -\frac{10}{9}\frac{a_D}{k_B T}\left(\frac{\rho}{\rho_0}\right)^{2/3} + \frac{2a_0}{k_B T}\left(\frac{\rho}{\rho_0}\right) - (1+\sigma)(2+\sigma)\frac{a_3}{k_B T}\left(\frac{\rho}{\rho_0}\right)^{1+\sigma} \\ &\quad - \frac{2}{9}\frac{k_B T}{\varepsilon_0}\left(\frac{T_0}{T+T_0}\right) + \left(\frac{V}{y}\frac{\partial y}{\partial V}\right)^2 .\end{aligned} \tag{6.44}$$

6.3.1 Internal energy and specific heat

We begin our investigation of thermodynamic functions with the internal energy and specific heat, which are related to the partition function by $U = k_B T^2 \frac{\partial}{\partial T} \ln Z_A$, $C_V = \left(\frac{\partial U}{\partial T}\right)_V$. These functions are physical manifestations of the effect of temperature changes on the system. Given these formulae, the determination of thermodynamic quantities can be reduced to a computation of the cumulant moments of the fragmentation multiplicity $m = \sum_j \pi_j$ and some derivatives of the thermodynamic parameters x, y. The result for x, y in general is

$$\frac{U}{k_B T} = (\langle m\rangle_A - 1)\frac{T}{x}\frac{\partial x}{\partial T} + (A - \langle m\rangle_A)\frac{T}{y}\frac{\partial y}{\partial T} , \tag{6.45}$$

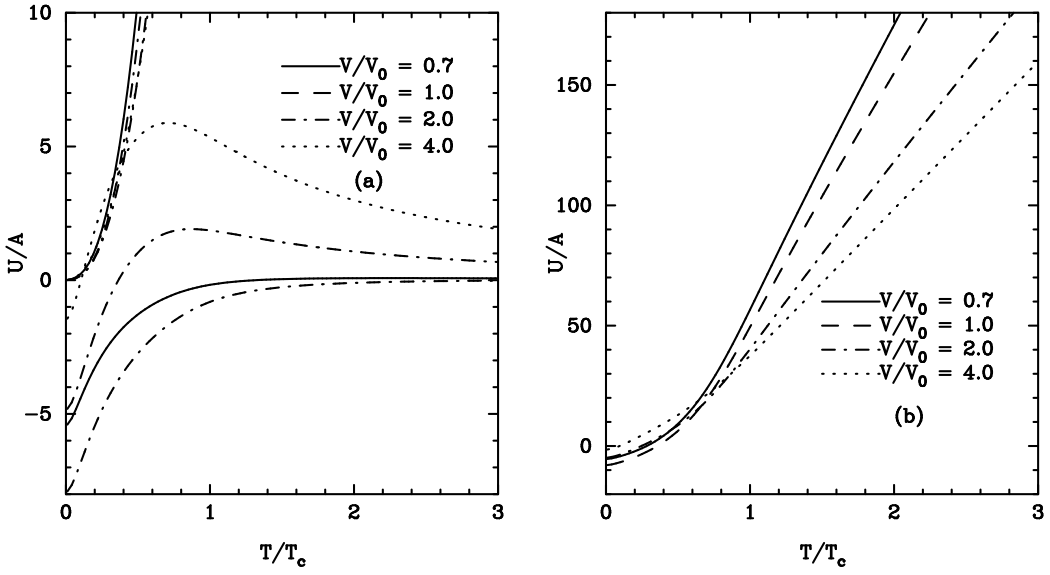
$$\begin{aligned}\frac{C_V}{k_B} &= (\langle m\rangle_A - 1)\left(\frac{2T}{x}\frac{\partial x}{\partial T} - \left(\frac{T}{x}\frac{\partial x}{\partial T}\right)^2 + \frac{T^2}{x}\frac{\partial^2 x}{\partial T^2}\right) \\ &\quad + (A - \langle m\rangle_A)\left(\frac{2T}{y}\frac{\partial y}{\partial T} - \left(\frac{T}{y}\frac{\partial y}{\partial T}\right)^2 + \frac{T^2}{y}\frac{\partial^2 y}{\partial T^2}\right) \\ &\quad + (\langle m^2\rangle_A - \langle m\rangle_A^2)\left(\frac{T}{x}\frac{\partial x}{\partial T} - \frac{T}{y}\frac{\partial y}{\partial T}\right)^2 .\end{aligned} \tag{6.46}$$

For the nuclear model specified by equations (6.31) and (6.34), applying the above equations yields

$$\frac{U}{k_B T} = (\langle m \rangle_A - 1)\frac{d}{2} + (A - \langle m \rangle_A)\frac{2k_B T}{\varepsilon_0}\left(\frac{T_0}{T+T_0}\right)^3 . \tag{6.47}$$

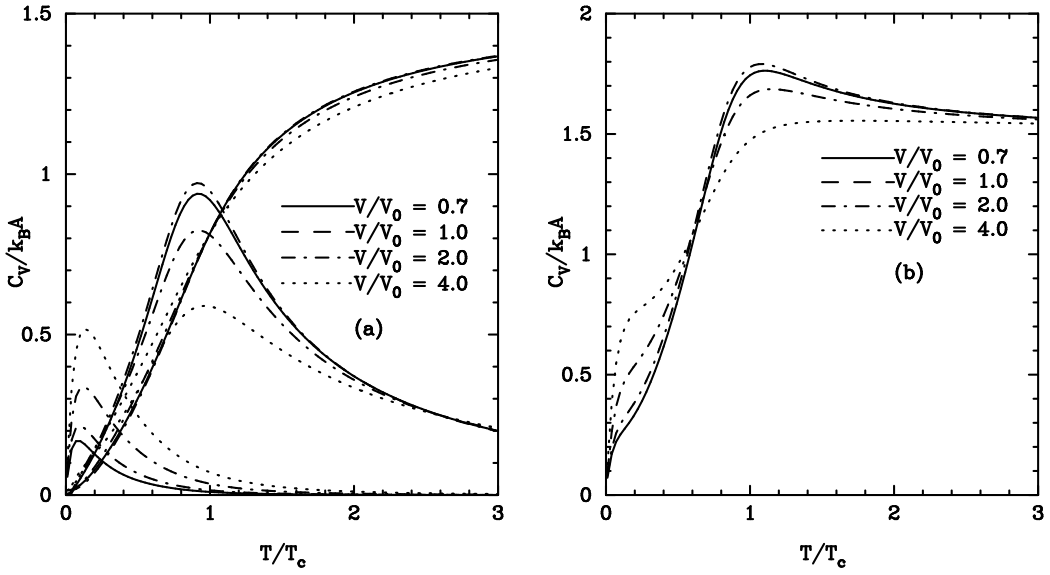
$$\frac{C_V}{k_B} = (\langle m \rangle_A - 1)\frac{d}{2} + (A - \langle m \rangle_A)\frac{2k_B T}{\varepsilon_0}\left(\frac{T_0}{T+T_0}\right)^3 + \mathrm{Var}(m)\left(\frac{d}{2} + \frac{a_V}{k_B T} - \frac{k_B T}{\varepsilon_0}\left(\frac{T_0}{T+T_0}\right)^2\right)^2 , \tag{6.48}$$

Figure 6.5: The internal energy per particle for $\varepsilon_F = 40$ MeV, $\sigma = 1$, $A = 100$, and $T_0 = 12$ MeV. Part (a) breaks the energy into the x and y components, part (b) graphs the total energy from both contributions.



Figures 6.5,6.6 sketch the behavior of these functions over a wide range of temperatures and densities. For low T, $C_V \propto T$ and is that of a heated nucleus of nucleons treated as a nearly degenerate Fermi gas. At higher T, nucleons and clusters are emitted from this nucleus, increasing the number of degrees of freedom and the specific heat. At a relatively low temperature this effect causes a transition from a degenerate Fermi gas to a Bose gas-like state. This change in C_V shows up in the figure as a shoulder. At very high T the nucleus of A nucleons dissolves into A independent nucleons and $C_V = \frac{1}{2}dk_B A$. The "cusp" like behavior of C_V can be understood as a critical point in the infinite A limit as discussed in the next paragraph. A rounded peak is seen instead of the cusp because of the finite size of the system.

Figure 6.6: The specific heat C_V per particle for $\varepsilon_F = 40$ MeV, $\sigma = 1$, $A = 100$, and $T_0 = 12$ MeV. Part (a) breaks the specific heat into the x and y multiplicity components and the fluctuation term, part (b) graphs the total specific heat from all three contributions.



6.3.2 Pressure and compressibility

The pressure and isothermal compressibility defined by $P = -k_B T \frac{\partial \ln Z_A}{\partial V}$ and $\kappa_T^{-1} = V\left(\frac{\partial P}{\partial V}\right)_T$ reflect the effects of volume changes on the system, and are therefore complementary to the internal energy and specific heat. In this model they are given by,

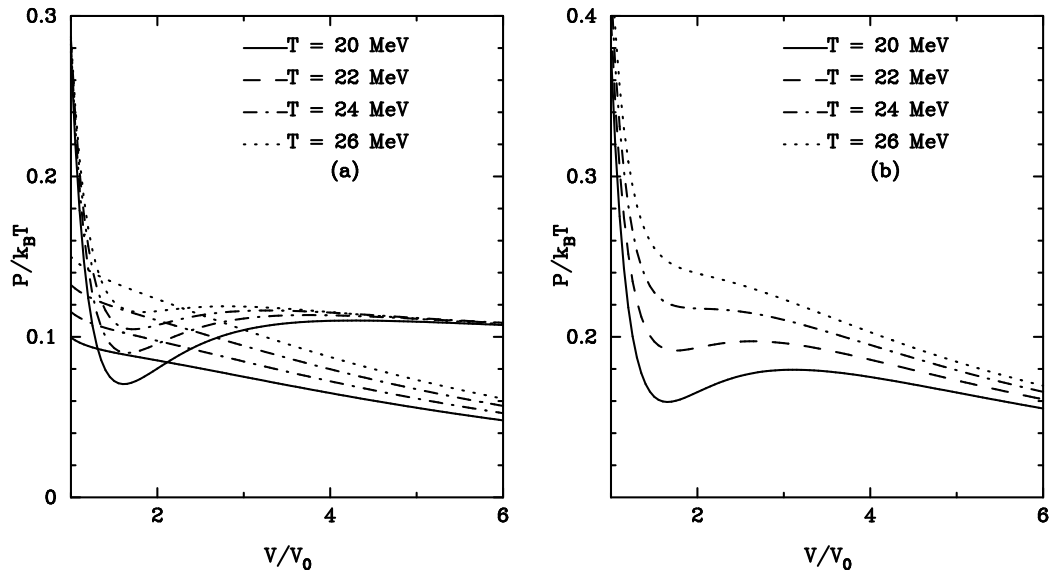
$$\frac{PV}{k_B T} = (\langle m\rangle_A - 1)\frac{V}{x}\frac{\partial x}{\partial V} + (A - \langle m\rangle_A)\frac{V}{y}\frac{\partial y}{\partial V}\,, \tag{6.49}$$

$$\begin{aligned}\frac{1}{\kappa_T} = -\frac{k_B T}{V}\Bigg[&(\langle m\rangle_A - 1)\left(\frac{V^2}{x}\frac{\partial^2 x}{\partial V^2} - \left(\frac{V}{x}\frac{\partial x}{\partial V}\right)^2\right)\\ &+(A - \langle m\rangle_A)\left(\frac{V^2}{y}\frac{\partial^2 y}{\partial V^2} - \left(\frac{V}{y}\frac{\partial y}{\partial V}\right)^2\right)\\ &+ (\langle m^2\rangle_A - \langle m\rangle_A^2)\left(\frac{V}{x}\frac{\partial x}{\partial V} - \frac{V}{y}\frac{\partial y}{\partial V}\right)^2\Bigg]\,.\end{aligned} \tag{6.50}$$

The equation for the pressure is more often called the equation of state (EOS). Using the nuclear parameters of equations (6.31) and (6.34) gives us the specific forms

$$\begin{aligned} PV &= (\langle m\rangle_A - 1)k_BT + (A - \langle m\rangle_A) \\ &\quad \times \left(\frac{2}{5}\varepsilon_F(\rho)\left(1 + \frac{5\pi^2}{12}\left(\frac{k_BT}{\varepsilon_F(\rho)}\right)^2 \frac{T_0}{T+T_0}\right)\right. \\ &\quad \left. - a_0\left(\frac{\rho}{\rho_0}\right) + a_3(1+\sigma)\left(\frac{\rho}{\rho_0}\right)^{1+\sigma}\right) , \qquad (6.51) \\ \frac{1}{\kappa_T} &= \frac{k_BT}{V}\left[(\langle m\rangle_A - 1) - (A - \langle m\rangle_A)\left(\frac{V^2}{y}\frac{\partial^2 y}{\partial V^2} - \left(\frac{V}{y}\frac{\partial y}{\partial V}\right)^2\right)\right. \\ &\quad \left. - (\langle m^2\rangle_A - \langle m\rangle_A^2)\left(1 - \frac{V}{y}\frac{\partial y}{\partial V}\right)^2\right] . \qquad (6.52) \end{aligned}$$

Figure 6.7: The nuclear pressure for $\varepsilon_F = 40$ MeV, $\sigma = 1$, $A = 100$, and $T_0 = 12$ MeV. Part (a) breaks the pressure into the x and y components, part (b) graphs the total pressure from both contributions.



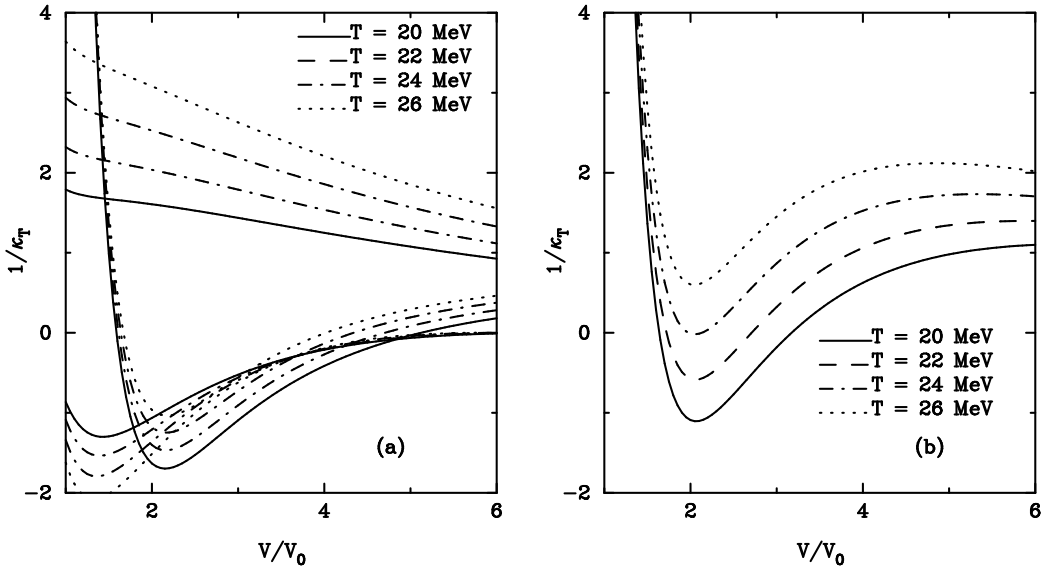
Note that the equation of state is particularly simple. The first term is the ideal gas law, while the second term contains the low temperature degeneracy pressure and interaction terms from the Skyrme potential. Figure 6.7(b) illustrates the behavior of P with V/A in the transition region where a phase instability develops. In this region, the equation of state behaves in many ways like a van der Waals gas, i.e. the appearance of a negative compressibility indicates a phase instability, usually identified as a first

order liquid-gas phase transition

$$\left(P + \frac{a}{V^2}\right)(V - b) = nk_BT \; . \tag{6.53}$$

The compressibility in particular is interesting. At low temperatures and standard densities, $9\rho/\kappa_T$ is about 240 MeV, a typical value for nuclei. This increases as the temperature is raised, albeit slowly, until around 40 MeV is passed and the system becomes more gas-like. At that point the compressibility increases essentially linearly with temperature, like an ideal gas.

Figure 6.8: The nuclear isothermal (in)compressibility for $\varepsilon_F = 40$ MeV, $\sigma = 1$, $A = 100$, and $T_0 = 12$ MeV. Part (a) breaks the incompressibility into the x, y and fluctuation components, part (b) graphs the total (in)compressibility from all three contributions.



6.3.3 Entropy and thermodynamic potentials

Clearly there is no practical limit to the number of thermodynamic functions. For example, the specific heat at constant pressure C_P can be evaluated from C_V and the isothermal compressibility and thermal expansion coefficient α,

$$C_P = C_V + \frac{TV\alpha^2}{\kappa_T} \tag{6.54}$$

where α is given by

$$\begin{aligned}
\alpha &= \kappa_T \left(\frac{\partial P}{\partial T}\right)_V , \\
&= \kappa_T \frac{k_B}{V}\Bigg[(\langle m\rangle_A - 1)\left(\frac{V}{x}\frac{\partial x}{\partial V} - \frac{TV}{x^2}\frac{\partial x}{\partial T}\frac{\partial x}{\partial V} + \frac{TV}{x}\frac{\partial^2 x}{\partial T \partial V}\right) \\
&\quad +(A - \langle m\rangle_A)\left(\frac{V}{y}\frac{\partial y}{\partial V} - \frac{TV}{y^2}\frac{\partial y}{\partial T}\frac{\partial y}{\partial V} + \frac{TV}{y}\frac{\partial^2 y}{\partial T \partial V}\right) \\
&\quad +(\langle m^2\rangle_A - \langle m\rangle_A^2)\left(\frac{T}{x}\frac{\partial x}{\partial T} - \frac{T}{y}\frac{\partial y}{\partial T}\right)\left(\frac{V}{x}\frac{\partial x}{\partial V} - \frac{V}{y}\frac{\partial y}{\partial V}\right)\Bigg] , \qquad (6.55)
\end{aligned}$$

Given this, the adiabatic compressibility κ_S can all be fairly easily expressed,

$$\kappa_S = \kappa_T \frac{1}{1 + \frac{VT\alpha^2}{C_V \kappa_T}} . \qquad (6.56)$$

In spite of the wide variety of functions however, physicists tend to concentrate on only a few, especially the thermodynamic potentials such as the already mentioned internal energy as well as the enthalpy H and Helmholtz and Gibbs free energies F, G,

$$H = U + PV , \qquad (6.57)$$

$$F = -k_B T \ln Z_A , \qquad (6.58)$$

$$G = -k_B T \ln Z_A + PV , \qquad (6.59)$$

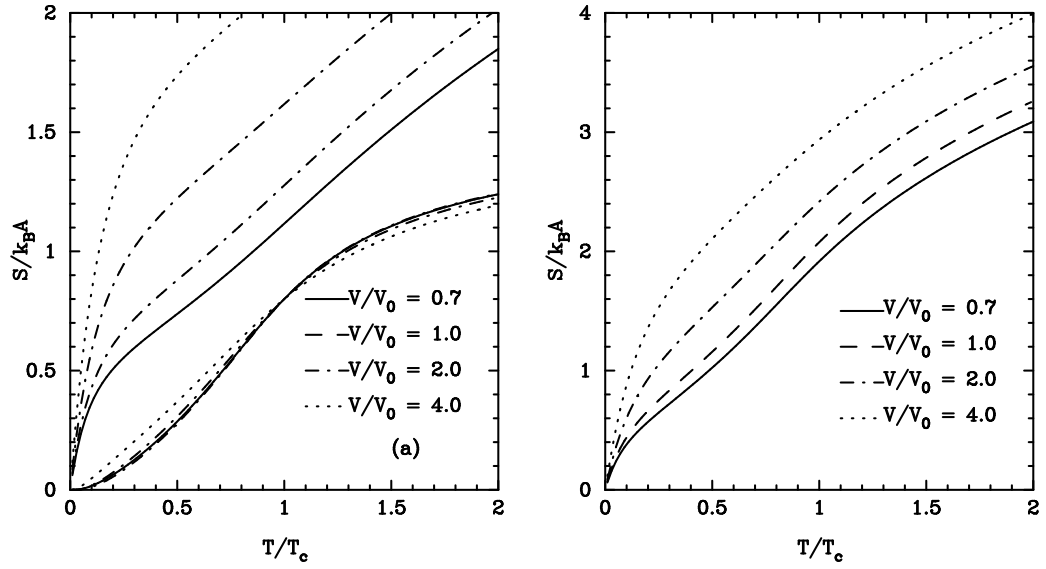
since minimizing these potentials will give the equilibrium condition for a system held at a certain fixed point in state space. The behavior of the energy is typical of these, and we will not investigate them further.

Additionally we can consider the entropy, a function which measures the intrinsic disorder of the system and is defined by

$$\frac{S}{k_B} = \tau \ln n + \ln Z_A + \frac{U}{T} \qquad (6.60)$$

where $\tau \ln n$ is simply the constant term (i.e. independent of V) required to set the entropy to zero at zero temperature. Figure 6.9 plots the entropy per particle for the nuclear model. Not surprisingly, lower densities and higher temperatures lead to higher entropies. The slight dip in the curve evidence at higher densities is related to the phase instability seen in the equation of state curves.

Figure 6.9: The nuclear entropy per particle for $\varepsilon_F = 40$ MeV, $\sigma = 1$, $A = 100$, and $T_0 = 12$. Part (a) break the entropy into two parts, the lower of which is the x dependent part of U/k_BT. Part (b) plots the total entropy.



6.4 Phase transitions in nuclei

The nature of the hadronic phase transition is of course of great interest to nuclear physicists. Is it like a liquid-gas transition, or a percolative transition, or of some other type, such as Bose-Einstein condensation? Or, could several transitions coexist, perhaps at different points in the state space. This section shows that indeed the model developed in the preceding section contains two distinct transitions, one associated with a thermodynamic instability (6.4.1) and another associated with a singularity in the partition function, a classical phase transition which can be interpreted both as a Bose-Einstein condensation (6.4.2) and as a percolation transition (6.4.3). Some care is taken to show that the methods of percolation theory which have been used to analyze nuclear fragmentation can be applied to this case exactly.

6.4.1 Liquid-gas thermal phase transitions in nuclei

The presence of power-law behavior in the distribution of fragments in early fragmentation experiments (J.E. Finn *et al.* [105], R.W. Minich *et al.* [221], A.S. Hirsch *et al.* [147]) suggested a phase transition was occurring in nuclear matter. The experimentalists who

first measured this suggested it was evidence of a liquid-gas phase transition in analog with the Fisher droplet model [106,107]. Later experimental results [63,235] continued to show such a dependence. Theorists (M.W. Curtin *et al.* [67], H. Schulz *et al.* [269], P.J. Siemens and G.F. Bertsch [271,28], H.R. Jaqaman, A.Z. Mekjian and L. Zamick [154,155] J.I. Kapusta, A.L. Goodman, and A.Z. Mekjian [159,122] and S. Levit and P. Bonche [33,187]) analyzed the nature of such a liquid-gas phase transition in nuclei in various bulk models. They estimated the critical temperature and volume as $T_c \approx 20$ MeV and $\rho/\rho_0 \approx 0.5$. However, the actual transition was expected to happen at a lower temperature due to Coulomb instabilities and other effects (cf. H.R. Jaqaman *et al.* [156,153] and L. Satpathy *et al.* [266]). Today the case continues to be made that the phase transition is essentially liquid-gas like [206,241].

A liquid gas phase transition is determined as the temperature at which the isotherm P vs. ρ has an inflection point, namely

$$\left(\frac{\partial P}{\partial \rho}\right)_T = \left(\frac{\partial^2 P}{\partial \rho^2}\right)_T = 0 \ . \tag{6.61}$$

For example, in one of the simplest versions of the equation of state [122]

$$P = \rho k_B T - a_0 \rho^2 + a_3 \rho^3 \tag{6.62}$$

it is easy to determine $\rho_c = a_0/6a_3 \approx 0.49\rho_0$ and $k_B T_c = a_0 \rho_c \approx 21.5$ MeV.

The model considered here essentially adds excitation energy and clustering effects to the above simple model. Consider the isothermal (in)compressibility curves in figure 6.8. The curve for $T = 24$ MeV satisfies the condition of having its minimum occur at $1/\kappa_T = 0$, around $\rho/\rho_0 \approx 0.5$. This is the critical instability point. Apparently the competing processes of internal excitation and fragmentation do not significantly affect the location of this point, which has only been shifted upward by a few MeV. Coulomb effects however have still been neglected, although they can considered in the two-component version of this model. Nonetheless, in spite of the size of the effect in this particular model, it is clear that we can expect the clustering degrees of freedom to affect the thermodynamic stability of nuclei, and that such effects should not be neglected.

6.4.2 Bose-Einstein condensation in nuclei

As this model of nuclear fragmentation is closely related to the ideal Bose-Einstein gas model, it would not be surprising to discover evidence of a Bose-Einstein like phase transition in the physics. Indeed, as we shall see, considered as a statistical system, this model exhibits a phase transition in the fixed density but infinite A limit, at which the specific heat per nucleon is maximal. This is the phase transition discussed in chapter four, characterized by the appearance of large clusters and zeros of the partition function. Real nuclear systems are far from infinite collections of nucleons, but the evidence of such phase transitions can be obtained from a finite scaling analysis in the region of the phase transition [48, 120]. This section reviews the characteristics of the transition.

Let us repeat an arguments from section 4.3, tailored specifically however to this nuclear fragmentation model. The thermodynamic limit $A, V \to \infty$ with $\rho = A/V$ finite is of interest since it specifies the the nature of any phase transitions. In this model, we can work in the grand canonical limit and consider the question of the behavior of the largest cluster. In the grand canonical limit $\langle \pi_k \rangle$ is given by

$$\langle \pi_k \rangle = \frac{x}{y} \frac{e^{\mu k/k_B T}}{k^\tau} = \frac{x}{y} \frac{z^k}{k^\tau} , \tag{6.63}$$

which implies the mass constraint

$$\frac{A}{x/y} = \sum_k z^k k^{1-\tau} . \tag{6.64}$$

Here $A/(x/y)$ is finite in the thermodynamic limit since $x \propto V$ and $y = y(\rho, T)$ is finite. For $z \leq 1$, the sum is always less than or equal to the case $z = 1$, for which the sum gives $\zeta(\tau - 1)$, i.e. the Riemann zeta function. When $z > 1$ the sum diverges. Now $A/(x/y)$ is a function of ρ, T which are fixed, so z is the only parameter we can adjust. If $A/(x/y) \leq \zeta(\tau - 1)$ then we can find a $z \leq 1$ such that the mass constraint is met. Then by equation (6.63), $\langle \pi_\infty \rangle \to 0$, and correspondingly there is no chance that an infinite cluster can exist. On the other hand, if $A/(x/y) > \zeta(\tau - 1)$ then no z can be found to satisfy the mass constraint. Equation (6.63) with $z = 1$ still holds for finite sized clusters, but $\sum_k k \langle \pi_k \rangle$ does not then account for all the nucleons. The "missing mass"

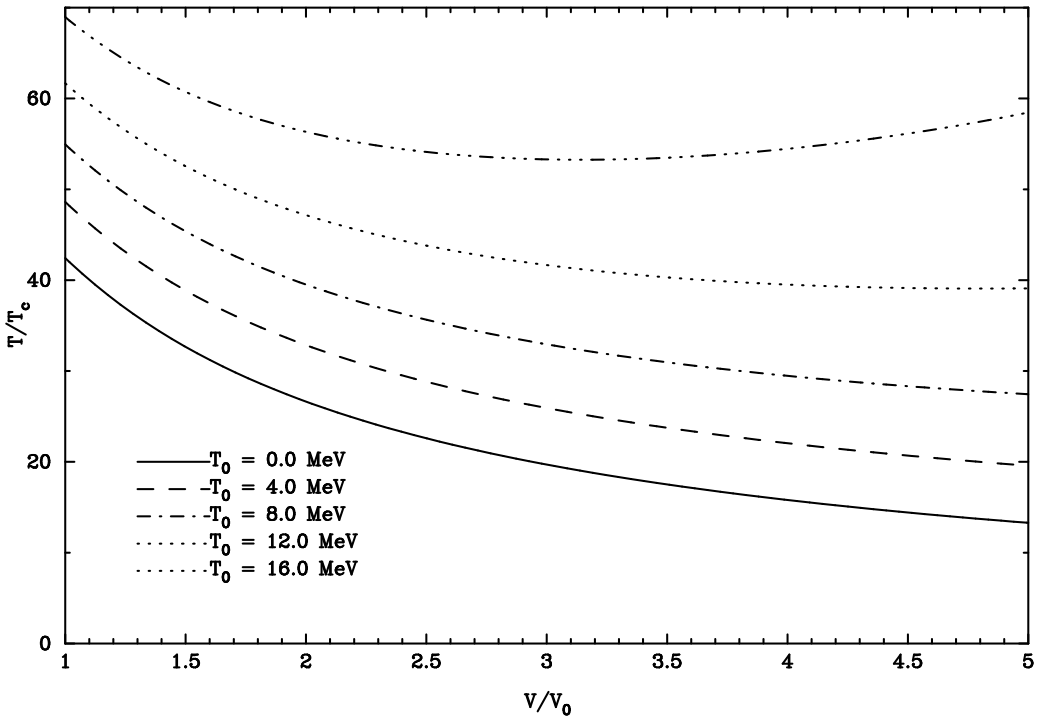
has accumulated into an infinite cluster, which the grand canonical solution neglects. So $(x/y)_c/A = 1/\zeta(\tau - 1)$ defines a critical point for this system, which is identical to the critical point of a Bose gas if $y = 1$. Since $\zeta(\tau - 1) < \infty$ only if $\tau > 2$, this also implies that the system has no critical behavior if $\tau \leq 2$. Above this point the grand canonical solution is valid. Below this point, an infinite cluster has absorbed a finite fraction of the mass of the system.

For nuclear matter, this is important since the critical point may be accessible if equilibrium conditions are realized in heavy-ion collisions. A specific concern is whether this theory has the same characteristic as the infinite cluster in percolation theory [279], i.e. for $p > p_c$ the infinite cluster exists while for $p < p_c$ it does not exist.

The consequences of this kind of transition were explored in chapter four, the most important of which is that at the transition the variance of the multiplicity is maximal, and its derivative is discontinuous. Since the specific heat and compressibility of the models depend on this variance (see section 6.3.1 and 6.3.2), they are the thermodynamic quantities which will reveal this non-thermodynamic phase transition. Specifically, we can expect the specific heat of nuclei to be maximal at this transition. It is important to note however that although the transition can be seen in the thermodynamic functions, it is mostly unrelated to the thermodynamics, and is rather strongly dependent on the clustering degrees of freedom. In other words, the liquid-gas phase instability seen in the previous section we expect to appear even if there is no clustering allowed in the model, since that is originally how such an instability was studied. The phase transition seen here though is intimately connected to the ability of the nucleons to form clusters of varying sizes. Without such freedom, the transition would not happen. In fact, considering figure 6.10 which plots the dependence of the critical temperature with density, we see that this clustering transition occurs at a much higher temperature than the liquid-gas instability. As such this is a much different kind of transition than the liquid-gas instability discussed in the previous section, and is somewhat speculative. However, it is a natural consequence if we assume that the power law behavior seen in the experiments is a persistent feature below the critical point.

Universality indicates the model near the critical point is specified uniquely by its

Figure 6.10: Critical temperature as a function of density at various cutoff temperatures for $\tau = 2.5$. The rise at high V is due to the lack of a cutoff in the internal excitations at low density.



critical exponents. We already mentioned the critical exponent τ, but other exponents are needed to determine the critical behavior. By the above discussion, the fraction of mass not in the infinite cluster, $m_x = \lim_{A\to\infty} 1 - \langle k_{max}\rangle/A$ satisfies $m_x < 1$ for $T \leq T_C$ and $\rangle M_1 = 1$ for $T > T_C$. Thus $\langle \pi_\infty \rangle = 1 - m_x$ is zero for $T > T_C$. Near $T = T_C$, $\langle n_\infty \rangle \sim (T - T_C)/T_C$. The analog of m_x in the Bose system is the fraction of Bose particles in excited states, while $\langle n_\infty \rangle$ is the fraction in the condensed ground state. For the Bose system the order parameter is taken as the square root of the number of Bosons in the ground state, and in analogy $\sqrt{\langle n_\infty \rangle} \propto (T - T_C)^{1/2}$, which gives the second critical exponent $\beta = 1/2$. The clustering point of view defines the exponents differently, and as this transition is really a change in the clustering behavior, we should define the exponents in terms of the clustering. This we do in the next section.

6.4.3 Percolative phase transitions in nuclei

We have already mentioned that the Bose-Einstein condensation transition can be viewed as a percolative transition since at that point there is an appearance of a very large cluster. This section examines that transition point more carefully in terms of percolation, firstly noting the similarities between the two and secondly stressing some of the differences. A brief introduction to percolation theory is given, and the exact method for computing expectation values in the Gibbs model which exclude the largest cluster introduced in section 4.3.1 is further developed and applied. This method allows for the computation of the reduced variance and other quantities of interest introduced by Xavier Campi and a comparison shows that the percolation model and the Gibbs model with $x_k = x/k^{5/2}$ differ mostly only in small respects in these ensemble averages. As percolation is such a popular model in nuclear fragmentation, these similarities suggest a simple Gibbs model may be used in its stead. The advantage of such a substitution can be seen at once, as the Gibbs model has an explicit thermodynamic parameterization and exact solution which the percolative models lack.

Percolation theory was introduced to nuclear fragmentation in the mid-1980s by Xavier Campi and J. Debois [46,74] and by Wolfgang Bauer *et al.* [21]. They suggested that a bond percolation model in three dimensions might explain the data for nuclear fragmentation, since the model intuitively seemed to connect to many theorists simplified picture of a nucleus fragmenting. Such models date back to Flory's work on polymer physics [109–112] in 1941, but interest and systematic study of their properties did not begin in earnest until the 1960s. Although such models contains a minimum of physics (indeed there is only one parameter), they could explain many aspects of the nuclear fragmentation experiments, and as such they have become benchmarks to which other fragmentation models must compare favorably. Moreover, the analogy suggested that there was a critical transition in nuclear fragmentation and showed ways of extracting information on that transition from the experimental data.

Percolation models can be defined simply. Let L be a (now) finite lattice (in 2D, 3D, etc.) with a particular topological structure (e.g. simple cubic, hexagonal) defined by

the number and location of nearest neighbors and N the number of vertices. The lines connecting nearest neighbor vertices we will call bonds, and the vertices themselves are simply called sites. The site percolation problem is defined as follows. Randomly select pN sites on the lattice and denote them filled. What is the probability that the filled sites form a lattice spanning cluster (LSC), i.e. that there exists a path from one side of the lattice to the other through adjacent filled lattice sites. The bond percolation problem is the same, except one randomly fills the bonds and computes the probability that their exists a path from one side to the other.

In some sense the (above described) percolation model is the simplest possible statistical model with clustering and fragmentation. There is but one parameter p and the underlying topology to consider. This simplicity has made it an attractive model for fragmentation models, since the states of the system geometrically can be identified with particular cluster configurations. For example, 125 nucleons can be considered to reside on a $5 \times 5 \times 5$ lattice, the bonds connecting the sites forming clusters which correspond to the clusters emitted during the fragmentation process. Suppose Π is a configuration and let us denote by π_k the number of clusters of size k. Then we have

$$\sum_k k\pi_k = pN \tag{6.65}$$

for any configuration Π.

Let $q = 1 - p$ and $n_k = \pi_k/N$. Consider a simple quadratic lattice, whose sites are filled with a probability p. Obviously $\langle n_1 \rangle$ is given by the probability that a particular site is filled, with the four edges around it empty, i.e.

$$\langle n_1 \rangle = pq^4 \ . \tag{6.66}$$

Similarly,

$$\langle n_2 \rangle = 2p^2q^6 \ , \tag{6.67}$$

$$\langle n_3 \rangle = 4p^3q^7 + 2p^3q^8 \ , \tag{6.68}$$

and in general

$$\langle n_s \rangle = p^s \sum_t g_{st} q^t \ , \tag{6.69}$$

where g_{st} is the number of clusters of size s and perimeter t, and we denote $g_s = \sum_t g_{st}$. So a determination of the properties of the percolation problem can be reduced to an enumeration of clusters (known as "lattice animals"). Enumerating such clusters can be done by a variety of computer methods, and for the simple quadratic site problem, g_{st} is known for all $s \leq 24$.[10]

Traditionally, the critical transition is identified by the appearance of a "percolating" cluster, in other words a cluster which spans the entire lattice, connecting one side with the other. In one dimension, $p_c = 1$ for such a cluster, since any empty site or bond in one dimension breaks the connection, and unless $p = 1$ such a break will occur. In higher dimensions, $p_c < 1$, since the lattice can support a number of holes and still be connected.

Once the critical point is identified, the transition can be characterized by studying the behavior of various functions around the point. Reduced moments (section 4.3.1) are usually used, although they sometimes go by different names. For example, below the critical point one defines the following functions

$$K(p) := \sum_{s \geq 1} \langle n_s \rangle = \sum_n k_n p^n \,, \tag{6.70}$$

$$S(p) := \frac{1}{p} \sum_{s \geq 1} s^2 \langle n_s \rangle = \sum_n b_n p^n \,. \tag{6.71}$$

Since sn_s is the probability a given monomer is part of an s-cluster, $S(p)$ denotes the expected cluster size, and $nK(p)$ denotes the expected number of clusters. In terms of reduced moments these are the zeroth and second moments, and there behavior around the critical point specifies the nature of the transition.

Two general approaches have been taken in the evaluation of these (and other) functions. The first is Monte Carlo simulation, whereby the systems are sampled and approximations are determined subject to the dual limitations of the length of the simulation and the size of the lattice. The other technique applied is that of exact

[10] The $s = 23, 24$ cases I calculated myself as an exercise using an algorithm by S. Mertens [219] and 27 days of CPU time on an idle computer. The results are in table 6.3. The principal motivation was to deduce the total number of lattice animals of size 25, since the numbers up to 24 had been known since 1981 [250]. Despite an increase in computer power of a factor of at least one hundred since that computation, the results had not been extended. The result was $g_{25} = 20457802016011$.

series expansions. An expansion valid for low p and low q can be developed using the lattice animals, and by using Padé approximants the two series can be combined to give an estimate of the location of the critical point and its critical parameters. In fact this method typically leads to the best approximations for the critical point. The exact series method is somewhat related to the exact methods applied to the Gibbs models, although the recursion relations that result are nowhere near as powerful as in the Gibbs case. Tables 6.4 and 6.5 give such expansions in two and three dimensions.

Analyzing the critical point and its exponents in this manner has engaged many researchers over the years, and table 6.6 summarizes the results. Our interest is to apply the same analysis to a different model, namely the canonical Gibbs model. This is motivated from the successful application of purely percolative models to nuclear fragmentation. As we already noted, X. Campi and W. Bauer suggested that the bond percolation problem in three dimensions captures the essence of nuclear fragmentation. S. Das Gupta [69] has suggested the three dimensional site problem for other reasons, but both have identical critical behavior. This is an appealing picture and Campi developed functions which distinguished this model from other models, including the Gibbs model with $x_k = x/k$. Applying his functions to the nuclear fragmentation data yielded the following somewhat puzzling result: The simple percolation model best fit the data.

The method X. Campi and H. Krivine [47,51,50] introduced for distinguishing fragmentation models from one another is quite simple and elegant. By comparing various expectation values in which the largest cluster is excluded but the particle number and fragment multiplicity are held fixed (i.e. microcanonical ensembles), they showed that the percolation model has a distinctly different behavior than many competing nuclear fragmentation models. Specifically, percolation could be quickly distinguished from equipartitioning, intranuclear cascade and the Gibbs model with $x_k = x/k$. Moreover, actual fragmentation data [175] agreed with the percolative model in this respect more so than any other other model of fragmentation.

Specifically, Campi and Krivine [47, 51, 50] define the reduced variance γ_2 for a

fragmentation event as

$$\gamma_2(\boldsymbol{\pi}) = (m-1)\frac{\sum_k k^2\pi_k - k_{\max}^2}{(A-k_{\max})^2}\ , \tag{6.72}$$

where $k_{\max}$ is the size of the largest cluster. Its expectation value can be computed by breaking events into classes specified by $k_{\max}$, and summing the expectation values over those classes with the appropriate weight, i.e.

$$\langle\gamma_2\rangle_A^{(m)} = (m-1)\sum_{k_{\max}} \Pr(k_{\max})\frac{\sum_k k^2\langle\pi_k\rangle_A^{(m)}(k_{\max}) - k_{\max}^2}{(n-k_{\max})^2}\ , \tag{6.73}$$

where $\Pr(k_{\max})$ is the probability of $k_{\max}$ being the largest cluster size and $\langle\pi_k\rangle_A^{(m)}(k_{\max})$ is the expectation value of π_k when $k_{\max}$ is fixed. It is this expectation value which when plotted against m indicates the distinction between the percolation model and other models of fragmentation.

Now to compute expectation values in which the largest cluster size is fixed we need to compute the partition function for such ensembles. Suppose that each fragmentation outcome happens with a probability proportional to the Gibbs weight in the microcanonical ensemble (equation (3.25)). Clearly the partition function is given by all the terms in the unrestricted microcanonical partition function which have $x_{k_{\max}}$ as the highest x_k in the term. Consider

$$\begin{aligned}\Delta Z_A^{(m)}(k_{\max}) \equiv\ & Z_A^{(m)}(x_1,\ldots,x_{k_{\max}},0,\ldots,0) \\ & - Z_A^{(m)}(x_1,\ldots,x_{k_{\max}-1},0,\ldots,0)\ .\end{aligned} \tag{6.74}$$

We see that $\Delta Z_A^{(m)}(k_{\max})$ is the partition function for ensembles with fixed maximum cluster size $k_{\max}$, since the first term collects all terms with $x_{k_{\max}}$ or lower, and the second term eliminates those terms which don't have an $x_{k_{\max}}$. From this result we can determine $\Pr(k_{\max})$ and $\langle\pi_k\rangle_A^{(m)}(k_{\max})$, which are given by

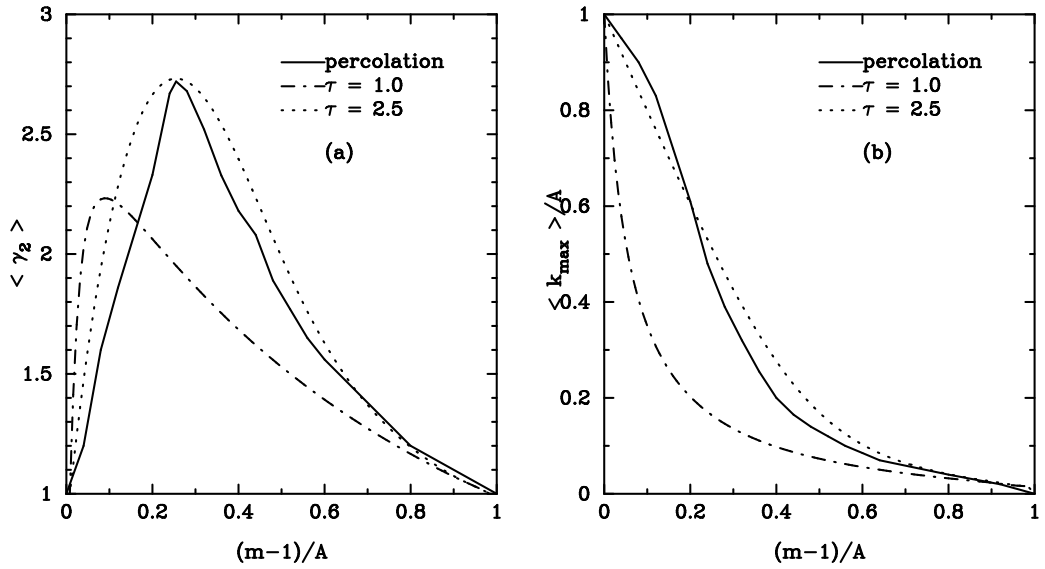
$$\Pr(k_{\max}) = \frac{\Delta Z_A^{(m)}(k_{\max})}{Z_A^{(m)}(x_1,\ldots,x_A)} \tag{6.75}$$

$$\langle\pi_k\rangle_A^{(m)}(k_{\max}) = \begin{cases} 0 & k > k_{\max} \\ x_k\dfrac{Z_{A-k}^{(m-1)}(x_1,\ldots,x_k,0,\ldots,0)}{\Delta Z_A^{(m)}(k_{\max})} & k = k_{\max} \\ x_k\dfrac{\Delta Z_{A-k}^{(m-1)}(k_{\max})}{\Delta Z_A^{(m)}(k_{\max})} & k < k_{\max} \end{cases} \tag{6.76}$$

This method is quite general and can be applied to other models. For example equipartitioning models can also be analyzed by this method with some minor modifications.

With these identities there is sufficient information to compute $\langle \gamma_2 \rangle_A^{(m)}$ for any x_k. We use $x_k = x/k^\tau$ for a number of reasons, especially the behavior of its mass yield (section 4.2.2). Campi and Krivine [50,51] following Mekjian [215] considered this model with $\tau = 1.0$ and showed that its reduced variance and other related expectation values had a distinctly different behavior than the percolation model. Plotting the expected reduced variance vs. $(m-1)/A$, $\langle \gamma_2 \rangle_A^{(m)}$ has a single peak. The location, height and width of this peak for the two models (and other models they considered) are completely different, suggesting the usefulness of this plot in distinguishing fragmentation models.

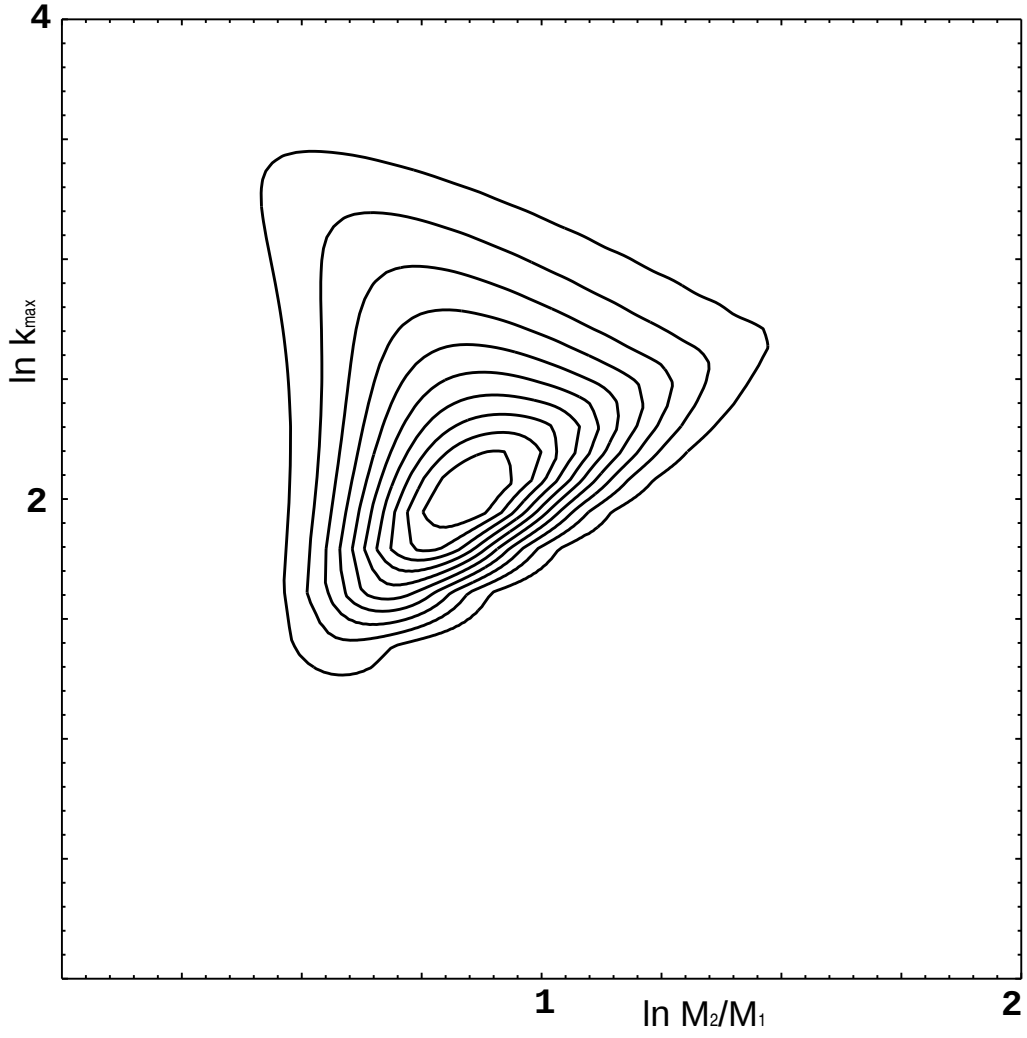
Figure 6.11: Reduced variance $\langle \gamma_2 \rangle_A^{(m)}$ (a) and largest cluster size $\langle k_{\max} \rangle_A^{(m)}/A$ (b) vs. $(m-1)/A$ for $\tau = 1.0, 2.5$ and the percolation model at $n = 125$.



Since that time our interest has turned to the model with $\tau = 2.5$, since it has an explicit phase transition and better mass yield characteristics than $\tau = 1.0$. Computing the reduced variance for this case allows us to compare this model to Campi's percolation model. This is shown in figure 6.11. A cursory inspection shows that the percolation and Gibbs models now substantially agree in many respects. The height and location of the peak of the reduced variance $\langle \gamma_2 \rangle_A^{(m)}$ is nearly the same in both models, as indicated in figure 6.11. The only significant difference is the width of the

peak which tends to be somewhat larger in the Gibbs model than in the percolation model. Plots of $\langle k_{\max}\rangle_A^{(m)}$ vs. $(m-1)/A$ are also very similar for both models, and the scaling behavior of the position, width and height with changing A also agree.

Figure 6.12: Campi probability contour plot for $Z = 79$, $\tau = 2.5$ at the critical point $x = x_c$. The axes are logarithmic, with the largest cluster size on the y-axis, and the ratio of the reduced moments M_2/M_1 on the x-axis. The central rings are higher in probability than the outer rings.



Another plot suggested by Campi [46] is to divide the event space by the maximum cluster size of the event k_{max} and the reduced second moment M_2 and plot the probability of the canonical model being at any particular point on the graph. This can be also be done exactly for Gibbs models in a way completely analogous to the way given above. Define the partition function $Z_A(m_2;\mathbf{x})$ as the sum of the Gibbs weight

equation (3.25) over all partition vectors $\boldsymbol{\pi}$ which satisfy $\sum_k k\pi_k = n$, $\sum_k k^2\pi_k = m_2$. This can be computed by the following recursion,

$$AZ_A(m_2;\mathbf{x}) = \sum_k kx_k Z_{A-k}(m_2 - k^2;\mathbf{x}) \,, \tag{6.77}$$

with $Z_0(m_2;\mathbf{x}) = \delta_{m_2,0}$. If we define ΔZ as in equation (6.74), we find again the partition function conditioned on k_{max} being fixed, which is proportional to the probability of having an event with a particular m_2 and k_{max}. Figure 6.12 plots this probability profile as a contour plot, which reveals the events are centered on a particular region in this phase space. The slopes of the edges of this region are related to the critical exponents according to Campi [46].

Clearly there are differences between percolation theory and a Gibbs model, but the differences are not as vast as originally suggested by early computations. Indeed the reduced variance cannot reliably distinguish percolation from a simple Gibbs model. A different method is needed to distinguish these models. In retrospect, however, the agreement is not completely unexpected. The Gibbs model with $x_k = x/k^{5/2}$ is closely related to the Flory-Stockmayer polymer model (section 5.2). This model in turn is equivalent to the percolation problem on a Cayley lattice [280], and as such is expected to share some of the features of a percolation model on a finite dimensional lattice.

On the basis of the results we have found here, the Gibbs model is a reasonable alternative to the percolation model in nuclear fragmentation. Its exact solution and explicit thermodynamic parameterization make it a physically and computationally attractive model. The success of percolation theory in describing the data suggests a closer inspection, but the Gibbs model presented here seems equally adept at reproducing certain features of the fragmentation experiments. The two approaches at this point complement each other, and further investigation should distinguish their strengths and weaknesses.

6.5 Particle production and the quark-gluon plasma

The techniques developed here can be extended upward in energy where conservation of particles is no longer satisfied due to particle production. Although the number of

particles is not conserved, there are other conserved quantities which can serve equally well to determine the combinatorial objects. These conservation laws can then be used to determine recursion relations (i.e. algorithms) for enumerating and evaluating partition functions in the exact same manner as in the fragmentation models.

An example of this kind of general combinatorial object is given by configurations specified by conservation of baryon number and energy. Suppose we have only one kind of baryon, and its corresponding anti-baryon. Let π_k denote the number of k-sized baryon cluster, and π_{-k} the number of k-sized anti-baryon clusters. Our constraints are then

$$\sum_j j(\pi_j - \pi_{-j}) = B \ , \tag{6.78}$$

$$\sum_j \epsilon_j(\pi_j + \pi_{-j}) = E \ , \tag{6.79}$$

where ϵ_j is the amount of rest mass associated with a cluster of j baryons. This constraint defines a combinatorial object enumerated by

$$\sum_{BE} n(B,E) x^B y^E = \prod_{j\geq 1} \frac{1}{(1-x^j y^{\epsilon_j})(1-x^{-j}y^{\epsilon_j})} \ , \tag{6.80}$$

where $n(B,E)$ is the number of states with baryon number B and energy E. In practice, we want the energy constraint to be weak, or in other words it should be an inequality (we can place excess energy into other excitations, such as kinetic energy). In that case simply include all the partitions specified by $0 \leq E' \leq E$ in our set, $n'(B,E) = \sum_{E'=0}^{E} n(B,E')$, and hence the generating function is given by

$$\sum_{BE} n'(B,E) x^B y^E = \frac{1}{1-y} \prod_{j\geq 1} \frac{1}{(1-x^j y^{\epsilon_j})(1-x^{-j}y^{\epsilon_j})} \ . \tag{6.81}$$

Table 6.3: Perimeter polynomials g_{st} for the simple quadratic site problem, $s = 23, 24$.

t	$g_{23,t}$	$g_{24,t}$
16	52	9
17	3332	1305
18	65780	35042
19	727668	471844
20	5664918	4247869
21	33997116	28833567
22	165477100	157180878
23	670599744	710668754
24	2299264494	2721780421
25	6735207164	8928596723
26	16966106238	25302085602
27	36913936804	62249333336
28	69541499676	133467703607
29	113548417344	249857740898
30	160644611412	408726736300
31	196680985596	583979560584
32	207928717388	727863766037
33	189230716408	789728235716
34	147656366202	743811652776
35	98293011684	605934392800
36	55499021646	425061844840
37	26400293856	255427953321
38	10503415084	130711144096
39	3465612328	56582637908
40	939643714	20570991840
41	206860352	6228635528
42	36480976	1556205378
43	5049744	316990696
44	537118	51921985
45	42128	6701488
46	2372	667174
47	84	49240
48	2	2616
49		88
50		2

Table 6.4: Simple quadratic lattice site percolation series expansions, g_n, k_n, b_{n-1} for $n = 1(1)25$. Results were computed with g_{st} from [289,219] and a private computation of g_{st} for $s = 23, 24$ by the author. The results were checked against published values in [250, 219, 286].

n	g_n	k_n	b_{n-1}
1	1	1	1
2	2	-2	4
3	6	0	12
4	19	1	24
5	63	0	52
6	216	0	108
7	760	0	224
8	2725	1	412
9	9910	-1	844
10	36446	2	1528
11	135268	-4	3152
12	505861	11	5036
13	1903890	-26	11984
14	7204874	62	15040
15	27394666	142	46512
16	104592937	333	34788
17	400795844	-780	197612
18	1540820542	1828	4036
19	5940738676	-4256	929368
20	22964779660	9894	-702592
21	88983512783	-23007	4847552
22	345532572678	53682	-7033956
23	1344372335524	-125690	27903296
24	5239988770268	295221	-54403996
25	20457802016011	-694759	170579740

Table 6.5: Simple cubic lattice bond percolation series expansions, g_n, k_n, b_{n-1} for $n = 1(1)13$. Results were calculated from g_{st} in [288, 291] and checked against published values in [287, 290].

n	g_n	k_n	b_{n-1}
1	3	3	3
2	15	-15	30
3	95	20	150
4	681	-12	714
5	5277	6	3342
6	43086	21	14994
7	365313	-18	67686
8	3186444	183	294522
9	28414802	-328	1304682
10	257908020	2034	5566038
11	2375037477	-5142	24376170
12	22136623447	26539	102447990
13	208438845633	-81183	445619106

Table 6.6: Percolation critical exponents. The results are exact in two dimensions due to M.P.M. den Nijs [232]. The three dimensional results are from series expansions due to D.S. Gaunt and M.F. Sykes [119].

Exponent	$d = 2$	$d = 3$	Cayley tree
α	-2/3	-0.64 $\pm$ 0.05	-1
β	5/36	0.454 $\pm$ 0.008	1
γ	43/18	1.73 $\pm$ 0.03	1
τ	187/91	2.21 $\pm$ 0.03	5/2

Chapter 7

Conclusion

A number of models for fragmentation and aggregation were discussed in this dissertation. They were characterized by the distinguishability of the components of the system, the ensemble associated with the conservation laws (e.g. microcanonical, canonical or grand canonical), and the underlying statistics of the objects (e.g. Gibbs or equipartitioning). For these models, exact and approximate solutions were developed for the partition functions. Traditionally the computation of the partition function solves all related statistical problems, and that tradition is upheld for these models. For example, relations between the expected cluster yields and the partition functions were developed that allow results to be obtained directly from the partition functions. It has long been known that in the canonical and microcanonical ensembles, the partition functions can be somewhat unwieldy being polynomials with as many terms as there are partitions of the system. However, for moderate numbers of particles (typically in the hundreds to thousands), it is possible to construct these solutions exactly using a computer and a recursive algorithm for several families of statistical weights. Historically this fact was of little consequence since the systems to which these models were applied had far greater numbers of particles and could be modeled well by the grand canonical or maximal entropy method, which have more tractable solutions. The idea of applying these models to systems with far fewer numbers of particles, such as in nuclear fragmentation, challenged this paradigm and promoted the development and application of exact methods for canonical and microcanonical ensembles.

That is the essential point to be made. Historically there was little reason to recognize the exact solutions, both because the grand canonical and maximal entropy solutions captured the essential physics in the regions of interest and because until the

1970s computers with sufficient memory and computational power were unavailable. This lack of recognition of the exact solutions makes it difficult to assign priority to their discovery, but it seems clear that the fundamental recursive relations arose first in symmetric function theory, where interest in "finite systems" was extensive, and have since been rediscovered several times. Such algorithms reveal that the canonical models are typically weakly sensitive to the finite size of the system, and such effects are essentially inconsequential in systems with large numbers of particles. The exception to this behavior occurs when phase transitions manifest themselves, but in this case the system can usually be dissected into two phases, each of which can be treated grand canonically. For this reason, there was little reason to criticize the grand canonical or maximal entropy solutions. By contrast, nuclear systems are sufficiently small that such effects can be appreciable, and as a result models which strictly conserve particle number are needed, i.e. canonical and microcanonical solutions.

So the successful application of methods from symmetric function and recursion theory allows us to rely less on the predictably problematic grand canonical ensemble in describing systems with small numbers of particles, and to avoid the computationally expensive Monte Carlo sampling methods. Herein, chapters two, three and four established these techniques which chapters five and six applied to a variety of models. Chapter two introduced in a self-contained fashion the subject of combinatorics as it applies to the restricted problem of describing systems which fragment or aggregate. Chapter three, building on the results of chapter two, introduced a number of statistical models to apply to physical systems, and proceeded to analyze various approaches to solving such models. One in particular, the canonical Gibbs model, considered in chapter four, was the model principally used in real world applications due to its roots in the Gibbs formulation of the ideal Boltzmann gas.

Chapter five introduced several historical and non-historical models which benefit from these methods. The ideal Bose gas, the Feynman theory of the λ transition in liquid helium, the Flory-Stockmayer theory of polymer gelation, Ewens' sampling formula for the frequency of alleles and a schematic model for the dynamics of group formation were all shown to be related to the canonical Gibbs model of chapter four. The

minimal information approach to fragmentation and the enumeration of involutions, Young tableaux, and loop-free graphs and digraphs were also shown to be related to the equipartition, separable, and interacting Gibbs models of chapter three. Although the grand canonical approach is often sufficient for these systems, a canonical or microcanonical approach often simplifies some of the computations. For example, it was shown that the Mayer cluster expansion for the high temperature behavior of the Bose gas can be more quickly and easily computed in the canonical model.

Chapter six applied the Gibbs model to the phenomenon of nuclear fragmentation. There it was shown that relatively simple models of fragmentation can explain the behavior of the mass and isotopic yields. Furthermore, the Gibbs models affords the possibility of exploring the effects of the fragmentation itself on the thermodynamic properties of nuclear matter. Of greatest interest is the question of whether a phase transition occurs in nuclear matter. A simple model incorporating some features of the nuclear forces indeed shows several aspects of phase-transitional behavior, including the appearance of a liquid-gas phase instability and the creation of large clusters. Indeed, the model is not especially different from the percolation model used by many experimental groups, although it has the advantage of having its thermodynamic properties explicit in the model. A deliberate comparison of this model was made with percolation theory in order to compare and contrast the two models.

One of the aims of this dissertation was to develop exact techniques to solve a wide class of fragmentation models. As a result, the greater portion of the introductory part of the dissertation explored the consequences of a particularly effective technique, the recursion implicit in the conservation laws. Clearly the conservation laws reveal themselves in a particular symmetry in the partition functions, and those symmetries indeed are the source of the unusual effectiveness of the recursive techniques. It should not be lost on the reader that the methods for extracting expectation values from the partition functions depend both on the availability of the partition functions, and also on a clear connection between these functions and the quantities to be measured. Such a connection is not guaranteed, and in fact is often difficult to elicit without some forethought and careful decomposition of the problem into solvable subproblems. For

the mass and isotopic yields, the connection was rather simple, but in the case of the reduced moments and informational entropy, the connection was more subtle.

Another aim was to use the models to understand the physics of nuclear fragmentation. The simple statistical models considered generated a surprisingly rich thermodynamics of nuclei. Various regimes show features which are described by Fermi liquids, Bose-Einstein condensates, van der Waals liquid-gas phase equilibria, and percolating clusters. Such a wide variety of phenomena from such a simplified model suggests that such an approach might not compromise too much. Theoretical and experimental studies have all suggested that the nature of the hadronic phase transition is closely related to that of percolating and liquid-gas transitions, and the models proposed here are consistent with those kinds of transitions.

This dissertation systematized some of the methods implicit in the work of others, and greatly extended their usefulness. At all points effort was made to credit original authors, and collect results together which previously had been separate, although the results of such efforts are mixed. The work of many groups closely paralleled each other, and another aim of this dissertation was to highlight those parallels, and reveal how different problems in physics and mathematics converged on the same set of models.

There are several truly novel aspects of this thesis. In particular, the combinatorial projection algorithms are both elegant and useful. They show how to connect models under various projection options, a topic which has received little attention, but is very important, since experiments in nuclear fragmentation tend to apply such coarse graining to the final states by making less than ideal measurements. For example most fragmentation experiments measure only the charge distribution: the distribution of isotopes is not measured, except perhaps for a few selected isotopes. As such the ideas of isotopic and isobaric equivalences connecting integer and vector partition models, and to a lesser extent ideas from Pólya-de Bruijn enumeration theory, are extremely useful in helping to connect the theoretical predictions and the experimental results. The result that the equipartitioning of permutations under several types of coarse graining yielded the same canonical Gibbs model was a surprising result which is only beginning to be appreciated.

The computation of observables in these models was shown to be practical for a number of different measures. The informational entropy (section 4.1.4) and reduced moments (section 4.3.1) in particular were shown to be exactly computable in polynomial time complexity by relating them to the ordinary partition functions. This fact enabled a number of hitherto impractical calculations to be possible. Previous to this result, such computations could only be done by sampling or exhaustive enumeration, methods which are limited in either accuracy or the size of the system which can be considered. At various times both methods were applied to the problems of this dissertation although in the end they proved to be unnecessary. In fact, the method used to expedite both calculations can be reasonably expected to be applicable to many possible measurements.

Having identified some of the accomplishments of this work, it remains to comment on the future directions to which these results can reasonably be expected to be applied. Chapter five showed that the models appear outside of nuclear fragmentation in many cases, and the one of current interest which immediately suggests itself is the fragmentation of atomic clusters such as C_{60}. This is an area which has already benefited from ideas from the nuclear shell model (i.e. magic numbers), and data for the fragmentation of such clusters is already being studied. Other nuclear fragmentation groups have already shown some interest in this area [128].

The future direction of this research as applied to nuclear fragmentation is perhaps unfortunately in the direction of greater complexity. To date, the models I have considered have had a considerably simplified but still realistic physics. I have not felt overly compelled to abandon the simplified models as they contain enough of the essential physics yet avoid enough of the detailed knowledge of nuclear structure that they might be considered a reasonable compromise between the contrary demands of predictive power and descriptive economy. However, the physics community has been inclined to prefer the former over the latter, and some serious drawbacks of the model as presented in chapter six need to addressed. The Copenhagen and Berlin models of nuclear fragmentation overcome some of these drawbacks by explicitly including much more physics. These two models can also be solved by the canonical approach favored in

this dissertation, although to date this has not been tried. Instead, the microcanonical (energy conserving) and grand canonical approaches have been explored. The microcanonical approach requires Monte Carlo sampling, and the grand canonical approach allows unphysical particle number fluctuations. A canonical approach might prove to be nearly as accurate as the microcanonical, yet require significantly reduced computer resources to evaluate, a situation which would improve its range of applications. The Copenhagen model in particular seems to be amenable to such an approach, and the grand canonical approach has already been explored by another research group. These two models have been particularly influential, and a quickly computable canonical solution of either of them would enable the physics to be explored in greater detail and accuracy.

In conclusion, the apparatus and methods of combinatorics when applied to a number of statistical models of fragmenting and aggregating systems yield solutions of surprising versatility and power. They can be applied to a number of areas in physics, mathematics and biology. Most especially, their application to the problem of nuclear fragmentation yields a number of schematic and intensive models which explain many aspects of the experimental phenomena. Most interesting, it appears that a nuclear liquid-gas phase transition will appear in many such models, and such a transition may already have been experimentally observed. The idea that the fragmenting degrees of freedom can substantially affect the thermodynamics of nuclei was illustrated effectively by the use of simplified models. In the future the effects of clustering on bulk properties of matter can be efficiently included by adopting the methods developed here.

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