THERMODYNAMICS OF
HEATED ROTATING NUCLEI

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ABSTRACT

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The large number of degrees of freedom that become available as nuclei are heated to finite temperature means that an exact solution for the levels of the system is impossible in this region. The properties of individual states become less accessible, as only average quantities can be determined either theoretically or experimentally. Thus thermodynamic methods are a natural way of dealing with nuclei at high excitation, since they provide well known procedures for extracting such average quantities. One such average quantity which has been measured recently is the average shape of $^{166}$Er at high energy and spin, which is seen to have a rapid change from a prolate to an oblate spheroid.

The method we have chosen to use to investigate this system is a Landau expansion in terms of the quadrupole deformation parameters. We develop a general expansion with both temperature and rotation dependent terms, and investigate the behavior of its equilibrium solutions. Scaling variables exist, and we are thus able to give universal formulas for the thermodynamic properties of the nuclear system in terms of dimensionless variables. The phase structure of the general expansion is explored, and we find that both first and second order transitions are possible.

The Landau theory is then applied to the case of $^{166}$Er, in order to see if the experimentally observed transitions can be reproduced. Rotation dependent terms in the expansion are taken from the rigid body moment of inertia, while the rest of the coefficients in the expansion are extracted from finite temperature Nilsson calculations. The phase diagram for this nucleus is given, and it is found that the region where the deformation changes most quickly is comparable in spin and energy to the experimentally observed transition region.

The equilibrium behavior of the Landau expansion of the free energy gives the behavior of the mean field solution. However, in a nucleus, where there are few particles,
fluctuations about the mean field can be significant. Thus we have investigated methods of dealing with fluctuations of the order parameter in order to better understand the behavior of the nuclear free energy. A simple prescription for dealing with these fluctuations is presented, along with a more rigorous method, known as the uniform approximation. The uniform approximation is applied to solvable many body Hamiltonians whose mean field solutions are known to undergo phase transitions, in order to estimate its effectiveness. It is found that fluctuations in the order parameter give a significant correction to the mean field values of both the free energy and the level density.
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Table of Contents

Chapter 1:
Introduction ................................................................. 1

Chapter 2:
Review of Statistical and Nuclear Physics ......................... 8
2.1.1 Review of Statistical Mechanics ............................... 8
2.1.1 Variational Calculations ......................................... 8
2.1.2 The Landau Theory ............................................... 10
2.1.3 Statistical Mechanics of Rotating Systems ............... 12
2.1.4 Level Densities ...................................................... 13
2.2. The Fermi Gas and Fermi Liquid Models ....................... 16
2.3.1 The Nilsson Model ............................................... 21
2.3.1 Zero Temperature and Finite Spin ......................... 22
2.3.2 Finite Temperature Effects .................................... 24
2.4. Microscopic Calculations at Finite Temperature and Spin 26

Chapter 3:
Phenomenology of Rotating Heated Nuclei ......................... 30
3.1. The Landau Expansion for Rotating Nuclei .................. 30
3.2. The $D = 0$ Case .................................................. 37
3.3. The General Case .................................................. 49

Chapter 4:
Application to $^{166}$Er .................................................. 55
4.1. Introduction and Phase Diagrams .............................................. 55
4.2. Isotherms .............................................................................. 62
4.3. Isentropic Lines ..................................................................... 64

Chapter 5:
The Uniform Approximation and Applications ............................. 71

5.1. Direct Evaluation of the Fluctuations .................................... 72
5.2. Uniform Treatment of Fluctuations ....................................... 73
5.3. The Lipkin Model as a Test of the Uniform Approximation ....... 78
  5.3.1 The Mean Field Approximation ......................................... 81
  5.3.2 Fluctuations and the Uniform Mapping ............................. 83
  5.3.3 Inclusion of Fluctuations in the Order Parameter Only ...... 88

5.4. The Multilevel Lipkin Model .................................................. 92

Chapter 6:
Conclusions .................................................................................. 101

Appendix A:
The Rigid Body Moment of Inertia ............................................. 104

Appendix B:
Explicit Formulas for the Phenomenology ................................. 106
The study of nuclear physics has traditionally been limited to fairly low energy states. Certainly the best explored and explained phenomena are those which occur near the ground state and have either a collective or single particle nature. In this region, the nuclear level density is quite low, and discrete levels may be identified. Theoretical models like the shell model or the IBA can predict the spectra and interlevel transitions well, and these properties are fairly easy to measure experimentally.

When higher energy excitations are considered, there are numerous problems. States with a high degree of non-collectivity may appear, as new degrees of freedom open up with the available energy. The proliferation of states leads to level densities that are neither experimentally nor theoretically resolvable. On the theoretical side, even if only one or two shells are considered, the number of states a few tens of MeV above the ground state may number into the millions. Experimentally, the widths of the states become comparable to or greater than their spacing, and a continuum type of spectrum results.

Nuclei in states having both large spin and excitation energy can be formed in heavy ion collisions. In such collisions, nuclei can fuse, and then begin to lose energy through neutron evaporation. Once the evaporation threshold has been crossed, nuclei lose energy through gamma-ray deexcitation, from states which are still quite high in energy. The transition rates can be calculated by using Fermi's Golden Rule, which requires knowledge of the level density in the region of the transition. Thus to really understand the behavior of the nuclei in this region, the level density must be known.
Since the level density is so large, it is hopeless to look at the properties of individual states, since they will not be resolvable. Only average properties such as the average shape and level density should be significant in this regime. In order to average over a set of states, their distribution must be known. Statistical methods are used in many branches of physics to perform such averages, and in combination with thermodynamics, give a framework in which to calculate them. The level density is the partition function for the microcanonical ensemble. This, however, is not a convenient object to deal with, since the energy is fixed. If the energy is allowed to fluctuate, then the canonical ensemble results. Its partition function at a temperature $T$ is given by

$$Z = \text{Tr} e^{-H/T},$$ \hspace{1cm} (1.1)

where $H$ is the Hamiltonian for the system. Since the nuclear thermal equilibration time can be shorter than the characteristic time for reactions, it may in fact be correct to think of the nucleus as having a finite temperature. The free energy,

$$F(T) = -T \ln Z(T),$$ \hspace{1cm} (1.2)

is a fundamental relation in thermodynamics from which all of the thermodynamical information about the system can be extracted.

If the level density is discrete, then the trace in Eq. (1.1) is a sum. If, instead, there is a continuum, or, as in the present case, so many states that the level density is almost smooth, then the partition function can be written as a Laplace transform of the level density $\rho$:

$$Z(T) = \int_{0}^{\infty} dE e^{-E/T} \rho(E).$$ \hspace{1cm} (1.3)

Thus if we can calculate the partition function we will be able to extract the level density by applying an inverse Laplace transform to Eq. (1.3). If the nucleus also has a finite spin, then the partition function must be considered in the rotating frame.
This trace is very complex, especially when the full many-body theory is considered. One must solve for all the levels of a strongly interacting many body quantum system to completely determine it, which is impossible for all but trivial cases. Since the many-body problem is so difficult, some sort of approximation must be used. One simplification is to assume that the particles each move independently in some sort of average potential that simulates the original Hamiltonian. By applying a variational principle, we can find the best such single particle potential by minimizing the free energy with respect to some chosen set of parameters. This results in a mean field approximation to the problem, which transforms the many body problem into a single particle one. The single particle substitution changes the nature of the difficulty of the problem, without reducing the number of degrees of freedom, so further approximations are necessary. The most significant degrees of freedom are thus chosen, usually by examining the nature of the collective behavior. In the nuclear case, for instance, the enhancement of E2 transitions among members of rotational bands has led to the conclusion that quadrupole degrees of freedom are the most important in describing the nuclear shape and density. By choosing these quadrupole deformation parameters as the most important, the free energy will come to depend on them as well as the temperature and spin. We will thus be able to find the equilibrium free energy by extremizing the free energy with respect to the deformation. The equilibrium values of the deformation will then be interpreted as describing the average shape of the nucleus. Microscopic calculations of the shape of the nucleus at high spin and energy have been carried out, but these tend to be long and intricate calculations, while here we are more interested in a general theory that can reveal the general behavior that is to be expected in the nucleus.

The theoretical prediction of the equilibrium shape can then be compared to experimental measurements of the shape. The average shape of the nucleus can
be determined experimentally, but this is quite difficult. Information about the shape of the nucleus can be inferred from the moment of inertia, which can be derived from the rotational spectrum. Rotational information can be derived at high spin and energy with the use of $4 - \pi$ detectors, including information about backbending. Investigating the shape directly, however, would be preferable to such an indirect method. One way this has been done recently is by inferring the shape from the observation of giant dipole resonances (GDRs) that are built on excited states. These resonances are thought to occur as the protons and neutrons inside a nucleus oscillate against each other. They decay primarily by E1 radiation, and tend to be quite broad in energy, showing the distribution of strength across many levels. Although the lowest energy resonances are built on the nuclear ground state, such resonances may be built on excited levels as well. If the nucleus is spherical, then no matter which way the nucleonic oscillations orient themselves, their frequency will be the same. If the nucleus is deformed, though, the frequencies along the principal axes will be different, since the nuclear density is assumed to be constant. Hence $\gamma$-rays deexciting the GDR built on such a deformed state should have an energy splitting according to the frequencies possible. Measuring these energy splittings is thus a way to examine the deformation degrees of freedom at high spin and excitation. Experiments to make this measurement have been performed, but are quite difficult, since the splittings are not very large and since there is competition with neutron evaporation in the decays. In addition, the signals leading to the splitting only arise from those $\gamma$-rays which are emitted in an early stage of the decay and hence are at quite high energy. The cross-section for emission falls exponentially in this region, leading first to small cross sections, and second to the fact that an exponential factor must be introduced in order to compensate for this dropoff. Once the cross-section is multiplied by this factor, given by the statistical part of the level density, $\exp(E_\gamma/T)$, the GDR must be fit by distributions modeling
Figure 1: $\sigma_\gamma(E_\gamma) \exp(E_\gamma/T)$ at the GDR. Solid lines show the two-function fit, and dashed the single distribution fit. Left: $E^* = 49.2\text{MeV} (T = 1.45\text{MeV})$, right: $E^* = 61.5\text{MeV} (T = 1.4\text{MeV})$

the strength functions of the resonance. The energy splitting is indicated by the fact that for some spectra, a single Lorentzian or Gaussian does not fit the data as well as a double distribution.

Such measurements have been made on $^{166}\text{Er}$ at different energies and spin. In one experiment, this nucleus was observed at an excitation energy $E^* = 49.2\text{MeV}$ and spin up to $25\hbar$. The splitting and strengths of the two peaks led to the interpretation that the ground state deformation was the same as has been observed in the ground state. In another experiment, the nucleus was observed at $E^* = 61.2\text{MeV}$ and spin up to $40\hbar$. The observed splitting led to the conclusion that at this higher energy and spin, the nucleus had lost the ground state prolate deformation, and was now oblate.

The two scaled cross-sections are presented in Fig. 1. The differences in $E^*$ and spin are not very great here, so it is important to find out first if such a transition is possible in this nucleus, and second, whether the transition can occur within such a limited range of the parameters. Since this rather marked transition occurs quite quickly, this indicates the possibility of a phase transition in spin and temperature.
We seek a general framework to describe the average behavior of nuclei in this excitation region. The Landau-Ginzburg theory is one such framework. When a phase transition occurs, states below the transition temperature often have a lower degree of symmetry than do the higher temperature states. In this theory, the free energy in the lower temperature regime is expanded in a quantity, known as an order parameter, which expresses the degree to which the symmetry is broken. At a phase transition, this parameter vanishes, and thus the expansion is in terms of this quantity when it is small. The coefficients of the expansion are functions of the thermodynamic variables, and can be derived in a number of ways, often by using the results of microscopic calculations in the Hartree-Fock approximation or from the Nilsson model. The expansion thus makes macroscopic predictions using as input the results of microscopic calculations. By extremizing a Landau-Ginzburg expansion at every value of the thermodynamic variables, with respect to the order parameter, the equilibrium values of the free energy are found. If an equilibrium order parameter is discontinuous at the transition, the transition is first order, otherwise it is second order or higher.

The mean field approach necessarily assumes that the influence of individual particles is negligible. In ordinary thermodynamic systems, this is the case, but here, where there are less than 200 particles, fluctuations about the order parameter can be significant. Thus we have also investigated an approximate method of evaluating these fluctuations. We have made this approximation by using the uniform approximation, in which the behavior of the free energy that is due to the order parameters and not to the other degrees of freedom is simply modeled. Thus we calculate fluctuations in the order parameter only. We have not yet applied these corrections to the mean field density in the full nuclear case, but have tested the validity of such an approximation in the Lipkin model, which is a solvable many-body model that undergoes phase transitions in its mean field solution. Thus we
are able to calculate two significant corrections to the level density, as compared with standard calculations within simple nuclear models, the effect of shape changes through the Landau-Ginzburg expansion, and the effect of fluctuations in the order parameter.

This thesis is organized as follows. In Chapter 2, some background material in statistical and nuclear physics will be presented. The basic statistical formulas will be presented, along with a brief description of various nuclear models that help in understanding the behavior of nuclei at high spin. Microscopic calculations of $^{166}$Er at finite temperature and spin have been carried out within the Nilsson model in order to determine the parameters of the Landau expansion, and so this model will be introduced briefly as well. Chapter 3 will present the general Landau-Ginzburg theory that we have used to give a unified description of the phenomena seen in the microscopic calculations. In Chapter 4, this theory will be applied to $^{166}$Er with input from the Nilsson calculations. Chapter 5 will describe ways that fluctuations can be handled, in order to extend our description of heated rotating nuclei beyond the mean field approximation the Landau expansion provides. A simple way of treating them is presented, as well as the uniform approximation, which provides a more accurate accounting. The approximations that go into this kind of calculation are difficult to assess. Thus the uniform approximation has been applied to the Lipkin model, which undergoes a second order transition in its mean field solution, and to the generalized Lipkin model, which can exhibit both first and second order transitions. Finally, Chapter 6 contains conclusions, as well as suggests future work we would like to carry out in this theory.
Chapter 2.

Review of Statistical and Nuclear Physics

2.1. Review of Statistical Mechanics

2.1.1. Variational Calculations

For any choice of thermodynamic variables, the equilibrium free energy is extremal. This suggests that the use of a variational principle in finding the free energy can be productive. The variational principle is defined with respect to a trial density function $D$, and thus the free energy functional to be extremized will be a function of the temperature and this trial density,

$$ F(T, D) = \langle H \rangle - TS = \text{Tr}(HD) + T \text{Tr}(D \ln D) , \quad (2.1.1) $$

where $S$ is the entropy. The trial density should be normalized to 1, and combined with the extremization condition, $\delta F/\delta D = 0$, yields

$$ D = \frac{e^{-H/T}}{\text{Tr} e^{-H/T}} , \quad (2.1.2) $$

which is just the density matrix for the canonical ensemble. Substituting this into Eq. (2.1.1), the canonical free energy results, $F(T) = -T \ln \text{Tr} e^{-H/T}$.

The canonical density is difficult to calculate for a many-body problem. If a one-body operator is used instead of the full Hamiltonian, the density becomes much easier to evaluate. Then, taking $\rho$ as a single-particle density, and denoting traces over single particle states by $\text{tr}$, the entropy becomes

$$ S = - \text{Tr}(D \ln D) = - \text{tr}(\rho \ln \rho) - \text{tr}[(1 - \rho) \ln (1 - \rho)] , \quad (2.1.3) $$
the entropy for a gas of independent fermions.

The canonical distribution assumes fixed particle number. If instead, the particle number is allowed to fluctuate as well as the energy, then the grand canonical distribution results. The particle number can be fixed for a particular problem with the use of a chemical potential, and since this distribution is more useful for nuclear physics calculations, it will be used from now on. All of the above derivations will follow in exactly the same way, but they are more clearly presented with the canonical distribution.

The free energy can be minimized with respect to the single particle density. In this case, the particles are assumed to be moving independently in some single particle potential well. Since this potential mimics the effect of the average interaction between particles, it is known as a mean field approximation. The minimization yields

\[ \rho = \frac{1}{1 + e^{(h_\rho - \mu)/T}}, \]  

(2.1.4)

where \( h_\rho \) is a single particle Hamiltonian calculated by averaging the two-body interaction with the single particle density matrix \( \rho \). This is a self-consistent equation, and is difficult to solve. A further simplification occurs if Eq. (2.1.4) is used with a non-self-consistent density in the definition of the mean-field Hamiltonian \( h_\rho \). Then the free energy can be evaluated, and

\[ F(T, \rho) = \sum_i \{ \epsilon_i + T [f_i \ln f_i + (1 - f_i) \ln (1 - f_i)] \}. \]  

(2.1.5)

Here the \( \epsilon_i \) are the single particle energy levels, and the \( f_i \) are generalized Fermi occupation numbers,

\[ f_i = \frac{1}{1 + e^{(\epsilon_i - \mu)/T}}. \]  

(2.1.6)

The chemical potential \( \mu \) is fixed by requiring \( \sum_i f_i = A \).

Since there has been no reduction in the number of degrees of freedom, even the non-self-consistent problem is very difficult to solve. If the physically important
degrees of freedom can be identified, then a tremendous simplification can be made. The Landau theory provides a framework in which the free energy is expanded in order parameters which are chosen because they characterize the most important degrees of freedom of a system. In terms of what has been done so far, we will choose only a few parameters for $\rho$ to depend on, and vary only with respect to them. If these parameters are held fixed for a given calculation, then a constrained mean-field theory will be obtained.

2.1.2. The Landau Theory

Before we specify these parameters, we will give a brief review of the Landau theory which will later be applied to rotating nuclei. When a phase transition occurs, one phase generally is of a higher symmetry than the other. We can thus identify an order parameter $\eta$ which characterizes the deviation from the more symmetrical state of the system, and then expand the free energy in a power series in $\eta$ near the transition point. The coefficients in such an expansion are functions of the temperature and any other appropriate thermodynamic variables. The equilibrium value of $\eta$ is found at each set of variables by minimizing the free energy. If there is more than one minimum, then the lowest must be chosen. Since the expansion is only valid in the neighborhood of the transition, the order parameter is usually small, and hence the expansion is cut off at some low order. In many cases, physical considerations can be used to set various of the coefficients to 0.

The behavior of the coefficients can be such that the equilibrium order parameter smoothly goes to 0, yielding a second order or higher transition. However, it is also possible that the transition can occur in such a way that the value of $\eta$ which minimizes the free energy moves discontinuously to 0, giving a first order transition. In general, explaining both types of transitions with a single expansion
requires that more terms be kept, in order to insure the stability of the equilibrium solutions.

In this thesis we present a theory of heated rotating nuclei in the spirit of such expansions. The expansion will be in terms of rotational invariants of the system, leading to a general formalism which can be applied to explain a wide variety of nuclear behavior. In this theory, the angular velocity plays the role of an external field, and we shall see that both first and second order transitions are possible. The order parameter for the theory will be a tensorial quantity, so that complex phenomena can occur even when the expansion is truncated at a fairly low order. In liquid-gas phase transitions, where the external field is the pressure, a line of first order transitions ends at a critical point. In our theory, however, different behavior is found. Here a line of first order transitions reaches a point beyond which a line of second order transitions continue. The point where these two curves join is called a tricritical point. Such a point indicates the existence of another external field, which when turned on results in critical surfaces rather than lines. An example of a system with a tricritical point is a dilute magnet in the presence of an external magnetic field. When the critical temperature for the phase transition is plotted against the chemical potential, with no external field applied, a tricritical point is seen. When the external field is turned on, this point is part of a whole tricritical surface that has first order transitions for small values of the external field, but only second order for larger values. The details of our theory will be presented in Chapter 3, after a review of the nuclear physics which underlies it.

For a finite system, such as the nucleus, fluctuations around the equilibrium solution for the order parameter will be important. These fluctuations tend to smooth out the roughness of the transitions predicted by the mean-field free energy. The basic idea behind the simplest extension of the Landau theory is that the probability for the deformation parameters to have a given value \( \eta \) is given by
$e^{-F(T,\eta)/T}$, whether or not $\eta$ is an equilibrium value. Thus a better approximation for the partition function is given by

$$e^{-F(T)/T} = Z(T) = \int d\eta \, e^{-F(T,\eta)/T}. \quad (2.1.7)$$

If the expansion models the free energy well at its extrema, then the mean-field approximation to the partition function should be good, since the extrema contribute most to the integral. When these extrema are close together, such as near a phase transition, the saddle point approximation breaks down. The flatness of the free energy surface in the order parameter means that it takes much less energy to fluctuate away from the minimum, since differing configurations will have nearly the same energy, and hence fluctuations should be more important there. A way of using the free energy expansion to evaluate these fluctuations will be presented in Chapter 5.

2.1.3. Statistical Mechanics of Rotating Systems

We are concerned in this thesis with rotational as well as thermal effects. Thus the results of Sect. 2.1.1 must be extended to include rotating bodies. If a Hamiltonian $H$ describes a system in a fixed frame, the transformation to a frame rotating with angular velocity $\tilde{\omega}$ with respect to the first results in an effective Hamiltonian

$$H' = H - \tilde{\omega} \cdot \vec{J}, \quad (2.1.8)$$

where the angular momentum is given by $\vec{J}$. Just as the canonical results were transformed to the grand canonical ones by the addition of a term including $\mu$, we can extend the above results by using $H'$ instead of $H$. This is equivalent to including the effects of an external field $\mathcal{O}$.

If $\vec{J}$ is chosen to be parallel to the $z$-axis, the free energy will be a function of $T$ and $\omega$ given by

$$F(T, \omega) = -T \ln \text{Tr} \, e^{-(H-\omega J_z)/T}. \quad (2.1.9)$$
The variational principle is the same, but the free energy now is given by

\[ F(T, \omega, D) = \langle H \rangle - TS - \omega \langle J_z \rangle. \tag{2.1.10} \]

Now, more thermodynamic information is available. For example, the average spin is determined from Eq. (2.1.10) by \( \langle J_z \rangle = -\partial F/\partial \omega \). As well, a moment of inertia tensor can be defined. If the angular velocity \( \omega \) is small, the the free energy can be expanded to second order

\[ F(T, \omega) = F(T, \omega = 0) - \sum_{ij} \omega_i I_{ij} \omega_j, \tag{2.1.11} \]

defining

\[ I_{ij} = \frac{\partial^2 F}{\partial \omega_i \partial \omega_j} \bigg|_{\omega=0}. \tag{2.1.12} \]

A mean field theory of rotating nuclei can be developed as above, where the one body Hamiltonian is replaced by a cranking form as in Eq. (2.1.8), but where \( H \) and \( \vec{J} \) are replaced by single particle operators \( h_\rho \) and \( \vec{j} \). This is then a finite temperature cranked HF theory.

### 2.1.4. Level Densities

We are interested in the information the free energy can tell us. We have already seen that the minimum of the free energy determines the equilibrium behavior of a system. Thus we can find the value of the order parameters and determine the behavior of the system as it makes a phase transition using the equilibrium values. The free energy contains all of the thermodynamic information about the system, so we can derive other thermodynamic quantities from it. Once the free energy is known, we can find the level density as well.

For a system with no external field, the partition function is given by Eq. (1.3), and the level density can be found by applying an inverse Laplace transform to this
equation,

$$
\rho(E) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} d(1/T) \ e^{E/T} Z(T) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} d(1/T) \ e^{[E-F(T)]/T}. \quad (2.1.13)
$$

The full inversion is not often useful, since it requires knowledge of the free energy throughout the complex $1/T$ plane. If the free energy is known numerically for real temperatures, then there exist inversion techniques for the transform. Since these methods rely on inverting at discrete points, they are unstable with respect to the inclusion of high frequency components of the function.

A simpler approximation to Eq. (2.1.13) is the stationary phase approximation. As long as a stable Hartree-Fock solution exists, the exponent will be concave and there will be at most one saddle point. This yields

$$
\rho(E) = \frac{1}{2\sqrt{\pi} \Delta} e^{S(E)} \quad (2.1.14)
$$

where the entropy $S$ is given as a Legendre transform of $F/T$ with respect to $1/T$ by

$$
S(E) = (-F + E)/T \quad (2.1.15)
$$

so that the inverse Laplace transform is replaced by Legendre transform by the stationary phase approximation. $\Delta^2 = T^2(\partial E/\partial T)$ is the variance of the canonical distribution. In Eq. (2.1.15), the saddle point temperature satisfies $\partial(F/T)/\partial(1/T) = E$.

In the rotational case, we can write the partition function in analogy with Eq. (1.3) as

$$
Z(T, \omega) = \int dE \ dJ_\omega \ e^{(E-\omega J_\omega)/T} \rho(E, J_\omega). \quad (2.1.16)
$$

where $\rho(E, J_\omega)$ is the level density for an energy $E$ and spin projection $J_\omega$. Applying inverse Laplace transforms in both $1/T$ and $\omega/T$ to Eq. (2.1.16) gives $\rho(E, \omega)$. The stationary phase approximation can be applied to evaluate both integrals, and yields

$$
\rho(E, J_\omega) = \frac{1}{4\pi \sqrt{D}} e^{S(E, J_\omega)}. \quad (2.1.17)
$$
The entropy \( S(E, J_z) \) is obtained as a Legendre transform of \( F(T, \omega)/T \),

\[
S = -\frac{F}{T} + \frac{E}{T} - \left( \frac{\omega}{T} \right) J_z. \tag{2.1.18}
\]

Now \( \omega \) and \( T \) are found from \( E \) and \( J_z \) by \( J_z = -\partial F/\partial \omega \) and \( E = \partial (F/T)/\partial (1/T) \). \( D \) is the determinant of the variance matrix with respect to \( E \) and \( J_z \). Since we are interested in the level density at a given spin rather than spin projection, we can use the fact that \( J_z = J \) gives the highest angular momentum projection of a multiplet. Any states which have this same projection, but lie in a higher spin multiplet must also be counted in \( \rho(E, J_z = J + 1) \), and thus the difference of the level densities at these two spin projections will give a value proportional to the level density at the desired spin. This level density is thus given by

\[
\rho(E, J) \approx \frac{d \rho}{d J_z} \bigg|_{J_z = J}. \tag{2.1.19}
\]

This method relies on the stationary phase approximation giving a reasonable value for the integral. As \( T \to 0 \), the denominator of Eq. (2.1.13) vanishes, signaling the breakdown of that approximation. Thus this method is limited to fairly high temperatures.

Instead of using the approximate formula of Eq. (2.1.17), it is possible to project the spin exactly. This method relies on analytically continuing \( \omega \) to complex values, so that we evaluate \( Z(T, i\omega) \). Instead of integrating over the spin, we now take advantage of the fact that the spectrum of the angular momentum operator is not continuous, but discrete. We can thus evaluate the sum over the magnetic quantum number for each multiplet. This sum yields the character of the \( SU(2) \) representation \( J \):

\[
\sum_{m=-J}^{J} e^{-i \omega m/T} = \frac{\sin((J + \frac{1}{2})\omega/T)}{\sin(\frac{1}{2}\omega)/T}, \tag{2.1.20}
\]

so that the full partition function can be written as

\[
Z(T, i\omega) = \sum_{J} \frac{Z_J(T)}{(2J + 1)} \frac{\sin((J + \frac{1}{2})\omega/T)}{\sin(\frac{1}{2}\omega)/T}. \tag{2.1.21}
\]
$Z_J(T)$ is the partition function at a fixed spin $J$, $Z_J(T) = \text{Tr}_J e^{-H/T}$. This equation is in the form of a Fourier sum over the spins since the characters (2.1.20) satisfy orthogonality conditions similar to those seen in ordinary Fourier expansions. Eq. (2.1.21) is easily inverted to give $Z_J(T)$ in terms of $Z(T, i\omega)$

$$Z_J(T) = \frac{2J + 1}{2\pi} \int_0^{4\pi} d\left(\frac{\omega}{T}\right) \sin \frac{\omega}{2T} \sin \left(J + \frac{1}{2}\right) \frac{\omega}{T} Z(T, i\omega).$$

(2.1.22)

We can finally apply an inverse Laplace transform to $Z_J(T)$ with respect to $1/T$ to get $\rho(E, J)$.

2.2. The Fermi Gas and Fermi Liquid Models

We turn next to review the various nuclear models which can help to identify the order parameters and define the coefficient functions in the expansion. Special emphasis will be put on the prediction each model makes for the moment of inertia, since this will play an important role in the thermodynamic theory of heated rotating nuclei. The liquid drop and Fermi gas models will be briefly discussed, followed by a description of the pairing-quadrupole model, a many body model. Due to the problems inherent in analyzing such a model, a one body model related to it will be discussed next, the Nilsson model. A general discussion of cranking and finite temperature methods as applied to nuclear physics problems will also be presented.

Bulk properties of nuclei, such as the binding energy and the energies of some giant resonances, can be described by considering the nucleus as a charged liquid drop. The nucleus has a fairly sharp surface and is nearly incompressible, so a liquid drop should be a fairly good macroscopic analog to it. Since the nucleons are fermions, however, there will be some differences with ordinary liquids. For example, the mean free path and interparticle spacing are both much larger than might be expected from a purely classical drop. The static liquid drop model can be used e. g. to derive a formula for the binding energy for nuclei, but this is not...
the kind of property this thesis is concerned with. More important to the present work is how this model describes the density distribution of the nucleus.

One way to describe the nucleus is to parameterize its surface by giving the nuclear radius. Since the nucleus is assumed to be incompressible and to have a sharp surface, this description should be adequate. These assumptions also provide one constraint on such a description, that the nuclear volume as so described should be constant. Even those nuclei which are deformed are generally only slightly non-spherical, so it is natural to describe the nuclear radius in terms of small deviations from sphericity. Since fission degrees of freedom will not be discussed here, it is unlikely that necks will form, and hence the radius will be single valued. One such description of the surface is

\[ R = R(\theta, \phi) = R_0 \left( 1 + \alpha_{00} \sum_{\lambda=1}^{\infty} \sum_{\mu=-\lambda}^{\lambda} \alpha_{\lambda\mu}^* Y_{\lambda\mu}(\theta, \phi) \right), \]  

where \( R_0 \) is the radius of the spherical drop, and \( \alpha_{00} \) is a constant to insure volume conservation.

For many years it has been known that the most important multipole for nuclei in such an expansion is the quadrupole, and this work will consider only \( \lambda = 2 \). In this case, the five component spherical tensor \( \alpha_{\lambda\mu} \) of the quadrupole deformation parameters will be identified as the order parameters in the Landau theory. This tensor can be defined in a more general context as the expectation values of the quadrupole moment operator \( Q_{2\mu}, \alpha_{2\mu} \equiv < Q_{2\mu} > \). These five parameters do not all describe the shape of the nucleus, since they also give its orientation in space. If the axes of the coordinate system are chosen to coincide with the principal axes of the drop there will thus be only two degrees of freedom left corresponding to the intrinsic deformation of the drop. These two coordinates are real, and are usually denoted \( a_{20} \) and \( a_{22} = a_{2-2} \) (in this frame, \( a_{11} = a_{1-1} = 0 \)). The two non-zero
coordinates are generally used in the Bohr parameterization\(^{10}\), where

\[
\begin{align*}
\sigma_{20} &= \beta \cos \gamma \\
\sigma_{22} &= \frac{1}{\sqrt{2}} \beta \sin \gamma.
\end{align*}
\]  

(2.2.2)

It was not specified above which axis of the coordinate system coincides with which axis of the drop, and hence there must be a three-fold symmetry in the \(\beta - \gamma\) plane such that a rotation of \(\frac{2\pi}{3}\) yields the same shape with a different orientation. The physics will in general not depend on this orientation, so usually it is enough to consider one \(\frac{\pi}{3}\) sextant of the plane, since the others are gotten just by interchanging axes. In this work, however, this is not the case, since by considering rotation, a preferred direction is being chosen. Now the two directions perpendicular to the rotation axis are equivalent and there is instead a mirror symmetry in the \(\beta - \gamma\) plane. An entire half plane must now be considered, although as shall be seen later, not all parts of it admit stable rotations. A diagram showing the various possible shapes for different values of \(\beta\) and \(\gamma\) is given in Fig. 2, where the collective or non-collective nature of rotation about the 3-axis is also marked for the axially symmetric shapes.

For now, consider the nucleus generally. If the nucleus is a Fermi liquid, then irrotational flow is possible, i. e. in the laboratory frame, the particle flow has no curl. The transition probability for exciting a state is given by its \(B(E\lambda)\) value, and a sum rule for the \(E\lambda\) moment may be defined, giving the total overlap of excited states with the ground state through the \(E\lambda\) operator. For shape vibrations in general, it can be shown\(^9\) that the oscillator strength of a given vibration is a function of the ratio of the mass parameter of irrotational flow to the given flow. In a liquid drop model, all of the oscillator strength of each multipole goes into the corresponding surface vibration, and hence the flow must be irrotational.
The Fermi Gas and Fermi Liquid Models

Figure 2: The shape of the liquid drop as specified by the Hill-Wheeler coordinates. Our rotation axis is axis 3 on this graph. Coll or non-coll indicates whether the rotation is collective or non-collective, respectively. This graph is taken from Ref. 11.

The Hamiltonian for such a liquid drop can easily be written down\textsuperscript{12}. When written in general coordinates, the kinetic energy splits into two pieces, corresponding to vibrational and rotational modes. The vibrational part will not be discussed
at this time, while the other part may be written as \( \sum_k \omega_k^2 \mathcal{Q}_k \). Since the flow was shown to be irrotational, \( \mathcal{Q}_k \) can be identified as the moment of inertia corresponding to this flow. To lowest order in \( \beta \),

\[
\mathcal{Q}_k = \frac{3}{2\pi} m A R_0^2 \beta^2 \sin^2 \left( \gamma - \frac{2\pi}{3} k \right). \tag{2.2.3}
\]

Here \( m \) is the nucleon mass, \( A \) is the total particle number, and \( R_0 \) is the radius of the corresponding sphere. Note that this moment vanishes when the nucleus is spherical, as rotations about a sphere are not dynamical in quantum mechanics.

The liquid drop model can be used as well to calculate the free energy surface as a function of the order parameters \( \beta \) and \( \gamma \). The liquid drop energy at zero spin and temperature has two contributions, the Coulomb self energy, and the surface energy. These are measured in terms of their deviations from the spherical values, and in units of these values. The Coulomb energy \( \delta E_C \) is an integral over the potential between all points inside the drop, and can be expressed as an elliptic integral\(^{13}\). The surface energy \( \delta E_S \), which acts as a surface tension to hold the drop together, is just the surface integral over the drop. The final result is

\[
E_{LD} = 0.70521 \frac{Z^2}{A^{1/3}} \delta E_C (\beta, \gamma) + 17.9439 \left( 1 - 1.7826 \left( \frac{(N - Z)^2}{A} \right) \right) A^{2/3} \delta E_S (\beta, \gamma) \tag{2.2.4}
\]

where coefficients give the spherical values, and the extra surface term accounts for the reduced surface energy associated with increased nucleon asymmetry\(^{14}\). For the rotating case, an extra term is added, which is the rotational energy for the drop, assuming it to have a rigid body moment of inertia\(^{15}\), defined below. The \( \omega = 0 \) liquid drop model always has the spherical solution as its minimum, and the rotating case always has an oblate solution. Thus the liquid drop model does not have any phase transitions, since at 0 temperature the equilibrium shape already has the highest possible symmetry.
Another simple model for nuclear collective behavior is the Fermi gas model. Here, the nucleons are assumed to be a non-interacting gas constrained inside of a box, rather than a liquid which finds its own equilibrium shape. Thus single particle degrees of freedom can be included, but the deformation is not. Since each nucleon satisfies a free Schrödinger equation in a box at zero temperature, the Pauli principle forces all allowed states up to the Fermi level to be filled with an occupation number of 1. At a finite temperature, the occupation numbers will be of the form of Eq. (2.1.6), and the Fermi level will be replaced by the chemical potential \( \mu \).

The Fermi gas model also provides the other extreme for rotational behavior. If a Fermi gas, or in fact any system with a local potential, is rotated, then the velocity flow at any point is isotropic, and hence there is no net flow. Thus the moment of inertia will be the same as the rigid body, although the flow itself may not be rigid\(^\text{16} \).

The rigid moment of inertia about the \( z \)-axis is given by

\[
I_{zz} = \int \rho r^2 \sin^2 \theta \, dV. \tag{2.2.5}
\]

Upon integrating \( I_{zz} \), one gets

\[
I_{zz} = \frac{2}{5} m A R_0^2 \left( 1 - \sqrt{\frac{5}{4\pi}} \beta \cos \gamma + \frac{15}{28\pi} \beta^2 + \frac{10}{7\pi} \beta^2 \sin^2 \gamma \right). \tag{2.2.6}
\]

using Eq. (2.2.1) above for the radius. This result is to order \( \beta^2 \), rather than to first order as is usually done, and is discussed in Appendix A.

2.3. The Nilsson Model

2.3.1. Zero Temperature and Finite Spin
We now turn to discuss a more refined single particle model in which a deformed potential is used which depends on the parameters $\beta$ and $\gamma$. As discussed in the section on mean fields, this will be a constrained Hartree-Fock type of calculation. The nuclear interaction is mainly due to the nuclear shell model. There are, however, effects at low temperature and spin which suggest that in addition to this principal component, there are residual interactions as well. Many nuclei away from closed shells exhibit definite rotational behavior, thus indicating the existence of some sort of deformation. Since from other considerations the nucleus is known to be nearly spherical, it would seem reasonable to interpret these deformations in terms of small deviations away from sphericity. The rotational bands of such nuclei decay mostly by quadrupole radiation, suggesting that the nuclear deformation has a quadrupole nature as well. Another effect is derivable from the fact that even-even nuclei tend to have very few low-lying collective states, while nearby odd nuclei often have very many. This indicates the possible presence of a pairing interaction which serves to couple nucleon pairs to $J = 0$. This interaction lowers the energy of the pair, and hence requires a large amount of energy to break it, leading to high lying collective states. A model which incorporates these two effects is called the pairing-quadrupole model\textsuperscript{17}. The Hamiltonian for this model has three terms, a single body part for the spherical shell model, a two body quadrupole-quadrupole interaction, and a two body pairing interaction.

This many body Hamiltonian is easily written down, but is very difficult to solve in full. The Hartree-Fock-Bogolyubov approximation is often applied to it\textsuperscript{18} in order to make a more tractable single body problem. In this approximation, a self-consistent field is derived to model the quadrupole interaction, while the pairing interaction is treated as in the BCS method\textsuperscript{10}. Thus the spherical shell model is modified by a quadrupole field, leading to a deformed shell model, the Nilsson model.
This work is not concerned with nuclear ground states, but instead with rotational and thermal excitations of nuclei., and the Nilsson model must be modified by the inclusion of these two effects. The first of these is handled by the use of the cranking method, as in Eq. (2.1.8), with the Nilsson Hamiltonian in the lab frame. Thus in this model, nucleons are moving in a rotating potential well. Many important nuclear effects can be modeled by this formulation, including Coriolis antipairing and rotational alignment of broken pairs, both of which lead to reductions in pairing strength. The \( \omega \) in Eq. (2.1.8) is not an observable, but is usually considered as a Lagrange multiplier used to fix the average value of the spin. In analogy to classical mechanics, the moment of inertia \( \mathcal{S} \) can be defined by

\[
\mathcal{S} = \langle J \rangle / \omega. \tag{2.3.1}
\]

By considering the angular momentum term as a perturbation on the Hamiltonian, an expression for the moment of inertia can be derived, known as the Inglis formula:

\[
\mathcal{S} = 2 \sum_{im} \frac{\langle m | J_z | i \rangle^2}{\epsilon_m - \epsilon_i}, \tag{2.3.2}
\]

where \( m \) and \( i \) denote states above and below the Fermi level, respectively. This gives results quite similar to rigid body values when the pairing is absent as was argued at the end of Sect. 2.2.

Single particle models such as the Nilsson model tend to predict the average behavior of nuclear spectra incorrectly, while giving a very good idea of the fluctuations around these averages due to shell effects. Since the shell effects are more or less due to the valence particles, this is not surprising. A method has been developed by Strutinski to compensate for this inaccurate average behavior by substituting for it the average behavior of a charged liquid drop. Since the core particles are expected to behave primarily in a collective fashion, this should be a good approximation.
In this method, the average part of the single particle spectrum is found by averaging the discrete spectrum over a distribution that has Gaussians centered at each energy multiplied by interpolating polynomials. The order of the polynomial and the width of the Gaussian are varied until the smoothed energy is insensitive to further variations. Thus the Strutinski energy is given by

\[ E_{\text{Stru}} = E_{\text{sp}} - \tilde{E} + E_{\text{LD}} \]  

(2.3.3)

where \( E_{\text{sp}} \) is the summed single particle energy, \( \tilde{E} \) is the averaged single particle energy, and \( E_{\text{LD}} \) is the corresponding liquid drop energy. When the cranking Hamiltonian is used, then Eq. (2.3.3) is modified to give

\[ E_{\text{Stru}}(\omega) = E_{\text{sp}} - \tilde{E} + \frac{\omega^2}{2} (S_{\text{LD}} - S_{\text{Stru}}) + E_{\text{LD}} \]  

(2.3.4)

where now all values except the liquid drop ones are from energies calculated using Eq. (2.1.8) with the Nilsson Hamiltonian. The average value \( \tilde{E} \) is found to be roughly linear\(^{24}\), in \( \omega^2 \) and thus in practice is calculated only for the smallest and largest \( \omega \) points. Here \( S_{\text{Stru}} \) is the smoothed moment of inertia, and is taken as the constant of proportionality between \( \tilde{E} \) and \( \omega^2 \). \( S_{\text{LD}} \) is the rigid body moment of inertia. The Strutinski method thus combines the Nilsson model, which describes microscopic, single particle effects, with the liquid drop, a more macroscopic and collective model, to simulate the self-consistent Hartree-Fock calculations.

### 2.3.2. Finite Temperature Effects

The Hartree-Fock calculations at zero-temperature may be extended to non-zero temperatures by using a finite temperature variational principle as in Sect. 2.1. The grand canonical potential is used, and results in equations formally identical to the zero-temperature ones\(^ {25}\). Pairing can be included as well in both the finite and zero temperature calculations. The self-consistent potential in a theory of this type
can be found by effecting a linear transformation of the single particle basis. When pairing is present, the change of basis will involve states both above and below the Fermi level and is called a Bogolyubov transformation. Thus particle number is not preserved and the single-particle states are replaced by quasiparticle states.

The solution of a fully temperature dependent problem with pairing is very difficult, due to the high level of mixing between states from both pairing and finite temperature effects. Finite temperature BCS calculations show that even for $J = 0$, the pairing gap usually vanishes for temperatures of about 1MeV\textsuperscript{26}. In addition, Coriolis forces tend to reduce pairing even at low levels of spin, so that the pairing vanishes at even lower temperatures for a rotating system. Since the shape phase transition is expected to occur at higher temperatures and spins, the pairing has been set to zero for all calculations. Even with the absence of pairing, the self-consistent energies of the single particle solution must be solved for. However, it is observed that energies do not change very much with temperature\textsuperscript{27} and thus the $T = 0$ spectrum is used to calculate the entropy

$$S = - \sum_i \left[ f_i \ln f_i + (1 - f_i) \ln (1 - f_i) \right],$$

(2.3.5)

where the factors $\{f_i\}$ are given by Eq. (2.1.6). The chemical potential $\mu$ is set as mentioned above, by fixing the particle number at the desired value.

The energy which results from these finite temperature manipulations must also be smoothed. There are problems with this procedure at finite temperature\textsuperscript{28,27} especially in defining the liquid drop energy at finite temperature. For this reason, the Strutinsky smoothing at of the finite temperature energy has actually been done with zero temperature liquid drop values. Thus the free energy in the rotating frame will be

$$F = E_{\text{Stru}} - TS - \omega J.$$  

(2.3.6)
2.4. Microscopic Calculations at Finite Temperature and Spin

The Landau theory that we will develop should exhibit the same behavior as microscopic models, and thus we have investigated the behavior of the Nilsson model in order to derive a microscopic free energy. In the ground state, medium heavy nuclei such as $^{166}$Er often have a prolate deformation. However, as the temperature and spin increase, microscopic effects become less important, and macroscopic models are more accurate. Thus we expect that at some spin and temperature, the shape should shift from prolate to oblate.

The program used for the Nilsson levels is a standard one using fully triaxial deformations. The deformations are given in "stretched" coordinates rather than the Hill-Wheeler system used earlier. This choice of coordinates is used because the deformation terms vanish between nearby oscillator shells. The two coordinate systems are related by

$$\beta = \frac{1}{.946} \log \frac{1 + \frac{2\epsilon}{3}}{1 - \frac{\epsilon}{3}}. \quad (2.4.1)$$

The values from Eq. (2.3.6) are calculated for each point in $\epsilon$ and $\gamma$, for a variety of $\omega$ values. The minimum point of Eq. (2.3.6) is found and this point is considered the equilibrium deformation at the given $\omega$ and temperature.

The Nilsson model has been calculated for a grid of points in the $\epsilon - \gamma$ plane and for values of omega between 0 and .09 $\omega_0$. As explained in Sect. 2.2 and shown in Fig. 2, we choose the lower half plane for our calculations. The upper half-plane will yield identical results. The unit of rotation is the average oscillator shell spacing, $\omega_0 = 41 A^{-1/3} / h\text{MeV}$. These values were then used in finite temperature and Strutinski calculations to derive the free energy surface.

Sample contour plots are given in Fig. 3, for $T = 1.1\text{MeV}$, and in Fig. 4, for $T = 1.5\text{MeV}$. The top plot of each is at $\omega = 0$, the middle at $\omega = .03\omega_0$, and the bottom at $\omega = .06\omega_0$. The lines of $\gamma = -\frac{\pi}{3}$ and $\gamma = -\frac{2\pi}{3}$ are shown as well, to identify...
Figure 3: Contour plots for $T = 1.1\text{MeV}$. Contours are $.5\text{MeV}$ apart. From top to bottom, the rotational frequencies are $\omega = 0, .03, .06\omega_0$. Lines at $\gamma = -\frac{\pi}{3}, -\frac{2\pi}{3}$ are also shown. The spin $J$ at the equilibrium point is given.
Figure 4: As in Fig. 3, but for $T = 1.5\text{MeV}$
the lines of pure oblate and pure prolate shapes, respectively. In all calculations at \( \omega = 0 \), the expected threefold symmetry is seen, as the energy along the \( \gamma = -\frac{2\pi}{3} \) line is the same as for \( \gamma = 0 \). For \( \omega = 0.03\omega_0 \), the minimum has moved away from the prolate line, towards the oblate states at \( \gamma = -\pi \). This frequency corresponds to a spin of \( 15 - 20\hbar \), depending on the temperature. The higher temperature calculations show the minimum to be much broader and to have moved further from the pure shape. At all frequencies, the higher temperature saddle points are closer to the origin than the lower temperature ones. The prolate minimum at \( \gamma = 0 \) is no longer degenerate with the global minimum for any finite spin, as is clearly shown by the middle plot in both cases. Again, in the \( T = 1.5\text{MeV} \) calculation this point has moved more than in the lower energy calculations, showing one of the effects of increased temperature. By \( \omega = 0.06\omega_0 \), both of these temperatures show only one extremum in the plane, indicating that liquid drop effects dominate, and that shell effects have essentially vanished. The behavior to be expected from our theory is thus that at a fixed temperature, as the rotational frequency increases, the global minimum moves from the prolate axis at \( \gamma = -\frac{2\pi}{3} \) to the oblate axis at \( \gamma = -\pi \). The transition should be fairly quick, since in these calculations, while the minimum has clearly moved away from the prolate shape by \( \omega = 0.03\omega_0 \), there is much more movement in the same interval in \( \omega \), between \( \omega = 0.03 \) and \( \omega = 0.06\omega_0 \). For fixed spin and increasing temperature, the motion should be similar, but coupled to a sharply decreasing \( \epsilon \) with increasing temperature.

Thus in this microscopic model, shape phase transitions are indeed seen in \( T \) and \( \omega \). The calculations were done in one specific model and nucleus, but the behavior should be quite general. It is with the hope of describing the general behavior that we introduce in the next chapter in the framework of the Landau theory, a way to describe and analyze general transitions of nuclei in this region.
3.1. The Landau Expansion for Rotating Nuclei

We now proceed to develop a Landau expansion that will help to analyze the behavior of nuclei which have high energy and spin. An expansion of the nuclear free energy at zero spin and finite temperature in terms of quadrupole deformation parameters $\alpha^{(2)}$ was considered in Ref. 31. In this chapter, the nuclear free energy will be expanded in the same parameters, but at finite spin. This is a general theory, simple enough that it can be thoroughly analyzed, but at the same time has a rich variety of phase behavior.

In order to discover the appropriate form of the expansion, consider a free energy of the form

$$F(T,\omega) = -T \ln \text{Tr} e^{-\frac{(H-\vec{\omega} \cdot \vec{J})}{T}}.$$  \hspace{1cm} (3.1.1)

For $\omega = 0$, this $F$ is clearly a rotational invariant, since $H$ is. For $\vec{\omega} \neq 0$ fixed in space, $F$ is no longer rotationally invariant unless $\vec{\omega}$ is rotated as well. Thus $F$ will be rotationally invariant, when viewed from the vector $\omega^{(1)}$ and the tensor of deformation parameters $\alpha^{(2)}$. $F$ clearly should not depend on the sign of $\vec{\omega}$, and thus only even powers of it should appear. Limiting the expansion to second order in $\vec{\omega}$, Eq. (2.1.11) can be rewritten to give

$$F \left( T, \vec{\omega}, \alpha^{(2)} \right) = F \left( T, \omega = 0 \right) - I_0 (\vec{\omega} \cdot \vec{\omega}) - \left[ I^{(2)} (\omega^{(2)} [\omega \times \omega]) \right]^{(0)}, \hspace{1cm} (3.1.2)$$

where $I_0(T, \alpha^{(2)})$ is a general scalar built from $\alpha$, and $I^{(2)}(T, \alpha^{(2)})$ is a general rank 2 tensor built from the same quantities.
We will limit the expansions of $I_0$ and $I^{(2)}$ to second order in the $\alpha$. Then there are only two terms in $I_0$,

$$I_0 = F_0' + A'(\alpha \cdot \alpha).$$

(3.1.3)

The only possible second order tensorial terms of the correct order are the tensor itself and a single recoupling

$$I^{(2)}_2 = R\alpha^{(2)} + D\left[\alpha^{(2)} \times \alpha^{(2)}\right]^{(2)}.$$

(3.1.4)

Notice that $I_0$ and $I^{(2)}$ are the scalar and traceless second rank parts of the decomposition of the symmetric moment of inertia tensor $I_{ij}$.

We can now choose a specific direction for $\omega$, namely along the $z$-axis, and evaluate all of these terms in that frame. In general, then, the free energy will be a function of the deformation parameters $\beta$ and $\gamma$ and the Euler angles. The Euler angles will define the orientation of the intrinsic frame, in which the deformation tensor is diagonal, with respect to the rotation axis. Since $\alpha$ completely determines the moment of inertia tensor in this case, the intrinsic frame (defined to be the frame in which $\alpha$ is diagonal) is the same as the principal frame (in which the moment of inertia is diagonal).

The orientation is found by extremizing the free energy with respect to it. This calculation has the result that the rotation axis must be parallel to one of the principal axes. If the rotation $z$-axis and the principal $z$-axis are chosen to be the same, then, as is seen in Fig. 2, all possible shapes and orientations are given when $\gamma$ is in the interval $-\pi \leq \gamma \leq 0$, and the free energy reduces to $F(T, \omega) = F(T, \omega = 0) - I_{zz} \omega_z^2$. This means that for $\gamma = 0$, there is a prolate spheroid rotating about its axis of symmetry and for $\gamma = -\frac{2\pi}{3}$ there is a prolate spheroid rotating about an axis perpendicular to its axis of symmetry. The same rotations occur for an oblate spheroid for $\gamma = -\pi$ and $\gamma = -\frac{2\pi}{3}$, respectively.
The Landau Expansion for Rotating Nuclei

There are recognized to be two limits for the rotational behavior of the nucleus. If the particles move independently, as in the Fermi gas model\(^9\), then there will be no net flow in the rotating frame and the moment of inertia will be the classical rigid body one. At the other extreme, if the nucleus were completely superfluid, then the flow would be irrotational. In practice, experimental\(^{15}\) and theoretical\(^{32}\) results indicate the flow to be somewhere in between. Since the actual moment of inertia will be some mix of the two, the actual stability region should be a subset of the union of these two regions.

For a rigid body, the moment of inertia is given classically. This immediately shows that rotation of the shapes for \(\gamma = -\frac{2\pi}{3}\) and \(\gamma = -\pi\) is stable according to the above criteria, while for \(\gamma = 0\) and \(\gamma = -\frac{\pi}{3}\) it is unstable. To lowest order, the rigid body moment of inertia about the axis \(k\) is given by (see Sect. 2.2.)

\[
I_{kk} \propto \left(1 - \sqrt{\frac{5}{4\pi}} \beta \cos \left(\gamma - \frac{2\pi}{3}k\right)\right).
\]

The deformation dependent part of this expression is exactly the term proportional to \(R\) in Eq. (3.1.4) when considered in the principal frame. Thus we shall refer to the \(R\) term in Eq. (3.1.4) as the "rigid body" term. For rotation about the \(z\)-axis, the stability condition \(I_{zz} > I_{xz}, I_{yy}\), gives \(-\pi < \gamma < -\frac{2\pi}{3}\). Similarly, the irrotational moment of inertia is given to lowest order by

\[
I_{kk} \propto \beta^2 \sin^2 \left(\gamma - \frac{2\pi}{3}k\right),
\]

showing the stability region for this flow to be \(-\frac{2\pi}{3} < \gamma < -\frac{\pi}{3}\). This expression is seen to be the term that is multiplied by \(D\) in Eq. (3.1.4), and hence this term will be referred to as the "irrotational" term. For the total problem, the stable saddle points will lie in the region \(-\pi < \gamma < -\frac{\pi}{3}\), and there will never be stable rotation for shapes lying in the remaining third of the lower half-plane.
The nuclear free energy for the non-rotating case has been developed\textsuperscript{31} in terms of the quadrupole deformation parameters. The requirement that the free energy be a scalar formed from the 5 components of the quadrupole deformation $\alpha^{(2)}$ led to the expansion being limited to those terms that appear in Eq. (3.1.3) plus other terms up to fourth order in $\alpha^{(2)}$ given by $[\alpha^{(2)}, [\alpha^{(2)} \times \alpha^{(2)}]^{(2)}]$ and $(\alpha \cdot \alpha)^2$. All calculations are being carried out in the intrinsic frame, and hence we can parameterize the diagonal elements of the deformation tensor by $\alpha_{22} = \alpha_{2-2} = \frac{1}{\sqrt{2}} \beta \sin \gamma$, $\alpha_{21} = \alpha_{2-1} = 0$, and $\alpha_{20} = \beta \cos \gamma$. With these choices the terms in the expansion are $\beta^2$, $\beta^3 \cos \gamma$, and $\beta^4$. Thus the free energy in this case was

$$F(T) = F_0 + \tilde{A}\beta^2 - \tilde{B} \beta^3 \cos 3\gamma + \tilde{C} \beta^4. \quad (3.1.5)$$

As a simpler example of the kind of analysis and behavior which we will see in the general theory, the behavior of the $\omega = 0$ mode will be reviewed.

For the non-rotating nucleus, Eq. (3.1.5) is quartic in $\beta$ and has only a single term in $\gamma$. From $\partial F / \partial \gamma = 0$, prolate or oblate solutions are found to be stable equilibria if $\tilde{B}$ is greater or less than 0, respectively. For $\tilde{B} = 0$, the equilibrium is independent of $\gamma$, and hence these nuclei are called “$\gamma$ unstable”. Note that there are no triaxial saddle points, and hence this equation implies there are no stable triaxial extrema. Thus we take $\gamma = 0$, and consider the free energy as a function of $\beta$ only.

The other equation, $\partial F / \partial \beta = 0$, gives rise to the interesting phase structure of the problem. This is a cubic equation, which always has a solution of $\beta = 0$, and depending on the value of $\tilde{A}_s = \tilde{A}\tilde{C}/\tilde{B}^2$, has another zero or two real solutions. The real solutions for $\beta$ are given by

$$\beta = \frac{\tilde{B}}{\tilde{C}} \left( 1 \pm \sqrt{1 - \frac{32\tilde{A}_s}{9}} \right). \quad (3.1.6)$$
Thus all quantities in the model depend functionally on $A_s$, with the combination $B^\beta / C$ serving to scale the solutions of $\beta$. Substituting Eq. (3.1.6) into the expression for the free energy shows that $B^4 / C^3$ scales the magnitude of the free energy itself. The $\beta = 0$ or spherical solution shows that this phenomenology agrees with the observation that the spherical solution is always a solution of the non-rotating mean field equations. The non-spherical solutions break the rotational symmetry of the problem. This is an example of the general phenomenon that below a phase transition, states generally have a lower degree of symmetry than the states after the transition has occurred. The Landau parameter, in this case $\beta$, gives a measure of how nearly symmetrical the lower states are. The vanishing of $\beta$ is therefore a signal that the symmetry has been restored.

The parameter $A_s$ thus serves as a control parameter, its sign showing the nature of the equilibrium state. The behavior of the free energy as $A_s$ varies is shown qualitatively in Fig. 5, and is described below. For $A_s < 0$ there is an oblate local minimum, a prolate global minimum, and the spherical point is a saddle point. As $A_s$ increases, the oblate point moves towards $\beta = 0$, and at $A_s = 0$ the oblate and spherical points merge. The temperature at which this occurs is denoted $T_c$. As $A_s$ becomes positive, the spherical saddle point becomes a minimum and a prolate saddle point moves towards the prolate minimum, as is seen in the lower left hand graph of Fig. 5. As the temperature increases from $T_c$, the spherical minimum steadily deepens. For $A_s = 1/4$, at a temperature $T_1$, there is a first order phase transition as the free energy of the spherical and prolate minima become equal. Thus the global minimum shifts from the prolate point, which has been moving towards $\beta = 0$, to the spherical point, and hence the equilibrium $\beta$ changes discontinuously. Finally, at $A_s = 9/32$, at a temperature $T_2$, the two prolate extrema merge, leaving only the spherical saddle point for all higher temperatures. Thus the rotational symmetry of the problem is restored above the transition. $A_s$ determines the critical
The behavior of the free energy as it passes through 0, and near the critical temperature may be expanded as $\tilde{A}_s \sim T - T_c$.

Now the general free energy, including both the $\omega = 0$ terms described above and the new terms that arise from coupling to $\tilde{\omega}$ can be written down. This is

$$F(T, \omega) = F(T, \omega = 0) - (F_0'\omega^2 + A'\omega^2\beta^2 - R\omega^2\beta \cos 3\gamma + D\omega^2\beta^2 \sin^2 \gamma)$$

$$= (\tilde{F}_0' - F_0'\omega^2) + (\tilde{A} - A'\omega^2)\beta^2 - B\beta^3 \cos 3\gamma$$

$$+ C\beta^4 + R\omega^2\beta \cos \gamma - D\omega^2\beta^2 \sin^2 \gamma$$

$$= F_0 + A\beta^2 - B\beta^3 \cos 3\gamma + C\beta^4 + R\omega^2\beta \cos \gamma - D\omega^2\beta^2 \sin^2 \gamma.$$
where $A$ and $F_0$ can depend on $T$ and $\omega^2$ and $B, C, R$ and $D$ depend only on $T$. The coefficients up to this point have not been specified, and are functions of the thermodynamic variables $T$ and $\omega$. The equilibrium deformation is determined from the condition that $F$ is extremal for any choice of these variables. These coefficients can be fit to experimental or theoretical results, and thus illustrate the generality of the theory. We will see that the qualitative behavior of the system in the $T - \omega$ plane can be investigated without any detailed knowledge of these coefficients.

As in the $\omega = 0$ case, this free energy will have a variety of phase transitions in the minima that $F$ predicts. In a real nucleus, however, due to the finite number of particles, there can be no real phase transitions, since fluctuations about the mean field solutions will serve to smooth out the discontinuities. In Chapter 5, a method will be presented of dealing with these fluctuations in an approximate way, although the present work will not apply that method to this problem. In the rest of this chapter, the actual dependence of the coefficients of expansion on $T$ will not be specified, as this is application dependent. One such example will be presented in the next chapter, when the phenomenology presented here will be applied to the nucleus $^{166}$Er, whose behavior at finite spin and temperature has recently been investigated experimentally, as described in the introduction.

The phase structure of $F$ in this parameterization can now be analyzed. Most of the equations are fairly long and tedious, although for the most part they are polynomials of fourth degree or less. Because they are of such low order, most of them can be solved analytically, and hence there are explicit expressions for most of the important critical curves and points. The text of this chapter will include few of these formulas, but most of them are given in Appendix B.

3.2. The $D = 0$ Case
If $R = D = 0$, then a non-zero $\omega$ serves to renormalize the parameters, and thus the behavior of the saddle points will be the same, but occurring at slightly different temperatures. Even though the rigid body limit does not strictly correspond to $D = 0$, this case will be considered first, and will be referred to as the rigid body limit, since to lowest order in deformation this is correct. The previous discussion of the $\omega = 0$ case is a special case of this, and hence any new behavior must arise smoothly from the known phenomena as $R$ is fixed and $\omega$ increases from 0. First of all, there will be a new term in $\gamma$ in the free energy and thus the possibility of triaxial solutions arises. The complete rotational symmetry that was present in the $\omega = 0$ case is no longer present. Now, there is just rotational symmetry about the $z$-axis. We expect always to have solutions that preserve this partial symmetry, namely shapes that are axially symmetric around the $z$-axis. Thus there always should be solutions with $\gamma = 0$ or $-\pi$. Above the transition, the global minimum must have this symmetry, and since the solution $\gamma = 0$ is not stable with respect to orientation, the global minimum at high temperature is expected to have $\gamma = -\pi$.

Below the transition, the mean field solution should break this symmetry, and hence we expect to have solutions which lie off the line of $\gamma = 0$ or $-\pi$. Upon examining $\partial F / \partial \gamma = 0$ in this case, two classes of solutions arise,

$$
\sin \gamma = 0 \\
\beta \cos \gamma = \frac{3}{16} \left( 1 + \left( -\frac{32}{9} \frac{AC}{B^2} + 1 + \frac{64}{27} \frac{B^3}{C^2 R \omega^2} \right)^{1/2} \right) .
$$

(3.2.1)

The second solution is again seen to be a function of the scaled value of $A$ and a scaled value for $\omega$, which will be derived later. The former corresponds to the solutions for the $\omega = 0$ case which lay on the $\gamma = 0$ axis and are now the symmetry preserving solutions mentioned above. Due to the 3-fold symmetry in the $\beta - \gamma$ plane of the $\omega = 0$ case, there were prolate and oblate extrema lying on the $\gamma = -\frac{2\pi}{3}$ and
The $D = 0$ Case

$\gamma = -\frac{2}{3}$ lines as well. Now these solutions become triaxial and correspond to the second class of solutions in Eq. (3.2.1).

The solutions with $\gamma = 0$ will be considered first. When $\omega \neq 0$, there is a linear term in $\beta$ and hence $\partial F/\partial \beta = 0$ can no longer have a solution at $\beta = 0$. For $A_s \ll 0$ there will be a prolate minimum lying below an oblate minimum. Due to the stability arguments given above, however, this prolate minimum cannot exhibit stable rotation. The maximum on the $\gamma = 0$ axis, which was formerly spherical, is now prolate. As $A_s$ increases, the two prolate points move towards each other, and eventually coalesce, usually for $A_s < 0$. Meanwhile, the oblate point moves towards $\beta = 0$. This point remains a minimum, and although it can never hit 0, it tends to that value asymptotically as $A_s$ continues to increase.

Now the two triaxial extrema may be considered. They both start out as minima in the $\beta$ direction, but the one associated with the oblate axis is not stable with respect to the direction of rotation. For $\omega \neq 0$, these points can never have $\gamma = -\frac{2}{3}$ or $\gamma = -\frac{2\pi}{3}$, although they tend to these values asymptotically as $A_s \to -\infty$. The former point moves smoothly to the $\gamma = 0$ axis with $\beta > 0$, and at some $A_s$ merges with one of the two prolate points on that axis. This behavior can be seen in any of the graphs in Fig. 6, where the motion of the extrema with increasing $A_s$ is shown. These three points (the triaxial saddle point and the two prolate extrema with $\gamma = 0$) are all non-physical. They all lie in the sextant $-\pi/3 < \gamma < 0$, and hence are shapes which are unstable with respect to the rotation axis. They are important in the context of this work for two reasons, however. First, they provide a check of the general theory as $\omega \to 0$. Also, in the uniform mapping, to be described in Chapter 5, it is necessary to specify the behavior of all extrema of the free energy (even the unstable ones), since they completely characterize the mapping that will be performed.
Figure 6: Motion of the saddle point as $A_e$ varies. Global minima are shown by filled circles and other extrema by open circles. The motion of the extrema with increasing temperature is indicated by arrows. The triaxial solution in the right hand side of the plane always hits $\gamma = 0$ before the phase transition. Lines of $\gamma = -\frac{\pi}{3}, -\frac{2\pi}{3}$ shown for reference. All values are scaled.
We next concentrate on the sextant \(-\pi \leq \gamma \leq -\frac{2\pi}{3}\), where the physical solutions lie. Depending on the value of \(\omega\), two things can happen. If \(\omega\) is less than some critical value \(\omega_c\), then there is a first order phase transition. In this case, the stable triaxial minimum is moving towards the \(\gamma = \pi\) axis, but before it gets there, from the oblate solution on that axis emerges another extremum which is a maximum in \(\gamma\). This is seen in the upper left hand graph of Fig. 6, as the open circle in the stable region moves from the \(\gamma = -\pi\) axis towards the stable triaxial point. The oblate point now becomes a local minimum, and at some \(A_s\), a first order phase transition occurs between the oblate point and the original triaxial minimum. As \(A_s\) increases further, the two triaxial points merge, leaving only the oblate minimum, which moves slowly towards the origin. If \(\omega\) is larger than the critical value, however, there is a second order phase transition as the minimum that starts near \(\gamma = -\frac{2\pi}{3}\) moves continuously and merges with the oblate shape at \(\gamma = -\pi\) before the other solution can emerge. The critical \(\omega\) can thus be found as the point at which a first order transition with a zero difference between the two points occurs and is

\[
\omega_c^2 = \omega_R^2 = \frac{81}{256} \frac{B^3}{C^2 R^3}. \tag{3.2.2}
\]

The critical value is denoted \(\omega_R\) here to differentiate it from the one in the general case, with \(D \neq 0\).

The motion of the extrema is demonstrated in Fig. 6, where their behavior may be followed with increasing \(A_s\). The \(\gamma = -\frac{\pi}{3}\) and \(\gamma = -\frac{2\pi}{3}\) lines are also shown for reference. The location of the global minimum is given by filled circles and other extrema by open circles. Note that while points in the right third of the lower half plane may be stable with respect to \(\beta\) and \(\gamma\), they cannot be stable with respect to the direction of rotation. The points on this graph are universal in the sense that they have been scaled by \(B/C\), and are given as functions of the dimensionless \(A_s\) and \(\omega/\omega_R\). These scalings are temperature dependent, although their temperature
dependence is expected to be much weaker than that of $A_s$. Such plots may be generated for any value of $\omega/\omega_R$. The values of $A_s$ for which the two triaxial points merge and for which the triaxial maximum appears in the first order transition case may be easily derived, and hence a phase diagram in $A_s$ and $\omega/\omega_R$ may be generated, analogously to a $T - P$ diagram in ordinary thermodynamics. We would prefer to have phase diagrams using $T$ rather than $A_s$, but without a specific model for the temperature dependence of the coefficients, such quantities cannot be calculated. In the next chapter, a specific mapping will be discussed. As noted above, however, $A_s$ should be a good substitute for $T - T_c$. Also, due to the existence of the scaling variables $A_s$ and $\omega/\omega_R$, the curves in this phase diagram will be universal as well.

For any $\omega$, there is a temperature below which the oblate solution is no longer a minimum, and thus marks the limit of local stability of that solution. For $\omega/\omega_R < 1$, this is the point at which the triaxial point emerges from the oblate minimum, since for lower temperatures, the oblate point is a minimum in $\beta$, but not $\gamma$. In the second order region, this is actually the transition temperature, since the oblate point is never a local minimum before it becomes the equilibrium point. This limiting stability line for the oblate solution is derived by requiring $\cos \gamma = -1$ (see Appendix B) and is given by

$$A_s^{(1)} = \frac{9}{8} \left(1 - \left(\frac{1}{4} \frac{\omega}{\omega_R} - 1\right)^2\right).$$  \hspace{1cm} (3.2.3)

It is shown in Fig. 7 as the solid line to the right of the tricritical point, and the lowest solid line to the left of the tricritical point. We next turn to the limiting stability line for the stable triaxial solution. In the second order region, the stable triaxial solution is always a global minimum, and hence its stability limit is given by Eq. (3.2.3) as well. In the first order region, where $\omega/\omega_R < 1$, the triaxial solution can still be stable, even where it is no longer the global minimum. In fact, it will be
Figure 7: Phase diagram in the $\omega - \tau$ plane. In this and following figures, the variable $\tau$ corresponds to $A_s$ in the text. The transition lines are shown by solid lines, the tricritical point by a cross. First order transitions lie to its left, and second order to its right. Lines of constant $\beta$ are shown by dashed lines, and constant $\gamma$ by dotted. The insert shows the region near the first order transition.
stable until this minimum and the triaxial saddle point which stabilizes the oblate solution collide. The stability line in this region is then given by

\[ A_s^{(2)} = \frac{9}{32} \left( 1 + \frac{3}{4} \left( \frac{\omega}{\omega_R} \right)^2 \right). \]  

(3.2.4)

This line is the uppermost solid line in the region \((\frac{\omega}{\omega_R}) < 1\) in Fig. 7. It is clear that the first order transition line must lie between these two curves. There is no simple expression for this line since the roots of a cubic equation are involved, but it is easily found numerically. All three lines merge at the critical \(\omega\), as the first order transition line vanishes there, and for larger \(\omega\), the oblate and triaxial stability lines are the same.

The critical \(\omega\) is thus a tricritical point, since continuous lines of first and second order transitions meet there. The tricritical point indicates the existence of another external field, which, if varied, would generate surfaces of tricritical transitions, where lines of second and first order transitions meet. For some sufficiently large value of this field, there will only be second order transitions for all values of \(A_s\) and \(\omega\). This extra degree of freedom must be one which couples directly to the order parameter, which is, in this case, the quadrupole deformation. The field which does this is the gradient of an electric field, as may be seen by the fact that the quadrupole moment is a tensor, and hence a tensorial quantity must be coupled to it. If this quantity could be varied, we would expect to see the critical \(\omega\) decrease to 0 as the gradient increased. This, however, is not an easy quantity to produce on a nuclear scale, much less while insuring that there is a hot nucleus nearby.

For every temperature and angular velocity, then, there exists a stable minimum, as predicted by the phase diagram. When \(\omega/\omega_R > 1\), the minimum is oblate for \(A_s > A_s^{(1)}\) and triaxial for the rest, while for \(\omega/\omega_R < 1\) the same is true with respect to the first order transition line. Lines of constant \(\beta\) and \(\gamma\) can then be drawn in these regions, and thus the location of the global minimum for each \(A_s - \omega\) pair.
can be read off. This is done in Fig. 7, with lines of constant $\beta$ given by dashed lines and constant $\gamma$ by dotted ones. All of these plotted quantities are universal, as they have been scaled appropriately. There is no scaling for $\gamma$, so this quantity is automatically universal, but $\beta$ does have a scaling of $B/C$ in specific calculations. Thus to apply these calculations to a given nucleus, it is only necessary to multiply these results by the temperature dependent scaling. Note that there are no lines of constant $\gamma$ in the oblate region as $\gamma$ is fixed there. One of the most striking things about this graph is how slowly both coordinates change with temperature, except near the transition. The experiments mentioned in the introduction exhibit this kind of behavior. The lower energy experiment found essentially the same deformation at $T = 1.4\text{MeV}$ as had been seen at $T = 0$, while the other experiment found a completely different shape at a temperature just $0.05\text{MeV}$ higher. The Nilsson calculations as well show that the transition occurs quite quickly, although, like the experiments, they cannot really identify the nature of the transition. Thus it seems reasonable to expect from this theory as well very little change in deformation until the transition occurs. Also from this figure, the behavior described above with constant rotation and varying temperature may be deduced, as well as the behavior with constant temperature and varying spin.

Whereas there are basically two kinds of behavior at constant angular velocity, there are many more at fixed $A_s$. For low temperatures, triaxial saddle points move smoothly to the oblate axis where a second order phase transition occurs. For small positive $A_s$ there is an oblate minimum at $\omega/\omega_R = 0$ which undergoes a first order transition to a triaxial point. This minimum then moves to the oblate axis, where a second order transition again occurs. Even larger $A_s$ results in oblate points which have second order transitions to triaxial minima which reach some maximum $\gamma$ and then move back to the oblate axis. For the largest $A_s$, there is no transition at all, and an oblate minimum moves steadily out its axis. In all
Figure 8: Motion of the saddle points with varying omega. Extrema are denoted as in Fig. 6.
cases, with increasing $\omega/\omega_R$, there is increasing $\beta$. This richness of transitions has not been seen experimentally, but it would be extremely interesting to see more experiments done in this region in order to see how well this theory predicts the actual behavior. Examples of these phenomena are given in Fig. 8.

The average spin $J$ is given by

$$J = -\frac{\partial F}{\partial \omega}, \quad (3.2.5)$$

thus defining the spin corresponding to a given angular frequency and and temperature. When Eq. (3.1.7) is substituted into Eq. (3.2.5), we see that $J = \mathcal{S}\omega$, where the moment of inertia $\mathcal{S} = I_{zz}$ is now a function of the deformation at the equilibrium. Since this is at the equilibrium point, the calculation of the moment of inertia is greatly simplified by using $\partial F/\partial \alpha = 0$.

For $D = 0$, and $F'_0 = A' = 0$, we find

$$J = -2\omega R \beta \cos \gamma \quad (3.2.6)$$

so that $\mathcal{S} = -2R\beta \cos \gamma$ for the equilibrium solutions. Now the solutions found above can be substituted and contours of constant $A_\mathcal{S}$, which are "isotherms", can be drawn in the $\omega - J$ plane. Because there is a region where both triaxial and oblate solutions exist (near the first order transition) there will be a region of this plane where a Maxwell construction must be made. This region will be bordered by curves found from the equations for the transition lines for $A$.

These "isotherms" are drawn in Fig. 9, where, to expand the scale, $J/\omega$ is plotted rather than $J$. $A_\mathcal{S}^{(1)}$ is the line extending from the origin, and $A_\mathcal{S}^{(2)}$ is the horizontal line at $J/\omega = 243/2048$. Note that $J$ is scaled by $\frac{C^3}{B^4 \omega_R^3}$. Above $A_\mathcal{S}^{(1)}$ are triaxial minima, while below either transition line are oblate points. The lines of constant $A_\mathcal{S}$ are given by solid lines for triaxial and oblate solutions and thus the system’s behavior in terms of spin at fixed temperature and varying angular frequency may be followed. Note that backbending-like behavior is possible.
Figure 9: "Isotherms" in the $J/\omega - \omega$ plane. All values are scaled appropriately. The unstable region lies below $J/\omega = 243/2048$ and to the left of the transition line. The isotherms drawn in this region correspond to the unstable triaxial solutions which occur in the first order transition region.
In an ordinary isothermal liquid-gas phase transition, the pressure must decrease with increasing volume for physical states. As the pressure decreases, the phase transition occurs as the chemical potentials of the two phases become equal. The volume then changes discontinuously. There are metastable states of the system for which the liquid is superheated or the vapor supercooled, but the system will have lower free energy by going to one of the ordinary phases. These are the forbidden metastable states in analogy to the ones in our theory. An example of a $P - V$ diagram for the liquid-gas phase transition analogous to our $J/\omega - \omega$ plot is shown in Fig. 10. The triaxial minimum is a local minimum after the first order phase transition and is thus a metastable point. Similarly, the oblate point is a local minimum after the triaxial saddle point emerges.
3.3. The General Case

The situation for $D \neq 0$ has some differences from the case already considered. The system still undergoes both first and second order transitions, and a critical frequency can be defined at which the nature of the transition changes. Now the critical frequency depends on both $R$ and $D$ and is given by

$$\omega_c^2 = \frac{1}{10} \omega_R^2 \left( 2\omega_R^2 - 3\omega_D^2 + \sqrt{64\omega_R^4 - 12\omega_D^2\omega_R^2 + 9\omega_D^4} \right)$$  (3.3.1)

where $\omega_R$ is given in Eq. (3.2.2) and $\omega_D^2 = \frac{9}{4}B^2/CD$ and is the corresponding critical point for $R = 0$ and $D \neq 0$. Eq. (3.3.1) reduces to $\omega_D$ in the limit $R = 0 (\omega_R \to \infty)$, but since $\omega_c$ is not a convenient scaling variable, $\omega$ will continue to be scaled by $\omega_R$.

There is a scaled form for $D$ as well,

$$D' = \frac{9}{64} \frac{BD}{CR} = \frac{\omega_R^2}{\omega_D^2}$$  (3.3.2)

so that all expressions are functions of $A_s, D'$ and $\omega/\omega_R$ only.

All of the above results are generalizable, and thus for any $D'$ we have universal plots in the $A_s - \omega/\omega_R$ plane as before. For example,

$$A_s^{(1)} = \frac{1}{2} \left( \frac{1}{8} \left( 3 + D' \left( \frac{\omega}{\omega_R} \right)^2 \right) \left( 16D'^2 \left( \frac{\omega}{\omega_R} \right)^4 + 9 \left( \frac{\omega}{\omega_R} \right)^2 \right)^{\frac{1}{2}} + 3D' \left( \frac{\omega}{\omega_R} \right)^2 \right. \right.$$

$$+ \left. \frac{1}{2} D'^2 \left( \frac{\omega}{\omega_R} \right)^4 - \frac{9}{64} \left( \frac{\omega}{\omega_R} \right)^2 \right)$$  (3.3.3)

and

$$A_s^{(2)} = \frac{9}{8} \left( 1 + \frac{3}{4} \left( \frac{\omega}{\omega_R} \right)^2 + 6D' \left( \frac{\omega}{\omega_R} \right)^2 + D'^2 \left( \frac{\omega}{\omega_R} \right)^4 \right).$$  (3.3.4)

A universal phase diagram for $D' = .02$ is given in Fig. 11. The trajectories of the extrema can be followed in the $\beta - \gamma$ plane as before. Note that now as $\omega \to \infty$ Eq. (3.2.3) tends to $-9/128 \left( \frac{\omega}{\omega_R} \right)^2$ but in the same limit, Eq. (3.3.3) tends to $9/2D' \left( \frac{\omega}{\omega_R} \right)^2$. For the $D = 0$ case this meant that trajectories at fixed $A_s$ could be
Figure 11: Phase diagram for $D' = .02$. Lines and the tricritical point denoted as in Fig. 7. Note that the transition line increases monotonically for $\omega/\omega_c > 1$. 
such that there was never a triaxial minimum. Now, for all $A_s$, for a sufficiently large $\omega$, there will always be a one such minimum. As a matter of fact, since the two cases must connect smoothly, for small enough $D'$, the minimum can be oblate, then triaxial, then oblate again, and finally triaxial once more, all at a fixed $A_s$. Trajectories of the extrema for $D \neq 0$ are given in Fig. 6 for fixed $\omega$ and varying temperature, and in Fig. 8 for fixed temperature and varying rotation.

Another important difference for $D \neq 0$ is that all triaxial trajectories will have $\gamma = \frac{-2\pi}{3}$ for a finite $A_s$. Thus lines of constant $\gamma$ in the $A_s - \omega/\omega_R$ plane must include angles between $-\frac{\pi}{2}$ and $-\frac{2\pi}{3}$. Since as $A_s \to -\infty$, $\gamma \to -\frac{2\pi}{3}$ as before, the lines of constant $\gamma$ in this range do not hit the $\omega/\omega_R = 0$ axis. The isotherms also can be drawn. Since, unlike previously, all lines of constant $A_s$ must end up in the triaxial region rather than the oblate, the isotherms must have different asymptotic behavior in order to insure this. Hence all isotherms are observed to curve away from the transition line as they enter the triaxial region. There is still an unstable region of non-physical states, which will again require the use of a Maxwell construction in order to avoid these states. First order transitions in such a figure would be shown by vertical lines across the unstable region drawn between points which have the same free energy. These points are not on the border of the unstable region since the border represents the disappearance or reappearance of triaxial solutions, and except at the critical frequency, these will not be points of transition. These isotherms are shown in Fig. 12.

To summarize, the free energy given by Eq. (3.1.7) thus describes a variety of behavior. For example, both first and second order transitions are possible. In general, with fixed rotation and increasing temperature, the mean field solution given by the minimum of Eq. (3.1.7) is expected to be prolate or nearly so in its ground state and then eventually become oblate, with the deformation asymptotically vanishing. On the other hand, the deformation is seen to increase steadily.
Figure 12: Isotherms for $D' = .02$. Lines are denoted as in Fig. 9. Note that now triaxial isotherms curve away from the transition line for large $\omega/\omega_R$. 
with increasing rotation at a fixed temperature. For $D = 0$ the deformation always ends up oblate and increasing, as the nucleus seeks to minimize its rotational energy. Note that this is classical behavior, because the rotation is about a symmetry axis, and hence makes no sense quantally. For $D \neq 0$, the behavior with increasing rotation is again to increase deformation, but for large enough $\omega$ the shape will always be triaxial, and, as $\omega$ increases, will cross $\gamma = -\frac{2\pi}{3}$. The calculations of this chapter have only shown the location of the minimum, and have given no idea of its sharpness. In fact, the free energy surface is quite flat for most cases, and hence the phase behavior may be smoothed out by fluctuations.

The mean field solution trajectories which are traced out with increasing temperature at fixed spin yield an intuitive result for their general behavior. As expected, correlations leading to deformation disappear, yielding a more spherical shape with increasing temperature. The transition to the noncollective rotation of oblate shapes is understood microscopically from the fact that, as pairing breaks down, more of the nuclear spin will arise from aligned individual nucleon spins rather than collective rotation.

"Isotherms" in the $J/\omega - \omega$ plane have also been derived for the model, in the approximation of ignoring all of the $\omega$-dependence except that arising from the rigid body term, and exhibit backbending behavior in the region of the first order transition. This phenomenology is classical, but fluctuation corrections may serve to mock the quantum effects which are thought to underlie this behavior. Even on the yrast line, the breakdown of pairing which leads to backbending is a first order transition, as the quantum configuration of the system changes abruptly.

All in all, this seems to be an effective, simple theory for nuclei at low and medium spin and in the neighborhood of the critical temperature for the transition away from the ground state shape. It unifies behavior known from many microscopic calculations and provides a reasonable interpretation of the limited experimental
data available. It is important to note that in our phenomenology, we can only describe the lowest phase transitions possible. If more terms are included in the Landau expansion of the free energy, then other phase behavior should be possible at higher spin. For instance, it is known that at very high spins, the oblate nucleus can become triaxial again as it behaves more like the classical liquid drop, but this is at a sufficiently high spin that we would require extra terms.
Chapter 4.

Application to $^{166}$Er

4.1. Introduction and Phase Diagrams

The experiments described in the introduction motivate the choice of $^{166}$Er as a nucleus to which we now apply the theory of the previous chapter. Through these two experiments, as well as from the known ground state deformation, there is indication that the transition from prolate to oblate shape must occur fairly quickly. We also know that it must occur for spins around $15\hbar$ and temperatures near $1.4\text{MeV}$. In the previous chapter, the theory was shown to exhibit first and second order transitions, but the actual change from prolate to oblate shapes was rather quick as long as we were in the vicinity of the tricritical point. No specific temperature mapping was available, so the speed of transition was only known with respect to the scaling variable $A_s$. In Ref. 31, the scaled parameter $A_s$ is a steep function of $T$ near the transition point, and hence the transition could easily be expected to occur in a narrow range of temperature. As a first application of the model of the previous chapter, the case of $^{166}$Er with rigid body rather than microscopically derived coefficients of $\omega^2$ will be considered. The other coefficients will be extracted from finite temperature $\omega = 0$ calculations in the Nilsson model.

Before proceeding further, we will specify the units we will use in this part of the work. The free energy is given in MeV, while the moment of inertia goes like $[\text{mass}][\text{length}]^2$, and hence in nuclear units should have dimensions of MeV/$c^2\cdot\text{fm}^2$. Thus the natural units for the rotational frequency in this problem will be fm/$c$, and all values of the frequency quoted here will be in this unit. For comparison, in cranked Nilsson model calculations, the usual unit is the oscillator unit $\omega_0$, defined by $\hbar\omega_0 = 41A^{-1/3}\text{MeV}$. The conversion between the two sets is thus given
by the factor $41A^{-1/3}\text{MeV-fm}/(\hbar c) \approx 2A^{-1/3}$. Also, Nilsson model calculations are generally carried out in what are called “stretched” coordinates, while the moment of inertia calculated above was in the Hill-Wheeler coordinates. The radial coordinates in these two representations are related by Eq. (2.4.1).

In order to calculate the temperature dependent coefficients of the terms which do not multiply $\omega^2$, the ideas developed in the next chapter for the uniform approximation are applied. The basic idea of this scheme is that the actual free energy surface is mapped into a more tractable function. The mapping is $((\beta, \gamma) \rightarrow (\beta', \gamma'))$, where the primed coordinates are those of the more tractable function. The two surfaces, which have the same saddle point structure, are mapped by matching them at their extrema, which are the most important points of the surface for this application. The mapping can be achieved at any temperature, and thus allows us to expand the applicability of the Landau expansion to situations where the deformation parameters are no longer small. This assumes that the saddle point structure of the microscopically calculated surface remains identical with that of the expansion. For most calculations so far carried out, this seems to be true. This procedure was carried out over a range of temperatures, and the resulting values were then fit by a polynomial in temperature in order to extrapolate them to temperatures where there are difficulties in performing the mapping. These difficulties arise from the restoration of symmetry that occurs following the phase transition. For the expansion, this means the symmetry violating solutions become complex. The utility of the uniform expansion is seen when one wants to include effects such as fluctuations in the calculations. This technique will be explored in the following chapter at greater length.
The function that the actual free energy surface will be mapped to is the $\omega = 0$ expansion of the previous chapter, written in terms of the scaled variables. This is

$$F(T) = F_0 + c_F \left( A_s \beta^2 - \beta^3 + \beta^4 \right),$$

(4.1.1)

where $c_F = B^4/C^3$ is the scaling for $F$, and $A_s = AC/B^2$ is the scaled value of $A$. The scaling for $\beta$ will be denoted by $c_\beta = B/C$. Also, since these are the only terms we will be discussing for the moment we have dropped the tildes from them, with the understanding that unless explicitly mentioned, the coefficients do not multiply $\omega^2$.

For $\omega = 0$, all extrema must have $\gamma = \frac{\pi\omega}{9}$, and hence as in Ref. 31, just $\gamma = 0$ need be considered. $F_0(T)$ can be read off immediately from the microscopic calculations, as this is just the value at $\beta = 0$. For $\omega = 0$, the positions of the extrema are given explicitly by

$$\beta = \frac{B}{C} \left( 1 \pm \sqrt{1 - \frac{32}{9} A_s} \right)$$

(4.1.2)

and this can be substituted into Eq. (3.1.7) at $\omega = 0$. The three unknowns $A_s, c_F$, and $c_\beta$ are determined by the three conditions achieved by matching the two deformed minima and fixing the global minima to occur at the same value of the coordinate in both systems.

Once we calculated these quantities at chosen values of $T$, we fit them to polynomials in $T$. We fit $c_\beta$ by a linear function, while $c_F, A_s$ and $F_0$ were fit quadratically, as shown in Fig. 13. These fittings are especially useful in the calculation of quantities such as the entropy, where we require derivatives with respect to $T$. Since we have a simple form for the coefficients, the derivatives may be taken analytically and will be easily evaluated.

We will take the rest of the parameters that appear in Eq. (3.1.7) to be those for the rigid body moment of inertia. There are two reasons for considering the
Figure 13: Fits for the scaled parameters to the Nilsson calculations. The orders of the fits are given in the text. The calculated points are shown by dots.
rigid body parameters rather than extracting them from microscopic calculations. First, the temperatures considered here are all above the pairing transition, which generally occurs at $T \simeq 0.8\text{ MeV}^1$. This pairing transition is the point at which the gap equations have only the zero solution, and hence pairing correlations are no longer important. The pairing is intended to simulate the effects of the residual interaction, and its disappearance signals that the interactions among nucleons will be mostly given by some single particle potential, which is generally local. However, as mention in Chap. 2, local potentials lead to isotropic velocity flow at every point in the rotating frame, and hence no net flow. Thus local potentials have purely rigid body moments of inertia, and in fact this result is exact for potentials like the Woods-Saxon. For these models, as the temperature increases, the moment of inertia is thus seen to be more and more rigid body-like.

Unfortunately, in the present case, the Nilsson potential does have a non-local piece, the $l^2$ term, which arises from the spherical shell model part of the Hamiltonian. Hence calculations of the moment of inertia in this model, using for instance the Inglis formula, show a moment of inertia $30-40\%$ larger than the rigid body value$^{34}$. In order to retrieve the correct moment at high temperature or spin, a scaling can be applied$^9,35$ or the liquid drop part can be renormalized$^{36}$. Thus it is expected that the calculations in this thesis lie in the rigid body regime, and so we shall \textit{a priori} use the rigid body moment of inertia. This was given by Eq. (2.2.6), when compared with the general expansion Eq. (3.1.7) we get $F_0' = \frac{4}{9}mAR_0^2$, $A' = \sqrt{\frac{5}{4\pi}F_0'}$, $D = \frac{15}{28\pi}F_0'$ and $R = \frac{10}{7\pi}F_0'$. In the following, when we refer to $A'$, we will be referring to the scaled value, $A'C/B^2$.

We saw in the previous chapter that for $D' \geq 0.02$, the transition line increases monotonically as a function of $\omega/\omega_R$. The Nilsson calculations, however, indicate that with increasing spin, the transition temperature drops, as seen in the universal calculations for smaller values of $D'$. Since the rigid body value for $D' from
Eq. (2.2.6) gives $D' = 0.075$ at $T = 1\text{MeV}$, and the scalings force it to increase from there, we must choose the ordinary rigid body moment of inertia with $D = 0$ for the rest of the calculations.

In the last chapter, formulas were generally written as a function of $\omega$ in order to give $A_\omega$. Now the temperature dependence is much more complex than the frequency dependence, and it is easier to derive formulas for critical frequencies in terms of the temperature. All of the results of Chapter 3 can be inverted to give $\omega$ as a function of $T$, but, in addition, the $\omega$ dependent part of $A, A'$, must be taken into account. Since the rigid body calculations were carried out to order $\beta^2$, this is the only new $\omega$-dependent term introduced. We will also take into account the $\omega$ dependence of $F_0$, but this term only enters into calculations involving the value of the free energy and its derivatives with respect to $\omega$. The rigid body parameters were taken to be temperature independent, but when they get scaled, they will pick up temperature dependence from the scaling variables.

The transition lines can be now known as functions of $T$ and $\omega$ rather than of their scaled forms as before. As expected, in the region of concern, $A_\omega$ is a monotonic function of $T$, so the form of the transition lines and of the lines of constant $\beta$ and $\gamma$ should be similar. The $\omega$-dependent part of $A$ serves to reduce the its value at each spin, but should not change the shape of the lines too much, since it is not a very large correction. The transition lines play the same role as they did before, and are shown in Fig. 14 in the $T - J$ plane. Note that the critical value for the intersection of these two curves is independent of $A'$.

The previous chapter had no mapping from $T$ to $A_\omega$, and thus gave only general ideas about where in temperature the tricritical point lay, and over what range could the transitions expect to be seen. Now, the parameter space in which the first order transition can occur is known. It is a quite small range, from $T \approx 1.69 - 1.73 \text{MeV}$,
Figure 14: Phase diagram in the $T - J$ plane for $^{166}$Er.

Lines are as in Fig. 7. Note that here $\beta$ is unscaled.
and from $J \simeq 0 - 6\hbar$. The tricritical point is seen to lie at the end of this region, $T_c = 1.73\text{MeV}$ and $J = 6.5\hbar$.

Lines of constant $\beta$ and $\gamma$ can be drawn in the $T - J$ plane, so as to give the equilibrium configuration for each point in the plane. From the lines of constant $\gamma$ in Fig. 14, it is seen that even in the second order transition region, where $\gamma$ is continuous, it only changes rapidly in the neighborhood of the transition line, as long as we are in the region of the tricritical point. When fluctuations are taken into account, the first and second order regions should exhibit quite similar behavior. Two observations may be made about the location of the tricritical point in these calculations. The first is that the value is somewhat smaller than the spin at which the transition occurs in the experiments, but that transitions can occur at larger spins as well. This is quite encouraging in that a model with very little microscopic numerical input which is the result of a general theory has given good results. This indicates that the physical ideas we have based this on are probably the most important ones for the process we are investigating. The other observation is that the spin for the tricritical point is large enough that there can be significant structure to the phase diagram both below and above it.

In general, it is seen that the nuclear shape is almost entirely prolate or entirely oblate. Even in the second order region, as noted above, the $\gamma$ transition is very quick, or as it might better be put, there is only a very limited range of parameters for which triaxial shapes could be expected. Generally, the deformation tends to increase with increasing $\omega$, and decrease with increasing $T$, as was seen both in the universal calculations earlier, and in the microscopic Nilsson calculations.

4.2. Isotherms

True isotherms can now be calculated in the $J - \omega$ plane, and are shown in Fig. 15. Previously, in order to get a general idea of the nature of the isotherms,
Figure 15: Isotherms for $^{166}$Er with the rigid body parameters. The lines are as in Fig. 9.
only the $\omega$-dependence of the $R$ and $D$ terms was studied. Now, the $I_0$ and $I_1$ terms must also be included. The angular momentum is thus given by

$$ J = 2\omega \left( I_0 + c_F \left( I_1 \beta^2 - \frac{81}{256} \frac{1}{\omega R^2} \beta \cos \gamma + \frac{9}{4} D' \frac{1}{\omega R^2} \beta^2 \sin^2 \gamma \right) \right), \quad (4.2.1) $$

where $\beta$ is now the scaled value. As in the previous section, we take $D' = 0$. Once again, the behavior of the isotherms is seen more clearly by dividing the angular momentum by the rotational frequency, giving the effective moment of inertia, $\mathcal{I}$. From Fig. 15 it is seen that the isotherms begin to cross at large frequencies. This is an artifact of the behavior of $c_\beta / c_F$ and hence indicates a limit of the applicability of our fits. Not surprisingly, the spin increases monotonically and almost linearly with the rotational frequency.

4.3. Isentropic Lines

The free energy is now known explicitly as a function of temperature. This means that other thermodynamic quantities of the system can be studied in detail, especially ones which involve derivatives with respect to the temperature. While the detailed results obtained in this section are particular to the choice of mapping that has been made, the general formulas and ideas are not and should be applicable to any mapping. These calculations will also provide an experimental observable, namely the excitation energy, which, along with the observable already calculated, the angular momentum, will help to characterize the system in a useful fashion.

The first thermodynamic quantity that will be explored is the entropy. We are interested in the physical interpretation of isentropic lines. Rotational bands, except where backbending occurs, are assumed to be rotations of largely unchanging intrinsic configurations\textsuperscript{37}. The unchanging internal configuration means that no internal degrees of freedom are being excited and hence no heat is flowing in or
out of the system. Thus this is an isentropic process, and these processes may be identified with rotational bands with highly excited bandheads. Decays along such bands should then be favored, and it is important to understand their properties.

The entropy is found from the relation $S = -\partial F/\partial T$. Note that $F$ has been calculated in the rotating frame. In taking derivatives of $F$ with respect to $T$, only partial derivatives of $F$ with respect to $T$ need be taken, since $F$ is extremized already with respect to $\beta$ and $\gamma$. This yields

$$S = -\frac{\partial F_0}{\partial T} - \frac{\partial c_F}{\partial T} F - \frac{\partial c_F}{\partial T} F_0 - c_F \frac{\partial A_s}{\partial T} \beta^2 - \frac{\partial \omega_R^2}{\partial T} \frac{1}{\omega_R} \left( \frac{\omega}{\omega_R} \right)^2 \beta \cos \gamma. \quad (4.3.1)$$

Since the yrast line is a sequence of non-degenerate collective states, it is assumed that $S = 0$ for this band. However, since the behavior is collective, $T = 0$ as well. This is the only band for which an isentrope is exactly equivalent to an isotherm. Entropies at constant $\omega$ or temperature are easily calculated. Even though $\beta$ and $\gamma$ change smoothly in the second order transition region, the derivative of the entropy cannot be smooth there. For higher spins, though, as the transition temperature rises, the transition will become less and less marked.

The energy can now be calculated in the laboratory frame. In this frame, the energy $E$ is

$$E = F + TS + \omega J, \quad (4.3.2)$$

where $F$ is the free energy that has been discussed all along, namely the one in the rotating frame. The last term in this equation effects the transformation from the rotating to the fixed frame. Hence $E$ contains the rotational energy of the system as well. The excitation energy is now found from this quantity by subtracting the zero-spin, zero-temperature energy,

$$E^* = E - E (T = 0, \omega = 0). \quad (4.3.3)$$
Figure 16: Isentropes of $^{166}$Er with rigid body rotational parameters in the $E - J$ plane. The transition lines are shown by solid lines, and the tricritical point by a cross. The isentropes, given by the dot-dashed lines, are labeled by the value of the entropy.
Figure 17: Isentropes in the $T - J$ plane.
Isentropes in the $E - J$ and $T - J$ planes are shown in Fig. 16 and Fig. 17, respectively. All of the quantities that were fit to microscopic calculations were fit in the region of $T = 0.6 - 2$ MeV. Below this region, pairing becomes stronger, and the phenomenology developed here is no longer good. Thus, the values in the fits are not good down to $T = 0$ and the term $E(0)$ cannot be properly evaluated in this model. We use for the $E(0)$ point the energy of the Nilsson model with no pairing at zero temperature, which gives a value quite close to the one which using the fits gives.

As noted above, the $T = 0$ isotherm is the only one which is exactly equivalent to an isentrope. The isentropic lines are in general nearly isothermal, as $T$ is constant to within 5% over a range of $J = 0 - 60\hbar$, as seen in Fig. 17. If the entropy and spin are considered to be the independent variables for the problem, the energy is the appropriate fundamental thermodynamic quantity. Then the temperature can be defined by $T = (\partial E/\partial S)_J$. Since $J$ is discontinuous for an isentropic first order transition, the line of $T$ against $J$ must be discontinuous there. However, $J$ is continuous across a second order transition, so the isentropic temperature line will be also. Its derivative, however, will not, so we should see a change in the slope of such a line at a second order transition.

In the $E - J$ plane, the isentropes, which are like continuous "rotational bands," are seen to be nearly parallel, with a steadily increasing spacing for constant increments in $S$. Backbending has not been seen in this nucleus and the isentropes reflect this in their smooth behavior. As mentioned previously, $E = E(S, J)$ is a fundamental relation. Thus $E$ is always continuous for constant entropy as a function of $J$. The slope of these isentropes is $(\partial E/\partial J)_S = \omega$ which is continuous at second order transitions but not at first. Thus we expect to see no break in the slope of the isentropes for the second order transition. This behavior is seen in Fig. 16, where the transition lines are shown by the dashed lines. The angular
frequencies for different isentropes do not vary greatly in this range of $J$, and show that $\omega = 1.6 \times 10^{-3} c/\text{fm} \approx 0.3\omega_0$ is a large enough rotational frequency to give an angular momentum of $50\hbar$.

Now the theoretical predictions of this chapter may be compared with the experiments. The low energy experiment showed a prolate shape at an energy of 41MeV, or a temperature of 1.4MeV, using the Fermi gas definition of temperature. The deformation was essentially identical to that of the ground state. This is consistent with the calculations of this chapter, since the change in deformation predicted at that temperature is much too small to be detected experimentally, and probably would be erased anyway by fluctuations.

The experiment of the Copenhagen group measured the shape at the higher temperature of 1.45MeV and at several angular momenta and showed that the shape transition occurred at about $2\hbar$. This spin is quite close to our value for the tricritical point, where we expect the transition to be fastest, but our temperature is about $0.2\text{MeV}$ higher. Their temperature was derived by fitting the statistical part of the $\gamma$-ray cross section, rather than deriving it from a model as we have. This fitting resulted as well in an error bar of $\sim 0.2\text{MeV}$. Thus we cannot expect our temperatures necessarily to be the same, although if the nucleus is thermalized, then the two should be quite close. Our temperature for the transition is reflected in the Nilsson calculations. A transition from a prolate to an oblate shape was still seen at temperatures up to $1.6\text{MeV}$, although the surface was so flat that performing the fit was difficult.

Combining the experimental results and the observations we have made of the Nilsson calculations, it is somewhat surprising that the transition line rises for small spin values. The prolate to oblate transition has been seen in almost all of the Nilsson surfaces for sufficiently high spin, and thus the transition line should drop for these spins, so that the oblate region again becomes accessible at low temperature.
This was the behavior seen in Fig. 7, and has been reproduced for the calculations of this chapter by setting $D = 0$, but keeping the other rigid body terms. However, even in this case, the transition line rises slightly for small $\omega$ before falling. This means that for some temperature, it may be possible that the nucleus changes from oblate to prolate with increasing spin, rather than the other way around, the usual case.

All of the calculations to this point have dealt only with the equilibrium behavior of the nucleus. Statistical fluctuations may modify many of these predictions, especially as to the sharpness of transitions. Thus we turn next to ways to evaluate these fluctuations using the information we have already derived.
Chapter 5.

The Uniform Approximation and Applications

The exact evaluation of the partition function, for a general many-body Hamiltonian, is extremely difficult, so an approximation to it must be found. The criteria for such an approximation include that it should be computationally tractable, that it take into account the most significant degrees of freedom, and, in this case, that it provide a way to take account of fluctuations of these degrees of freedom around their equilibrium values.

In the previous chapters we have used the mean field approximation to try to understand the thermodynamic behavior of a heated rotating nucleus. We have selected as the most important degrees of freedom for this approximation the quadrupole deformation parameters of the nuclear density. By varying these parameters, we were able to derive a free energy surface whose minima we interpreted as the equilibrium deformation for a given choice of thermodynamic quantities. We took as the free energy its value at these minima. This procedure, however, did not take into account the sharpness of the minimum. In the region of a phase transition, the surface is quite flat, and hence the minimum may not be very well defined. Also, we are dealing here with a finite system. The mean field approximation assumes there are enough particles to give rise to a smooth potential for each nucleon, which for a small number of particles may not be accurate. For these reasons, fluctuations give important corrections to the thermodynamic quantities we have already calculated, and thus we would like to develop a method of dealing with them.

We have two ways of dealing with these fluctuations. In the first section of this chapter, we shall take them into account in a simple way by treating their probability in the lowest order. Afterwards, we develop a more rigorous treatment that is applicable even for very large fluctuations. This method is based on the uniform
approximation, and will be described in some detail. Because the approximations that go into the uniform method are not really amenable to an estimation of the error they induce, we have investigated the method carefully in solvable many body systems before applying it to the nuclear case. The application of the uniform approximation to solvable models whose mean field solutions undergo first and second order phase transitions is thus presented in the last sections of this chapter.

5.1. Direct Evaluation of the Fluctuations

The simplest approach to fluctuations in the order parameter $\alpha$ for the nucleus is to evaluate the probability as directly as possible. Since the free energy surface is considered to be the quantity that determines the equilibrium deformation, we can take $e^{-F(T, \omega, \alpha)/T}$ as the probability of the given deformation $\alpha$ at a given $T$ and $\omega$. The equilibrium point is thus the point of maximum probability, as would be expected from our interpretation of the Landau theory.

In Ref. 31, fluctuations were evaluated in the $\omega = 0$ case in this fashion. The inclusion of fluctuations in this way led to a significant smoothing of the behavior of the nucleus, especially near the phase transition. The free energy was modified, and the level density showed a significant correction as compared with the usual Fermi gas expression. The corrections arose from both the inclusion of fluctuations and the recognition of the effect of the changing equilibrium deformation.

In the previous chapters we have assumed that the intrinsic and rotating frames were fixed with respect to each other. If we are to properly account for all fluctuations in $\alpha$, we must include fluctuations in the Euler angles as well. Thus we must include all 5 deformation parameters, $\beta, \gamma$, and the Euler angles $\varphi, \theta, \psi$. For $\omega = 0$, the free energy cannot depend on the orientation of any axis and hence in Ref. 31 there was no need to take these degrees of freedom into account. Now, the dependence of $F$ on these variables must be explicitly evaluated. Since the rotation
frame is still the principal frame, the moment of inertia is diagonal, and \( F \) is given by
\[
F(T, \omega, \alpha_{2\mu}) = F(T, \omega = 0, \beta, \gamma) =
\]
\[
[I_{xx}(\beta, \gamma) \cos^2 \phi \sin^2 \theta + I_{yy}(\beta, \gamma) \sin^2 \phi \sin^2 \theta + I_{zz}(\beta, \gamma) \cos^2 \theta] \omega^2.
\]
(5.1.1)
Now not only the moment of inertia about the rotation axis appears, but the general moments of inertia,
\[
I_{kk}(\beta, \gamma) = R \beta \cos \left( \gamma - \frac{2\pi}{3} k \right) + D \beta^2 \sin^2 \left( \gamma - \frac{2\pi}{3} k \right)
\]
are also included. The other terms in the moment of inertia arise from the scalar part and hence do not depend on the orientation.

Thus the improved expression is
\[
e^{-F(T,\omega)/T} = Z(T, \omega) = \int d\mu [\alpha_{2\mu}] e^{-F[T,\omega,\alpha_{2\mu}]/T}.
\]
(5.1.3)
The measure in the integral is the invariant measure corresponding to all of the \( \alpha_{2\mu} \), and is given in terms of \( \beta, \gamma, \) and \( \Omega \) by
\[
d\mu [\alpha_{2\mu}] = \beta^4 \sin 3\gamma \sin \theta d\beta \, d\gamma \, d\phi \, d\theta \, d\psi.
\]
(5.1.4)
The integral over the Euler angles is similar to ones which appear in calculations of quadrupole Coulomb excitation, and thus Eq. (5.1.4) can be reduced to a standard form along with additional integration on \( \beta \) and \( \gamma \). This can be done numerically with our coefficient functions from the Landau expansion, and is one of the areas we would like to investigate in the future.

5.2. Uniform Treatment of Fluctuations

This section is based on an exact functional integral expression for the nuclear partition function \(^{38}\) which serves to linearize the problem, yielding
\[
e^{-F(T,\omega)/T} = Z(T, \mu) = \frac{\int D[\sigma] e^{-F[T,\omega,\sigma]/T}}{\int D[\sigma] e^{-F[T,\sigma]/T}}
\]
(5.2.1)
\[
\int D[\sigma] e^{-F[T,\omega,\sigma]/T}
\]
\[-73-\]
The integration is over all "time dependent" single particle density functions \( \sigma(\vec{r}, \tau) \) which in general have all possible variations in space and time. \( F[T, \omega, \sigma] \) is a mean-field free energy

\[
F[T, \omega, \sigma] = \frac{T}{2} \int_{-\frac{T}{2}}^{\frac{T}{2}} d\tau \sigma(\tau, \nu \sigma) - P \ln \left[ 1 + T e^{-\int_{-\frac{T}{2}}^{\frac{T}{2}} (h_\sigma - \omega \tau)} \right]
\]

(5.2.2)

where \( P \) is the \( \tau \)-ordering operator and \( h_\sigma = t + \nu \sigma \) is the mean-field single-particle Hamiltonian. This substitution has changed the difficulty in dealing with the partition function, since the problem has been reduced to a set of single body problems, rather than a many-body problem. Unfortunately, there are an infinite number of these one body problems to be solved, complete with all of their dynamics. The exact evaluation of the path integral would require the solution of all of these, and hence further approximations are required. The first approximation that will be made is to make the \( \sigma \) independent of \( \tau \), or static. Since the \( \tau \)-dependence arose from an ordering effect, the non-commutativity of the kinetic energy and the potential energy, ignoring this makes the approximation "classical".

There still are an infinite number of degrees of freedom since the static density \( \sigma(\vec{r}) \) is still a function of \( \vec{r} \) and hence the problem is only marginally more tractable. The next stage is to identify those degrees of freedom which are most important, and find a way to express the partition function in terms of them. The integrand in the above static partition function can be viewed as a functional in the field \( \sigma \). By extremizing the exponent, one can find those configurations which yield the greatest contribution to the integral. This is precisely the procedure one follows in the saddle point approximation for ordinary exponential integrals. The same procedure may applied here, at least formally, to find extrema of the exponent and then sum over the the minima to find the saddle point approximation for this problem. One may even derive an expression for the curvature of the surface and thus get the first correction to the saddle point approximation.
Once again, this procedure, while simplifying the problem somewhat, does not go far enough. The best one can do with this approximation is discuss it formally, since its actual execution would require evaluating infinite dimensional determinants for the curvature expression and minimization over an infinite dimensional surface. Also, this approximation is not good near phase transitions, since the curvature becomes very small, and minima are no longer well separated. The saddle point approximation is fine as long as the saddle points are well separated, otherwise the curvature correction is meaningless as it arises from a gaussian approximation which is not valid when the extrema are close. Finally, no degrees of freedom have been selected as the most important, and hence all of them must be considered when evaluating the approximation.

Identifying the important degrees of freedom requires an understanding of the physics of the problem. For instance, if the nuclear density is expanded in multipoles, then it is well known that the quadrupole degrees of freedom are the most important, and thus it would be natural to deal only with them in the expansion of the free energy. The most important degrees of freedom are chosen, and the free energy is minimized with respect to all others at a fixed value of the chosen ones. By varying the important degrees of freedom, a free energy surface in the space of all their possible values can be defined. It is the saddle point topology of this surface that will be used to evaluate the free energy. Since the free energy is minimized with respect to all other degrees of freedom, it must be stable with respect to them, and hence the stability of the saddle points will be determined by their stability in terms of the important parameters.

Evaluating the free energy on this surface will be much simpler than before. The stationary phase approximation could be applied to the problem now, but only when the points are well separated. When the system is near a phase transition, this condition will not be satisfied, and hence we would like to apply the method
known as the uniform mapping, which is applicable even when the system is in the neighborhood of a phase transition.

The basic idea of the uniform mapping is to map the exponent of the integrand $F[T, \omega, \sigma]/T$ onto a simple function that has the same saddle point topology but is easier to evaluate. The free energy of Eq. (3.1.7) provides a natural mapping in our case, after we add to it quadratic terms to take account of all of the other directions for fluctuations that we have assumed were stable. Thus we map the field $\sigma(\vec{r})$ onto new coordinates $\alpha$ and $z_j$ such that

$$F[T, \omega, \sigma]/T = F(\xi, \alpha_{2\mu}) + \frac{1}{2} \sum_j z_j^2$$

rather than the fields $\sigma(\vec{r})$. The "control parameters" $\xi$ are general functions of $T$ and $\omega$ and in this case are the set $(F_0, A, B, C, D, R)$. They are determined by the conditions that saddle points of $F[\sigma]$ are mapped onto those of $F(\alpha)$. This is a specific choice of the general mapping

$$F[T, \sigma]/T = g(\xi_i, u_\nu) + \xi_0 + \frac{1}{2} \sum_j z_j^2,$$

where $g$ is some polynomial in $u_\nu$ whose saddle points are determined by the control parameters $\xi_i$ for a general free energy $F$. The $\xi_i$ are fixed by identifying the saddle points of $g$ with those of $F/T$, and are thus temperature dependent. The minimization of $F$ with respect to other than the selected parameters is insured by the $z_j$ term in Eq. (5.2.4). The numerator integral in Eq. (5.2.1) becomes after a change of variables

$$\int D[\sigma] e^{-F[T, \sigma]/T} \rightarrow \int \left( \prod_\nu du_\nu \prod_j dz_j \right) J(u_\nu, z_j) e^{-g(\xi, u_\nu) - \frac{1}{2} \sum_j z_j^2 - \xi_0},$$

where $J$ is the Jacobian of the transformation between $u_\nu$ and $z_j$. Now, $J$ will be expanded in such a way that no matter where the saddle points lie, the lowest order
Uniform Treatment of Fluctuations

terms will give a good approximation. The expansion of $J$ gives this approximation its name, in that the expansion is uniform about all of the saddle points. To see why $J$ must be expanded in this way, note that the saddle points move as the $\xi_i$ vary, so that the expansion of the Jacobian cannot be fixed to one point, e.g. a Taylor expansion about 0 would not be good for all values of $\xi_i$.

Thus two conditions are imposed on the expansion of $J$. First, the basis chosen must vanish around all of the saddle points. Second, the basis should be complete in the sense that all possible terms that have the symmetry of the problem should be expressible in it, i.e., if the functions $F$ and $g$ are even, $J$ will reflect this, and not all polynomial terms will be necessary for its expansion. A basis which satisfies these conditions is

$$\frac{\partial g'}{\partial \xi_i} \prod_{\nu} \left( \frac{\partial g'}{\partial u_{\nu}} \right)^{m_{\nu}} \prod_j z^{n_{j}} \quad \text{for } i = 0, \ldots$$  \hspace{1cm} (5.2.6)

where $g' = g + \xi_0$. Thus $J$ can be expanded as

$$J = \sum_{m_0, m_1, \ldots, n_0, n_1, \ldots} \left[ \sum_i a^{(i)}_{m_0 m_1 \ldots n_0 n_1} \frac{\partial g'}{\partial \xi_i} \prod_{\nu} \frac{\partial g'}{\partial u_{\nu}} \prod_j z^{n_j} \right].$$  \hspace{1cm} (5.2.7)

This expansion is exact, and, as stated above, good for all values of $\xi_i$. The approximation comes in taking only the $m_j = 0$ terms. Then the coefficients $a^{(i)} \equiv a^{(i)}_{000\ldots}$ are given as the solution to a set of linear equations by evaluating Eq. (5.2.7) at the saddle points. Note that since the first derivatives vanish at the saddle points, the Jacobian is given by

$$J = \left( \frac{\det \left[ \partial^2 g / \partial u \partial u \right]}{\det \left[ \partial^2 (F/T) / \partial \sigma \partial \sigma \right]} \right)^{\frac{1}{2}}.$$  \hspace{1cm} (5.2.8)

Now the integral in Eq. (5.2.5) can be evaluated. Due to the sum over $i$ in Eq. (5.2.7), the integral has been broken up into a sum of integrals of the form

$$I_k (\xi) = - (\partial / \partial \xi_k) \int \prod_{\nu} du_{\nu} e^{-\psi'(\xi, u_{\nu})},$$  \hspace{1cm} (5.2.9)
which, due to our choice of $g$ are fairly easy to evaluate. With the normalization in Eq. (5.2.1) the approximation becomes

$$Z(T) = \frac{[\det(v/T)]^{1/2}}{(2\pi)^{n/2}} \sum_{k=0}^{n} a^{(k)} I_k(\xi).$$  \hspace{1cm} (5.2.10)

Here $n$ is the number of degrees of freedom in the free energy surface.

For the problem treated in the previous chapters, the evaluation of Eq. (5.2.10) is still difficult. This is because the calculation of the Jacobian in Eq. (5.2.8) requires the complete knowledge of the free energy surface and its curvature at the equilibrium point, i.e. a finite temperature cranking RPA calculation must be performed to solve this exactly. Thus a further approximation is to take once again only the quadrupole degrees of freedom and calculate the fluctuations along those directions. This determinant is much more tractable and hence this calculation may be more reasonably done. The validity of such an approximation is not at all clear, and hence in the next section we will apply the uniform approximation, both in general and only in the direction of the order parameter in order to test its applicability.

5.3. The Lipkin Model as a Test of the Uniform Approximation

The Lipkin model is an $N$ fermion system with two $N$-fold degenerate single-particle levels, $-\epsilon/2$ and $\epsilon/2$. Denoting by $a_{p-1}^\dagger$ ($p = 1, \ldots, N$) the creation operators for the $N$ degenerate lower states and by $a_{p+1}^\dagger$, those for the higher states, the Lipkin Hamiltonian is:

$$\hat{H} = \frac{1}{2} \epsilon \sum_{p,s=\pm1} s a_{p,s}^\dagger a_{p,s} + \frac{1}{2} v \sum_{p,s,s',p'} a_{p,s}^\dagger a_{p',s'}^\dagger a_{p'-s',p-s}. \hspace{1cm} (5.3.1)$$
The first term in the Hamiltonian Eq. (5.3.1) is a one-body operator analogous to a kinetic energy term, while the second represents a two-body interaction characterized by a strength \( v \). It is possible to define quasi-spin operators

\[
J_\pm = \sum_p a^\dagger_{p\pm 1} a_{p\mp 1}, \\
J_z = \frac{1}{2} \sum_{ps} s a^\dagger_{ps} a_{ps},
\]

which form an \( SU(2) \) algebra. The Hamiltonian can then be expressed in terms of these operators:

\[
\tilde{H} = \epsilon J_z + v \left( J_z^2 - J_y^2 \right).
\]

Since \([\tilde{H}, J^2]\) = 0, the Hamiltonian can be diagonalized within each of the irreducible \( SU(2) \) multiplets separately. The ground state multiplet is characterized by \( j = N/2 \), and from now on that is the only one which will be considered. For all integrals to remain finite, the interaction should be negative definite, and the Hamiltonian Eq. (5.3.3) is modified by subtracting from it \( v J^2 \) (which is a constant for the ground state multiplet):

\[
H = \epsilon J_z - v \left( 2J_y^2 + J_z^2 \right).
\]

For this section, take \( \epsilon = 1 \) so that all energies are measured in units of \( \epsilon \). This model is known to have a second order phase transition in the particle number in its mean field ground state \( 41 \) for all \( \chi = (N - 1) v/\epsilon > 1 \).

The partition function of Eq. (5.2.1) can now be written

\[
Z(T) = \frac{\int D[\sigma_y(\tau)] D[\sigma_z(\tau)] e^{-F[T, \sigma_y(\tau), \sigma_z(\tau)]/T}}{\int D[\sigma_y(\tau)] D[\sigma_z(\tau)] e^{-\int_{-1/2T}^{1/2T} dr \left( 2\sigma_y^2(\tau) + \sigma_z^2(\tau) \right)}}
\]

where

\[
F[T, \sigma_y(\tau), \sigma_z(\tau)] = T v \int_{-1/2T}^{1/2T} dr \left( 2\sigma_y^2 + \sigma_z^2 \right) - P \ln \text{Tr} \left[ T e^{\int_{-1/2T}^{1/2T} dr H_\sigma} \right].
\]
is the free energy of the one-body Hamiltonian:

\[ H_\sigma = J_z - 2v (2\sigma_y J_y + \sigma_z J_z). \]  

(5.3.7)

Path dependent mean-field configurations do contribute to the exact partition function but even for this simple model are difficult to calculate, and hence the static approximation mentioned above in which only path independent configurations are included in Eq. (5.3.5) can be applied. The partition function can now be written in terms of ordinary integrals

\[ Z(T) \approx \frac{\int d\sigma_y d\sigma_z e^{-F[T,\sigma_y,\sigma_z]/T}}{\int d\sigma_y d\sigma_z e^{-v/T(2\sigma_y^2 + \sigma_z^2)}}, \]  

(5.3.8)

where

\[ F[T,\sigma_y,\sigma_z] = v \left(2\sigma_y^2 + \sigma_z^2\right) - T \ln \frac{\sinh (j + 1/2) \lambda/T}{\sinh \lambda/2T} \]  

(5.3.9)

is the free energy Eq. (5.3.6) in the time-independent mean field \(\sigma_y, \sigma_z\). Here \(\lambda\) is the magnitude of the vector

\[ \vec{\lambda} = (0, -4v\sigma_y, 1 - 2v\sigma_z). \]  

(5.3.10)

As claimed above, the approximation Eq. (5.3.8) is a “classical” approximation since it provides the leading term in a \(1/N\) expansion as shown by scaling the quasi-spin operators \(j_y = J_y/N, j_z = J_z/N\). Then the Lipkin Hamiltonian undergoes a similar scaling:

\[ \frac{H}{N} \approx j_z - \frac{v}{n} \left(2j_y^2 + j_z^2\right). \]  

(5.3.11)

Since \([j_y, j_z] = \frac{j}{N} j_z\), it is clear that any correction to the free energy per particle from time-dependent fluctuations is of order \(1/N\).

To test the static approximation Eq. (5.3.8) has been evaluated numerically. The ratio of the partition function Eq. (5.3.8) to the exact one is plotted in Fig. 18. The static approximation becomes better for higher temperatures, since, as the
"time" interval $1/T$ in Eq. (5.3.6) becomes shorter, the time dependent fluctuations become less important. However, even at temperatures down to $T \sim 2$, the error for $N = 50$ is only about 10%.

5.3.1. The Mean Field Approximation

The uniform approximation depends on the saddle point topology of the free surface, so that will now be investigated for the Lipkin model. The logarithmic term in Eq. (5.3.9) is in fact the partition function $\zeta$ for a single-body $SU(2)$ hamiltonian, i.e.

$$\zeta = \text{Tr} e^{-\mathbf{J}/T} = \frac{\sinh \left[ (j + \frac{1}{2}) \lambda / T \right]}{\sinh \lambda / 2T}. \quad (5.3.12)$$

Below some critical temperature, there are three saddle points, while above it there is only one, as can be seen in Fig. 19. There is always a saddle point at $\sigma_y = 0$ and $\sigma_z = -\zeta / \zeta$. Since $\sigma_y = 0$, $\lambda = |1 - 2v\sigma_z|$. This will be referred to as the "spherical" saddle point. The other two points, when they exist, are
Figure 19: Contour plots in the $\sigma_y - \sigma_z$ plane using Eq. (5.3.9) with $\chi = 1.47$ and $N = 50$. Temperatures are $T = .67, 14.3, 18, 33.3$, in units of $\epsilon$. All contours are spaced 1.2 units apart. Spherical saddle points are marked with asterisks($\ast$), and deformed ones with crosses($\times$). The top plots are below the critical temperature, the bottom left at it, and the bottom right above it.

degenerate, and shall be referred to as the “deformed” points. They are given by $\sigma_1^2 = \sigma_2^2 = -1/(2\nu)$ and by $\sigma_1^1 = -\sigma_2^2$ which solve

$$\frac{\lambda}{4\nu} = -\zeta' / \zeta, \quad \text{(5.3.13)}$$

where now $\lambda = 2\sqrt{1 + 4\nu^2 \sigma_y^2}$. At $T = T_c$ the three solutions coalesce and there is a single minimum at $\sigma_y = 0, \sigma_z = -1/(2\nu)$. Since $\sigma_y$ becomes non-zero as $T$ decreases from $T_c$ it may be identified as an order parameter. The transition occurs when the
solution to Eq. (5.3.13) is $\sigma_y = 0$, so that $T_c$ is determined from

$$\frac{\xi'}{\xi|_{T_c/2}} = \frac{1}{2v}. \quad (5.3.14)$$

The mean-field free energy, which is the global minimum of $F$ in Eq. (5.3.9), is plotted against $T$ in Fig. 20 (dotted-dashed line), where the deformed value is used below $T_c$ and the spherical one above $T_c$.

5.3.2. Fluctuations and the Uniform Mapping

As discussed earlier, merely looking at the minima of the surface in order to calculate the free energy should fail near a phase transition. In fact, when the free energy given by the global minimum is compared to the exact free energy, the worst deviation occurs in the region near the phase transition. The uniform approximation will give an analytic expression for the partition function in Eq. (5.3.8), so comparisons even in this region should be straightforward.

The mapping in this case will be from $F/T$ onto a polynomial with the same saddle point topology. Since $\sigma_y$ has been identified as the order parameter, only need one non-trivial degree of freedom is needed in the mapping, i.e. only one $u$. There is only one other degree of freedom and thus the mapping will be $\sigma_y, \sigma_z \to u, z$. The simplest choice for $g$ with the correct behavior is

$$g'(u) = g(u) + \xi_0 = \frac{1}{4}u^4 - \frac{1}{2} \xi_1 u^2 + \xi_0. \quad (5.3.15)$$

Here, $\xi_0, \xi_1$ are constants (which depend on $T$) and are known as the control parameters. When $\xi_1 > 0$, the right-hand side of Eq. (5.3.15) has one saddle point and two degenerate minima, while when $\xi_1 < 0$ it has a unique real minimum. Note that there is no linear term in $u$ since the two deformed saddle points are always degenerate and that at the transition temperature $\xi_1 = 0$. The constants $\xi_0, \xi_1$ are determined by the conditions that the saddle points of $F$ be mapped onto those of
The Lipkin Model as a Test of the Uniform Approximation

\[ F \left[ T, \sigma_y^0, \sigma_z^0 \right] / T = \xi_0 \]

\[ F \left[ T, \sigma_y^1, \sigma_z^1 \right] / T = -\frac{1}{4} \xi_1^2 + \xi_0. \]  

(5.3.16)

Here \((\sigma_y^0, \sigma_z^0)\) is the spherical saddle point and \((\sigma_y^1, \sigma_z^1)\) is one of the two deformed points. To evaluate the numerator integral in Eq. (5.3.8), first transform the integration variables to \((u, z)\):

\[ \int d\sigma_y \, d\sigma_z \, e^{-F[T, \sigma_y, \sigma_z]/T} = \int du \, dz \, J(u, z) \, e^{-g(u) - \xi_0 - \frac{1}{2} z^2}, \]  

(5.3.17)

where \(J(u, z) = \frac{\partial(\sigma_y, \sigma_z)}{\partial(u, z)}\) is the Jacobian of the mapping. The basis for the expansion of \(J\) is given by Eq. (5.2.6) and in this case consists of terms of the form \((u(u^2 - \xi_1))^m z^n\) multiplied by \(u^2\) or 1:

\[ J(u, z) = \sum_{m,n} \left\{ a_{mn} \left[ u \left( u^2 - \xi_1 \right) \right]^m z^n + c_{mn} u^2 \left[ u \left( u^2 - \xi_1 \right) \right]^m z^n \right\}, \]  

(5.3.18)

where \(a_{mn}\) and \(c_{mn}\) are the expansion coefficients. The coefficients \(a_{00}\) and \(c_{00}\), (denoted by \(a_0\) and \(c_0\) respectively from now on) are found from the values of the Jacobian at the three saddle points, using Eq. (5.2.8) (Since two of them are degenerate, the problem is not overdetermined). The partition function in Eq. (5.3.8) is then approximated by

\[ Z(T) = 2e^{-F_0/T} \left[ \tilde{a}_0 J_0(\xi_1, 0) + \tilde{c}_0 J_2(\xi_1, 0) \right], \]  

(5.3.19)

where

\[ \tilde{a}_0 = \sqrt{\frac{2}{\pi}} v a_0 / T = \sqrt{\frac{2}{\pi}} v_1 \sqrt{\frac{\xi_1}{-\det F^{ij}}}, \]

\[ \tilde{c}_0 = 2 \sqrt{\frac{2}{\pi}} v c_0 / T = 2 \sqrt{\frac{2}{\pi}} v \left( \sqrt{\frac{2\xi_1}{\det F^{ij}_1}} - \sqrt{\frac{\xi_1^2}{-\det F^{ij}_0}} \right). \]  

(5.3.20)
The calculated and exact free energies are shown in Fig. 20, where the free energy of Eq. (5.3.19) is essentially indistinguishable from the exact one.
In this case, the $I_n(\xi_1, 0)$ are universal analytic functions defined by

$$I_n(\xi_1, 0) = \int_{-\infty}^{\infty} du u^n e^{-u^4 + \xi_1 u^2}.$$  \hspace{1cm} (5.3.21)

The universal functions $I_n$ of two arguments were introduced in Ref. 31. Here there is a special case in which the second argument is zero. A non-zero second argument characterizes a first order phase transition which can occur when the two deformed minima are not degenerate. The function $I_0(\xi_1, 0)$ can be expressed in terms of the parabolic cylinder functions $U$ and $V$ or in terms of Bessel functions of fractional order, which are more useful for numerical calculations 42.

At a given temperature, all of the parameters which occur in Eq. (5.3.19), namely $\xi_0(\equiv F_0/T)$, $\xi_1$, $\tilde{a}_0$, and $\tilde{c}_0$, are completely determined from $F_0, F_1$ and $\det(F''_0), \det(F''_1)$ by Eq. (5.3.16) and Eq. (5.3.20). Note that these equations also hold above the critical temperature $(T > T_c)$. In that case, the only real saddle point is the spherical one ($\sigma_0^0, \sigma_0^0$) and the two "deformed" saddle points become complex. Although these saddle points are not physical, they still have to be taken into account in Eq. (5.3.16) in order to determine the mapping. Especially just above $T_c$ these points are close to the spherical one and, therefore, affect the saddle-point approximation. For these points $\sigma_z = -1/(2v)$ as before, but the $\sigma_y$ which satisfies Eq. (5.3.13) is purely imaginary. As $T$ continues to increase, $\lambda$ becomes purely imaginary, too. Now $\zeta$ is a periodic function on the imaginary axis, so Eq. (5.3.13) has many imaginary solutions $\lambda$, among which is chosen the one closest to the real axis.

The uniform free energy calculated from the partition function Eq. (5.3.19) is in very close agreement with the exact one, as Fig. 21 shows.

When $T \ll T_c$ or $T \gg T_c$ the saddle points are well separated and the uniform approximation should reduce to the ordinary saddle point results. When $T \ll T_c$, $\xi_1$ is positive and large. Using the asymptotic expansion of $V$ (see (19.8.2) in Ref. 42
The Livkin Model as a Test of the Uniform Approximation

Figure 21: As in Fig. 20, but for the fractional error in the approximations \((F - F_{\text{exact}})/|F_{\text{exact}}|\).

\[ p. 689 \) gives:

\[
Z(T) \sim 2\frac{2^{5/4} v}{\sqrt{\det F''_1}} e^{-F_1/T}. \tag{5.3.22}
\]

The result Eq. (5.3.22) is exactly what is obtained if Eq. (5.3.8) is evaluated by the saddle point method. (For \(T \ll T_c\) only the two deformed saddle points contribute and their contributions are equal.) In the limit \(T \to 0\) Eq. (5.3.22) yields

\[
\frac{F}{T} \simeq (F_1/T - \ln 2) - \frac{1}{2} \ln \left[ \sqrt{2}x^2/\left( x^2 - 1 \right) \right], \tag{5.3.23}
\]

where \(F_1\) is given by

\[
F_1 = -j \left( x + \frac{1}{2x} \right) + \frac{1}{2x} - \frac{j}{2j - 1} x,
\]

the zero temperature limit of Eq. (5.3.9). Note that \((F_1/T - \ln 2)\) is the approximation for \(F/T\) when fluctuations are neglected (taking into account the degeneracy of the two deformed points). From Eq. (5.3.23), it is seen that the fluctuation corrections for \(F/T\) in the limit \(T \to 0\) are finite and negative.
When $T \gg T_c$ then $\xi_1$ is negative and large in magnitude. Using (19.8.1), p. 689 of Ref. 42, and neglecting the $c_0$ term gives

\[
Z(T) \sim \frac{2^{3/2} e^{-F_0/T}}{\sqrt{\det F''_0}}
\]

which is again just the saddle point approximation of Eq. (5.3.8). Indeed, for $T \gg T_c$ there is a single real saddle point (the spherical minimum).

5.3.3. Inclusion of Fluctuations in the Order Parameter Only

For a general many-body system, the determinants in Eq. (5.3.20) are still infinite-dimensional. A cruder approximation is one in which only fluctuations in the constrained directions which play the role of order parameters are taken into account. For instance, these directions were chosen in Ref. 31 to be the quadrupole deformations of the nucleus. In the present model, the order parameter is $\sigma_y$, and the free energy “surface” is:

\[
\tilde{F}[T, \sigma_y] = \min_{\sigma_z} F[T, \sigma_y, \sigma_z] \bigg|_{\sigma_y = \text{const.}}. \tag{5.3.25}
\]

The free energy of Eq. (5.3.25) is thus derived from that of Eq. (5.3.9). The two free energies have the same features at the phase transition, since the constrained one is merely a subset of the one with more degrees of freedom. As for the fluctuations, it is expected that those in all “other” directions ($\sigma_z$ in this case) would to a large extent be cancelled in the numerator and denominator of Eq. (5.3.8) and that the approximation based on fluctuations in the important directions only,

\[
Z(T) \sim \frac{\int d\sigma_y e^{-\tilde{F}[T, \sigma_y]/T}}{\int d\sigma_y e^{-2\nu \sigma_y^2/T}} \tag{5.3.26}
\]

will be reasonable. The normalization integral in the denominator of Eq. (5.3.26) is obtained from that in Eq. (5.3.8) by minimizing the “action” in the $\sigma_z$ direction.
e. setting $\sigma_z = 0$), as was done in the numerator. Note that this normalization integral is also temperature dependent.

Eq. (5.3.26) can also be evaluated by the uniform approximation. The mapping is a one-variable mapping ($\sigma_y \to u$) such that:

$$F [T, \sigma_y] / T = \frac{1}{4} u^4 - \frac{1}{2} \xi_1 u^2 + \xi_0.$$  \hfill (5.3.27)

The final result for the approximated partition function has the same form as Eq. (5.3.19). The numerical control parameter $\xi_1$ is exactly the same as in the full problem. The only difference arises in the coefficients $\tilde{a}_0, \tilde{c}_0$ which are now given by

$$\tilde{a}_0 = \sqrt{\frac{v}{\pi}} \tilde{a}_0 = \sqrt{\frac{v}{\pi}} \sqrt{\frac{\xi_1}{\tilde{F}_0''}}$$

$$\tilde{c}_0 = 2 \sqrt{\frac{v}{\pi}} \frac{\xi_1}{\tilde{F}_1''} c_0 = \sqrt{\frac{v}{\pi}} \frac{2 \xi_1}{\tilde{F}_1''} \left( \sqrt{\frac{\xi_1}{\tilde{F}_0''}} - \sqrt{\frac{\xi_1}{\tilde{F}_0''}} \right).$$  \hfill (5.3.28)

Here $\tilde{F}_0''$ and $\tilde{F}_1''$ refer to ordinary second derivatives of $\tilde{F}$ with respect to $\sigma_y$ at the spherical and deformed configurations, respectively. The earlier expressions for $\tilde{a}_0$ and $\tilde{c}_0$ differ from Eq. (5.3.28) also by an additional $\sqrt{2v}$ normalization factor. This is related to the presence of a second direction for fluctuations in the former calculation, since in the limit $N = 0(j = 0)$, $F = 2v \sigma_y^2 + \nu \sigma_2^2, \tilde{F} = 2v \sigma_y^2$, and thus $\det \tilde{F}_0''$ contains an additional factor of $2v$ as compared with $\tilde{F}_0''$.

The free energy corresponding to this approximation is shown in Fig. 20 and Fig. 21 by a solid line. It can be seen that this approximation accounts for a large part of the correction that the full uniform mapping achieves. Hence we can expect fluctuations in the order parameters only to be the primary correction in other cases as well.

The transition approximation, a power series expansion of the free energy about the spherical solution valid for $T \sim T_c$, can be derived for the one-dimensional case, where the free energy $\tilde{F}$ can be expanded to sixth order around the spherical
Figure 22: Level densities in the Lipkin model versus energy. The level densities were calculated from Eq. (2.1.14) using the curves of Fig. 20 and Eq. (2.1.15). Energy is in units of \( \epsilon \), and level density in \( \epsilon^{-1} \). Curves are denoted as in Fig. 20. Arrows show the transition points in the various approximations.

The final results for \( a_0 \) and \( c_0 \) in terms of the derivatives of \( \tilde{F} \) at the critical point are:

\[
\begin{align*}
a_0 (T_c) &= \sqrt{\frac{6}{\tilde{F}(iv)}} \\
c_0 (T_c) &= -\frac{6^{3/4}}{40} \frac{\tilde{F}(vi)}{\left[\tilde{F}(iv)\right]^{7/4}}.
\end{align*}
\] (5.3.29)
Finally we can turn to the level density for the Lipkin model. First, we calculate the entropy in the standard fashion:

\[ S = - \left( \frac{\partial F}{\partial T} \right) \]  \hspace{1cm} (5.3.30)

and from it calculate the energy using \( E = F + TS \). The energy curves calculated in this way are all monotonically increasing with temperature; since \( E \) may also be defined by \( E = \frac{\partial^2 F}{\partial \beta^2} \), it follows that \( \frac{\partial^2 (\beta F)}{\partial \beta^2} < 0 \) and hence that the free energies are thermodynamically stable.

The entropy of the mean field solution is easy to calculate from Eq. (5.3.9) when it is noted that since the mean field solutions solve

\[ \frac{\partial F}{\partial \sigma_y} = \frac{\partial F}{\partial \sigma_z} = 0 \]  \hspace{1cm} (5.3.31)

for these configurations, only explicit partial derivatives with respect to \( T \) need be taken. Even though there is an explicit expression (5.3.19) for the uniformly approximated partition function, numerical derivatives must be taken in Eq. (5.3.30) in this case, due to the large number of terms in the analytic derivative. In the limits \( T \gg T_c \) or \( T \ll T_c \), the simpler expressions for the stationary phase approximation which the uniform approximation reduces to permit simpler formulas to be used. Specifically, the entropy as \( T \to 0 \) is

\[ S \to \ln \left[ 2^{9/4} \chi^2 / \left( \chi^2 - 1 \right) \right] \]  \hspace{1cm} (5.3.32)

which is not zero for \( \chi > 1 \). This is unlike both the mean field and exact entropies, which vanish at \( T = 0 \). The region near \( T = 0 \), however, is expected to be the range in which the uniform approximation is worst, so this result is not too surprising.

The level density can be calculated using Eq. (2.1.13). Since the energy curves are all convex, \( \Delta \) appearing in the expression for \( \rho \) is always real. As with the
entropy, analytic expressions are available for the mean field level density, and the uniform approximation requires numerical derivatives. For comparison, Eq. (2.1.13) was also calculated using the exact spectrum and the exact partition function. The thermodynamic quantities are then given by various sums over the energy spectrum, all of which are easily calculated. The results of these calculations are given in Fig. 22. The mean field level density gives about 50% of the “exact” stationary phase approximation for energies above the ground state energy, where Eq. (2.1.13) is singular due to the vanishing of its denominator, although the integral of the mean field level density over energy is still finite. The mean field level density also has a discontinuity at the critical temperature due to the second order transition there. The uniformly approximated level density has no such discontinuity, showing one of the effects of fluctuations near the phase transition. When the uniform level density is compared to the “exact” averaged level density, they are seen to be quite close. Since this is an average level density, these calculations were compared to a Strutinski smoothed average level density derived from the exact spectrum. Over most of the energy range, the two methods give very good agreement. Near the ground state, however, the Strutinski calculation is not singular. Because the other averaged level densities are singular there, they must drop more quickly to the nearly constant value they assume in the center of the spectrum than does the Strutinski one, which accounts for the largest discrepancy between them.

5.4. The Multilevel Lipkin Model

The two-state Lipkin model, where a second order phase transition was found at finite temperature, was considered in the last section. For the multilevel extension of the Lipkin model, both first and second order phase transitions are known to occur in the ground state variational solutions, and thus this model is a good candidate to investigate for finite temperature first order phase transitions.
The multilevel Lipkin model consists of $M$ fermions, which can lie in any of $N$ $M$-fold degenerate energy levels. The original Lipkin model is the special case of $N = 2$. Now denote by $a^\dagger_{ij}$ the creation operator for the $i$-th fermion in the $j$-th level and by $a_{ij}$ the corresponding annihilation operator. For the purposes of this section, $N = 3$ has been chosen, although the results are easily generalizable to arbitrary $N$. As for $N = 2$, take collective operators $A^\dagger_j$ and $A_j$, where

$$A^\dagger_j = \sum_{i=1}^m a^\dagger_{ij}, \quad A_j = \sum_{i=1}^m a_{ij}$$  \hspace{1cm} (5.4.1)

but now note that the $N^2$ operators $\hat{L}_{jk} = A^\dagger_j A_k$ form a $U(N)$ group. In the ground state variational calculations, the first order phase transition can only occur if there is a quadrupole interaction between any two of the excited states\textsuperscript{43}, which suggests a Hamiltonian of the form

$$H = \sum c_j \hat{L}_{jj} + \frac{V}{2} (\hat{L}_{23}^2 + \hat{L}_{32}^2).$$  \hspace{1cm} (5.4.2)

Since all of the operators are number-conserving, the single particle part of $H$ can be written in terms of the number operators

$$\hat{N}_2 = \frac{1}{2} (\hat{L}_{22} - \hat{L}_{11}), \quad \hat{N}_3 = \frac{1}{2} (\hat{L}_{33} - \hat{L}_{11}),$$  \hspace{1cm} (5.4.3)

and thus a $SU(3)$ group can be used instead.

The operators which enter into the quadrupole interaction are seen to be the $I_+$ and $I_-$ operators of the usual $SU(2)$ isospin subgroup of $SU(3)$. Since a negative definite interaction is again required, choose Eq. (5.4.2) minus $I^2$ and have as our final Hamiltonian

$$H = \epsilon_2 \hat{N}_2 + \epsilon_3 \hat{N}_3 - V \left(2I_y^2 + I_z^2\right).$$  \hspace{1cm} (5.4.4)
Note that $I_z = \hat{N}_3 - \hat{N}_2$.

The partition function for this system can be transformed as above to a functional integral representation in the form

$$Z = \int d[\bar{\sigma}] e^{-v/T(2s_b^2+\Delta^2) \text{Tr} Pe^{\int_{-1/2T}^{1/2T} dr H_\sigma}}$$

(5.4.5)

where $H_\sigma$ is a linearized form of $H$

$$H_\sigma = \epsilon_2 \hat{N}_2 + \epsilon_3 \hat{N}_3 - V \left( 4I_y \sigma_y + 2 \left( \hat{N}_3 - \hat{N}_2 \right) (\sigma_3 - \sigma_2) \right).$$

(5.4.6)

or, $H_\sigma = \vec{\sigma} \cdot \vec{\lambda}$ where

$$\vec{\sigma} = (\epsilon_2 - 2V\Delta, \epsilon_3 - 2V\Delta, -4V\sigma_y, \vec{0})$$

$$\Delta = \sigma_2 - \sigma_3$$

(5.4.7)

$$\vec{\lambda} = (\hat{N}_2, \hat{N}_3, I_y, I_z, \ldots).$$

Here $\vec{\lambda}$ is the set of $SU(3)$ generators.

Restricting consideration as earlier to time-independent fluctuations reduces the above integrals to ordinary ones rather than path integrals. To evaluate $\text{Tr} \log H_\sigma$, find the eigenvalues of $H_\sigma$ in the fundamental representation. After this set of eigenvalues is known, it is easy to express them in terms of the usual set of $SU(3)$ diagonal operators and thus

$$H_\sigma = a I_3 + b Y$$

(5.4.8)

where

$$a = \left( (\epsilon_3 - \epsilon_2 - 4V\Delta)^2 / 4 + 16V^2 \sigma_y^2 \right)^{1/2}$$

$$b = \frac{3}{4} (\epsilon_2 + \epsilon_3).$$

(5.4.9)

Note that $b$ is independent of $\sigma$ and that Eq. (5.4.8) is independent of the representation, or equivalently, the number of particles.

The previous section considered only the ground state band of $SU(2)$. In order to have a more realistic spectrum, now the partition function for the entire spectrum
of SU(3) is calculated. Since all of the levels are $M$-fold degenerate, the particles move as independent fermions, and the partition function is just the product of $M$ single particle partition functions,

$$Z_\sigma = (Z_{sp})^M$$

(5.4.10)

where

$$Z_{sp} = e^{2b/3T} + e^{-(b/3+a/2)/T} + e^{-(b/3-a/2)/T}.$$  

(5.4.11)

Thus the integral expression for $Z$ is

$$Z = \int d\sigma_y d\Delta e^{-F_\sigma/T}$$

(5.4.12)

where

$$F_\sigma = V \left( 2\sigma_y^2 + \Delta^2 \right) - TM \ln Z_{sp}.$$  

(5.4.13)

Again an appropriate polynomial must be found to map $F_\sigma$ onto and then used in the evaluation of the integral in Eq. (5.4.12). As in the SU(2) calculations, there are two equations which must be solved to find the saddle points. Again, one of them has two sets of solutions, requiring either $\sigma_y = 0$ or that $\sigma_y$ satisfy some analytic equation. These two kinds of solutions will be denoted as the spherical and deformed, respectively. For certain temperatures, however, in this case there will be a maximum as well. This maximum will also lie off the $\Delta$ axis and will be referred to as a deformed maximum. Also as before, all of the deformed solutions have the same $\Delta$.

Thus, below a certain temperature, $F_\sigma$ can have five extrema, one on the $\Delta$ axis, and the others in pairs located symmetrically with respect to that axis. For a suitable choice of parameters, a first order phase transition can occur as the global minimum of the surface shifts discretely from the deformed minimum to the spherical one. If the first order phase transition occurs, then as the temperature
rises, after the first order transition happens, the deformed maxima and minima will coalesce and vanish, leaving only the spherical minimum. If the parameters $V$ and $\epsilon_{1,2}$ are such that no first order transition occurs, then the deformed minima first move to the $\sigma_y = 0$ axis and merge with the spherical saddle point, making it a maximum as in the $SU(2)$ case. As the temperature increases further, the behavior is similar to the $SU(2)$ model, as the two deformed minima move symmetrically toward the axis and finally merge with the spherical point. This behavior can be reproduced by a sixth order even polynomial, and hence we have chosen as our mapping function

$$g(u, v) = u^6/6 - \xi_2 u^4/4 + \xi_1 u^2/2 + v^2/2 + \xi_0.$$  \hspace{1cm} (5.4.14)$$

As before, the control parameters $\xi_0$, $\xi_1$, and $\xi_2$ are fixed by mapping the saddle points of $g$ onto those of $F_0/T$. Above the phase transition, the complex saddle points of $g$ closest to the real axis are chosen in the mapping. The calculations leading to an expression of the form of Eq. (5.2.10) are similar to those of the previous section and will not be detailed here. The resulting expression is then

$$Z = e^{-\xi_0} \int dudv \left( a_0 + b_0 u^2 + c_0 u^4 \right) e^{-\left( u^6/6 - \xi_2 u^4/4 + \xi_1 u^2/2 + v^2/2 \right)}.$$  \hspace{1cm} (5.4.15)$$

The expansion parameters $a_0$, $b_0$, and $c_0$ are given by expanding the Jacobian at the saddle points to order $u^4$ and solving the resulting set of equations. As in the $SU(2)$ case, all of these procedures can be carried out analytically. Unlike previously, there is no closed form for the integrals appearing in Eq. (5.4.15), although they can be easily evaluated numerically.

The conditions for the first order phase transition to occur are not analytically solvable. Since above some temperature the spherical minimum is the only minimum, the first condition is that as $1/T \to \infty$, the deformed minimum must lie lower than the spherical one. As before, the requirement for a second order phase
transition would be that the conditions for both spherical and deformed solutions be satisfied simultaneously. This leads to

\[
\frac{\epsilon_3 - \epsilon_2}{4V} = \frac{2N \sinh \left( \left( \frac{\epsilon_3 - \epsilon_2}{2T} \right) \right)}{e^{b/T} + 2 \cosh \left( \left( \frac{\epsilon_3 - \epsilon_2}{2T} \right) \right)}.
\]  

(5.4.16)

The right hand side of Eq. (5.4.16) tends to 0 at both \( T = 0 \) and \( T = \infty \) and has one maximum. Hence there is a critical \( V \) for which the maximum is exactly equal to the left hand side. For \( V \) larger than this, a second order phase transition will occur, while for \( V \) smaller than this, but in the range satisfying the first condition, a first order transition will occur. This behavior is in marked contrast to the zero temperature phase transition, where the first order transition occurs for all \( V \) greater than some threshold.

The integrals in Eq. (5.4.15) are similar to the \( I_n \) functions of two arguments of Ref. 31. In fact, as pointed out earlier, if both arguments of these functions are non-zero, then they can be used to describe a first-order phase transition. The extended Lipkin model, however, has a symmetry to the free energy surface that would make the use of the earlier functions inappropriate. Thus in cases where the first order phase transition occurs in the above symmetric fashion, this kind of description is more useful.

All of these calculations can be carried out in straightforward manner, especially since those calculations which are not analytic are generally not difficult numerically. Above the phase transition, though, care must be taken in calculating the complex saddle points. Unlike the \( SU(2) \) case, when the deformed saddle points coalesce they have a nonzero real part, and thus it cannot be assumed that just above the critical temperature, the saddle point will be purely imaginary in \( \sigma_y \). Rather, the real solution at the critical temperature is used as a starting guess, and the complex plane near it is searched, although \( \Delta \) retains the same value for all deformed saddle points, as before. For sufficiently high temperatures, \( \sigma_y \) must be
purely imaginary, and it is easy to calculate the temperature at which this happens. All of this behavior is reproducible by an appropriate and smooth choice of control parameters in $g$.

The uniform approximation gives a very good result in this case, as can be seen in Fig. 23. On the scale of the figure, the uniform approximation and the exact calculation of the free energy are virtually indistinguishable. The mean-field value of Eq. (5.4.13) is also shown.

As above, the free energy is used to derive the level density as a function of the excitation energy. Since the free energy is well approximated by the uniform approximation, it is not surprising that the level density is closely reproduced as well.

Due to improved numerical calculations numerical derivatives of the uniformly approximated free energy were used in the inverse Laplace transform rather than derivatives of the exact free energy as was done earlier. As can be seen in Fig. 24 the level density is reproduced quite well in this approximation.
Figure 23: Free energy curves in the $SU(3)$ Lipkin model.

The curves are as in Fig. 20.
The Multilevel Lipkin Model

Figure 24: Level density in the generalized Lipkin model.

The curves are as in Fig. 20.
Conclusions

In this thesis, a unified treatment of nuclei at finite temperature and spin has been presented. The difficulties in calculating the properties of nuclei at high spin and excitation energy are well known, and are such that it is unlikely, without the sort of approximations presented here, that much sense can be made of this region. The high density of states essentially eliminates the possibility of an exact diagonalization without some a priori choice of degrees of freedom to reduce the size of the solution space. Even if such a limited diagonalization could be performed, the states are not experimentally distinguishable.

Thus we have chosen to apply thermodynamic methods to the nuclear system. Since individual states are not resolvable, it is probably more reasonable to look at ensemble averages as observables rather than the properties of any one state. This is the power of statistical methods, since they allow the calculation of such averaged expectation values in a straightforward way. In fact, these methods take advantage of the huge number of states. We use as a microscopic basis for our theory a mean field approximation to the many-body problem we wish to solve, since a theory of this type is so much more tractable. However, even in a simplified mean-field theory like the Nilsson model, calculations can be difficult, expensive, and not terribly transparent physically.

Thus we have been motivated to develop a simpler theory based on the Landau expansion of the free energy. This expansion is simple, analytically tractable, and has terms that are easily understood in terms of the physics involved. It thus forms a useful theory for understanding the phenomena that occur as nuclei rotate at high temperature. The interplay between the microscopic single particle degrees of freedom which cause much of the low energy behavior and the classical effects which
are observed at higher energies as more degrees of freedom open up, is especially well modeled. Phase transitions can be seen in this theory, and a wide variety of thermodynamic information, especially the equilibrium shape at a given $E$ and $J$ are easily derived. By using the scaling behavior characteristic of a Landau expansion, we are able to derive universal behavior for the system. It should be noted, however, that the theory does contain phenomenological parameters which cannot be determined macroscopically. These parameters enter into the scaling quantities and thus when a specific case is to be considered, information from the underlying microscopic theory must be supplied. In this way, the microscopic theory forms a statistical model for the macroscopic theory.

These calculations have been compared to experiments which have shown rapidly changing deformation in $^{166}$Er. The theory predicts a slightly higher temperature and excitation energy for the transition than was seen, but this more likely reflects the underlying microscopic Nilsson calculations rather than any fault of the theory, as the Nilsson calculations themselves show the transition at a higher temperature.

The nucleus has few enough particles that thermodynamic methods must be applied with care, as fluctuations are important and can change the expected behavior significantly. These fluctuation corrections are especially important in the region of a phase transition. The theory we have presented can in fact be used as the input to a general scheme to calculate these fluctuation effects. This scheme, called the uniform approximation, provides a simple, general method of going beyond mean-field theories in a tractable way. By modeling the mean field behavior in a simple fashion, this approximation allows integral expressions for the fluctuation calculations to be easily evaluated. Thus the mean-field calculations can be considered as the lowest order approximation to the true partition function of a system, while the uniform approximation provides the next order.
We have not yet applied the uniform approximation to the theory of Chapter 3, but have tested it on solvable model systems which undergo first and second order transitions in their mean fields. It has been found that these mean field solutions are improved by including fluctuation corrections by way of the uniform approximation.

This work has a number of directions we would like to pursue. We would like to be able to determine the moment of inertia coefficients of the Landau expansion by fitting them to the microscopic calculations, rather than taking them to be the rigid body values. The rigid body values do not allow the phase transition to an oblate shape that we have seen even at low temperatures in the microscopic calculations, and thus there should be a better choice available. We would like to evaluate the effect of fluctuations on the nuclear system by using the direct method of Sect. 4.1. Finally, with any choice of parameters, we would like to be able to apply the uniform approximation, and thus see how fluctuations can affect a real nuclear system.

The nuclear level density at high excitation and finite spin is another quantity we would like to calculate using the methods developed in this work. We expect that our work provides two significant corrections to the standard formula; we take into account the changing deformation, and we can evaluate the effect of fluctuations.

In summary, the generalized Landau-Ginzburg expansion presented here uses well known mean-field solutions to difficult problems in an attempt to understand nuclei in the neighborhood of a shape phase transition. The fluctuations that are bound to be important are the next problem we would like to attack, and the uniform approximation appears to be a very good way of dealing with them. Thus, in this thesis, we have attempted to present a unified set of tools that can help in understanding nuclei in this new region of theoretical and experimental interest.
Appendix A.

The Rigid Body Moment of Inertia

The rigid body moment of inertia to first order in the deformation is a well known result,

\[ I_{zz} = \frac{2}{5} m A R_0^2 \left( 1 - \frac{1}{2} \sqrt{\frac{5}{4\pi}} \beta \cos \gamma \right). \]  \hspace{1cm} (A.1)

In this appendix, we will present the extension to the next order in $\beta$. The classical moment is given by Eq. (2.2.5). To properly evaluate this equation to the next order, we must use the correction term of Eq. (2.2.1) as well. We first impose the volume conservation condition

\[ \frac{4\pi}{3} R_0^3 = \int dV. \]  \hspace{1cm} (A.2)

Substituting Eq. (2.2.1) and expanding the power of the radius that appears, it is seen that there are only two terms of the proper order. These terms are easily evaluated by using the orthogonality relations for spherical harmonics, and the result to second order is that

\[ a_{00} = -\frac{1}{4\pi} \sum_{\mu} |\alpha_{2\mu}|^2. \]  \hspace{1cm} (A.3)

In order to fully utilize the properties of the spherical harmonics, it is helpful to rewrite \( \sin^2 \theta = \frac{2}{3} \left( 1 - \sqrt{\frac{4\pi}{5}} Y_{20} \right) \). Then Eq. (2.2.5) becomes

\[ I_{zz} = \frac{2}{3} \int \rho r^2 dV - \frac{2}{3} \sqrt{\frac{4\pi}{5}} \int \rho r^2 Y_{20} dV. \]  \hspace{1cm} (A.4)

The density \( \rho = A/(\frac{4}{3}\pi R_0^3) \) is assumed constant and hence may be pulled out of the integrals. For the first integral in Eq. (A.4), due to the orthogonality of the harmonics, only those terms to second order which are products of conjugate terms in Eq. (2.2.1) will contribute. This term yields

\[ I = \frac{2}{3} \rho \frac{4\pi R_0^5}{5} \left( 1 + \frac{5}{4\pi} \beta^2 \right). \]  \hspace{1cm} (A.5)
The first term in this equation is seen to be the lowest order part of the usual expression, which is the moment of inertia of the corresponding sphere. Since these shapes are considered to be only slightly deformed, the largest contribution should be from this term.

The second term in Eq. (A.4) is more difficult to handle, due to the presence of the extra spherical harmonic. The integral of the product of three spherical harmonics can be found, and is given as the product of $3 - j$ symbols. Thus only certain terms contribute, and, since the extra spherical harmonic has magnetic quantum number 0, once again these are only the conjugate terms. After summing over the magnetic quantum numbers, the second term in Eq. (A.4) gives

$$I = -\frac{2\rho}{3} \sqrt{\frac{4\pi}{5}} \frac{R_0^5}{5} \left( 5\beta \cos \gamma + \frac{20}{7} \sqrt{\frac{5}{4\pi}} \beta^2 \left( 1 - 2 \sin^2 \gamma \right) \right). \quad (A.6)$$

The low order part of this result is seen to be the usual first order correction. Combining these two results then gives Eq. (2.2.6).
Appendix B.

Explicit Formulas for the Phenomenology

This appendix will give the formulas for the phenomenology of Chap. 2, although their derivation will be sketched rather than presented in detail. The conditions for an extremum of the free energy are that the partial derivatives vanish, i.e. \( \frac{\partial F}{\partial \gamma} = \frac{\partial F}{\partial \beta} = 0 \). From Eq. (3.1.7), this means

\[
0 = 4C\beta^3 - 3B\beta^2 \cos 3\gamma + 2\beta \left(A - D\omega^2 \sin^2 \gamma\right) + R\omega^2 \cos \gamma
\]

\[
0 = \beta \sin \gamma \left(12B\beta^2 \cos^2 \gamma - 2D\beta^2 \cos \gamma - \left(R\omega^2 + 3B\beta^2\right)\right)
\]

(B.1)

The second equation shows that \( \beta \sin \gamma = 0 \) is one solution, and substituting this into the first gives the result that the solutions with \( \gamma = 0 \) are independent of \( D \).

The triaxial solutions arise from the other term in the second equation, which yields a quartic in \( \beta \) when the solution for \( \cos \gamma \) that it gives is substituted in the first equation. This quartic then has the solution

\[
\beta^2 = \frac{9}{32} \frac{B^2}{C^2} \left(1 + 3D' \left(\frac{\omega}{\omega_R}\right)^2 - \frac{16}{9} A_s \pm Q\right)
\]

(B.2)

where

\[
Q = \left(1 - \frac{32}{9} A_s + 6D' \left(\frac{\omega}{\omega_R}\right)^2 + \frac{3}{4} \left(\frac{\omega}{\omega_R}\right)^2 + D'' \left(\frac{\omega}{\omega_R}\right)^4\right)^{\frac{1}{2}}.
\]

(B.3)

As stated above, \( \beta \) scales as \( B/C \), and depends only on \( A_s, D', \) and \( \omega/\omega_R \). In the rest of this appendix, \( \beta \) will be divided by its scale factor, and hence only the scaling variables will appear. By examining second derivatives, it is seen that the stable solution has a \(+\) sign, and this is the only solution that will be considered from now on, although similar analyses as will follow can also be carried out for the unstable solution. Note, however, that the unstable triaxial solution always moves smoothly to the \( \gamma = 0 \) axis. The stable solution has

\[
\cos^2 \gamma = \frac{1}{4} \left(1 + \frac{3}{8} \left(\frac{\omega}{\omega_R}\right)^2 - D' \left(\frac{\omega}{\omega_R}\right)^2 + D'' \left(\frac{\omega}{\omega_R}\right)^4 - D' \left(\frac{\omega}{\omega_R}\right)^2 Q\right)
\]

(B.4)
and thus $\gamma$ is not scaled at all, but depends only on the scaling variables. To see how $F$ scales, use the information from the above equations to get

$$
F = F_0 + A B^2 C^2 \beta^2 - B B^3 C^3 \beta^3 \cos 3\gamma + C B^4 C^4 + R B C \omega^2 \beta \cos \gamma - D B^2 C^2 \omega^2 \beta^2 \sin^2 \gamma \tag{B.5}
$$

and then divide by $B^4/C^3$ to get

$$
F_s = F_{0s} + A_s \beta^2 - \beta^3 \cos 3\gamma + \beta^4 + \frac{81}{256} \left( \frac{\omega}{\omega_R} \right)^2 \beta \cos \gamma - \frac{9}{4} D' \left( \frac{\omega}{\omega_R} \right)^2. \tag{B.6}
$$

Here the subscript $s$ denotes a scaled value, and clearly Eq. (B.6) depends only on the scaling variables. Note that for $D = 0$, Eq. (B.4) yields

$$
\cos^2 \gamma = \frac{1}{4} \left( 1 + \frac{27}{256} \left( \frac{\omega}{\omega_R} \right)^2 \right), \tag{B.7}
$$

and hence $\gamma \neq -\frac{2\pi}{3}$ for finite $\omega$. From these formulas, the definition of the stability lines $A_{s(2)}^0$ and $A_{s(1)}^0$ may now be given. $A_{s(2)}^0$ is the point at which the two triaxial points collide, and hence is the point at which the discriminant $Q$ vanishes. $A_{s(1)}^0$ is where the oblate solution becomes stable, and thus is the point at which $\cos \gamma = -1$.

Since there are explicit forms for the quantities $\beta$ and $\gamma$, they can be inverted and their constant lines in the $A_s - \omega$ plane may derived as well. The lines of constant $\cos \gamma$ are then:

$$
A_s = \frac{9}{16x^2} \left( 3x^2 D' \left( \frac{\omega}{\omega_R} \right)^2 - x(D' \left( \frac{\omega}{\omega_R} \right)^2 + D' \left( \frac{\omega}{\omega_R} \right)^2 + \frac{3}{8} \left( \frac{\omega}{\omega_R} \right)^2 - D'' \left( \frac{\omega}{\omega_R} \right)^2 \right) + (D' \left( \frac{\omega}{\omega_R} \right)^2 + x)(D'' \left( \frac{\omega}{\omega_R} \right)^2 (x + 1)^2 + \left( \frac{\omega}{\omega_R} \right)^2 x(x + 1)) \frac{3}{2} \tag{B.8}
$$

where $x = 4 \cos^2 \gamma - 1$. A few of the lines of constant $\cos \gamma$ are especially notable. For $\omega/\omega_R > 1$, $A_{s(1)}^0$ is the line for $\gamma = -\pi$. When $D \neq 0$, this curve has positive quadratic asymptotic behavior. Since these constant lines cannot cross, the lines for other values must more or less follow the same shape. All of the lines for
The lines of constant $\beta$ in the oblate region are obtained by solving $\partial F/\partial \beta = 0$ for $A_s$. In the prolate region, Eq. (B.2) must be inverted and yields

$$A_s = \frac{1}{2} \left( \left( \frac{27}{8} D' \left( \frac{\omega}{\omega_R} \right)^2 - 4\beta^2 \right) + \left( \frac{81}{64} D'^2 \left( \frac{\omega}{\omega_R} \right)^4 + 9\beta^2 + \frac{243}{256} \left( \frac{\omega}{\omega_R} \right)^2 \right)^{\frac{1}{2}} \right).$$  \tag{B.10}$$

Note that $\beta$ decreases with increasing $A_s$, but increases with increasing $\left( \frac{\omega}{\omega_R} \right)$. In the $J/\omega - \omega/\omega_R$ plane, $A_s^{(2)}$ and $A_s^{(1)}$ border the unstable region. The spin $J$ is given by

$$J'/\omega = -2R\beta \cos \gamma + 2D\beta^2 \sin^2 \gamma$$  \tag{B.11}$$

and a procedure similar to the one followed above shows that the natural scaling for $J'$ is $\frac{B_4}{C_3} \omega_R^2$. The transition lines are now transformed, yielding

$$J^{(1)}/\omega = \frac{81}{256} \left( \frac{3}{8} (1 - D' \left( \frac{\omega}{\omega_R} \right)^2 ) + \frac{81}{512} D'(3 - 3 \left( \frac{\omega}{\omega_R} \right)^2 + 2D' \left( \frac{\omega}{\omega_R} \right)^2 - 5D'^2 \left( \frac{\omega}{\omega_R} \right)^4 ) \right)$$

and

$$J^{(2)}/\omega = \frac{81}{256} \left( -\frac{1}{2} \left( D' \left( \frac{\omega}{\omega_R} \right)^2 - D'^2 \left( \frac{\omega}{\omega_R} \right)^4 + \frac{9}{16} \left( \frac{\omega}{\omega_R} \right)^2 \right) \right).$$
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