

LOW EXCITATION CORRECTIONS TO THE
DENSITY OF STATES

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OF STATES

By

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Abstract

We study a many particle system contained within a harmonic oscillator potential, with the single particle spacings equispaced and nondegenerate. We consider either fermions or bosons within this harmonic oscillator potential and derive the density of states for this system, with low excitation energy corrections. We extend our method for more than one species of fermions or bosons within this harmonic oscillator potential and compare our results with number-theoretic techniques. We move on to the degenerate harmonic oscillator potential and show that, for a fermion system, shell effects are contained within low excitation energy terms. We attempt to arrive at the density of states for an infinite number of bosons within the same potential.

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Chapter 1

Introduction

The aim of this thesis is to derive an asymptotic formula for the density of states of many boson and many fermion systems incorporating low excitation energy corrections. We focus on particles confined in a harmonic oscillator system, due to the relative simplicity in calculating the exact number of states. For particles within an equispaced, nondegenerate single-particle energy spectrum, the number of excited configurations for a given excitation energy becomes uncountable by hand and computationally difficult. Asymptotic formulas, obtained by Bethe [1], for the one species density of states,

$$\rho^{(1)}(E) = \frac{e^{\sqrt{\frac{2}{3}}\pi^2 g(\epsilon_F) E}}{\sqrt{48E}}, \quad (1.1)$$

and for the two species density of states,

$$\rho^{(2)}(E) = 6^{\frac{1}{4}} g_o \left(\frac{g_o^2}{4g_n(\epsilon_F^{(n)})g_p(\epsilon_F^{(p)})} \right)^{\frac{1}{2}} (g_o E)^{-\frac{5}{4}} e^{2\pi\sqrt{\frac{g_o E}{6}}}, \quad (1.2)$$

provide a reasonable approximation to the exact number of microstates for large excitations while the error is considerable for low excitations. In Eq. 1.1 and Eq. 1.2,

the excitation energy is denoted by E , the fermi energy for the i^{th} species of particles denoted by $\epsilon_F^{(i)}$, the individual single-particle level densities at the respective fermi energies given by $g_{(i)}$, and the sum of the individual levels densities given by g_o .

With the 1-D harmonic oscillator spectrum containing one species of spinless particles, the number of excited configurations is equal to the number of partitions of an integer. Hardy and Ramanujan obtained an asymptotic equation[2] for the number of partitions for large integers and work later done by Rademacher[3] to obtain an exact series expression for the number of partitions. However, it should be stated that Leboeuf was able to derive low excitation corrections to the density of states using number-theoretic results[4, 5]. By generalizing "the circle method" [6], Leboeuf arrived at a series expressions for the density of states for two sets of noninteracting particles in a 1-D harmonic oscillator spectrum.

The relevance of this work can also be found in evaporation spectra of the nucleus. In inelastic neutron scattering experiments of atoms with high, negative Q values[7], such that neutron producing reactions are impossible, Co and Ag were found to obey Bethe's formula relatively well with g_o as a fitting parameter for each nucleus. Work done by Ignatyuk et al.[8] matched g_o to several atomic numbers. Fluctuations were observed for g_o corresponding to the locations of magic numbers.

The number of configurations of heavy nuclei grows large and only a statistical framework can be used to reasonably model the nuclear properties[9]. Knowing the statistical partition function and the single-particle energy levels, Ericson[10] demonstrated the validity of a saddle-point technique in obtaining the correct density of states. Angular momentum and odd-even effects were included to the density of states calculation, but we ignore these effects in this thesis. In Chapter 2, we derive the Leboeuf's low excitation terms by using the saddle-point technique and by re-

taining the non-Gaussian terms to the entropy. Chapter 3 will repeat the calculation for bosons in a three-dimensional harmonic oscillator and a discussion of a fermion system in the same system. The author believes that a number-theoretic derivation for the density of states for fermions or bosons within a degenerate single-particle level system is not possible and only a statistical derivation for the density of states series expression is possible.

Chapter 2

Numbers and one dimensional systems

This chapter will review the basic concepts of partitioning an integer into its parts and the number of different partitions of that integer. The direct connection between the number of partitions of an integer to the number of excited states for fermions or bosons in a nondegenerate equispaced harmonic trap will be illustrated. We will use a canonical and Grand Canonical partition function to arrive at the density of states for either one species of particles in a harmonic trap or two species of particles in a harmonic trap.

2.1 Partitioning an integer

For an integer n , there exist a finite number of ways to add up to that integer. Each way is known as a partition. We give the different partitions for some low integer examples in Table 2.1. The number of different partitions, denoted by $p(n)$,

Table 2.1: **Partitions of an integer**

Integer	Partitions	Number of Partitions $p(n)$
1	1	1
2	1 + 1	2
	2	
5	1 + 1 + 1 + 1 + 1	7
	1 + 2 + 2	
	1 + 1 + 1 + 2	
	1 + 1 + 3	
	1 + 4	
	2 + 3	
	5	

grows exponentially large for large integers. For $n = 5$, the number of different partitions for 5 is 7, $p(5) = 7$. For $n = 200$, the number of different partitions for 200 is 3972999029388 and a list of the different partitions is space consuming.

Hardy and Ramanujan [2] derived a mathematical formula for the number of partitions,

$$p^{(asymptotic)}(n) \approx \frac{e^{\sqrt{\frac{2\pi^2 n}{3}}}}{\sqrt{48n}}, \quad (2.1)$$

for large integers n . Inserting 200 for n into Eq. (2.1), the result is $p^{(asymptotic)}(200) = 4.1 \times 10^{12}$ which is similar in order to the exact answer. Further work done by Rademacher [3] yielded an exact series expression for the number of partitions of an integer.

2.2 The equispaced nondegenerate harmonic oscillator spectrum

Connecting the theory of partitions to physical systems, we consider an equispaced and nondegenerate harmonic oscillator spectrum. For either noninteracting, spinless bosons or noninteracting, spinless fermions within this harmonic oscillator spectrum, the number of excited energy levels is equal to the number of partitions of an integer, provided that the number of particles within the harmonic oscillator spectrum is greater than the number of parts for a particular partition of an integer. As an example, for the integer 5, one possible partition is $1 + 1 + 1 + 1 + 1$ and cannot be realized for a system of 3 particles.

As shown in Figure 2.2, for given excitation energy in units of the single particle spacing of the system, $\hbar\omega$, the energy can distribute itself evenly among particles, primarily on one particle, or some mixture in between. There are two states possible for an excitation energy of two units of $\hbar\omega$. For the fermion system, Pauli exclusion principle prevents two identical fermions from occupying the same energy state and particle indistinguishability reduces the number of configurations for the excitation energy. But the total number of microstates remains the same for both systems.

Connecting Eq. (2.1) to the harmonic oscillator system, we are left with an asymptotic expression for the density of states of the system,

$$\rho\left(\frac{E}{\hbar\omega}\right) \approx \frac{e^{2\sqrt{g_0 E}}}{\sqrt{48 \frac{E}{\hbar\omega}}}, \quad (2.2)$$

with g_0 the collection of constants in the exponential. The above formula states that systems within an equispaced, harmonic oscillator system should grow exponentially with the square root of the excitation energy. In studies of the nuclear evaporation

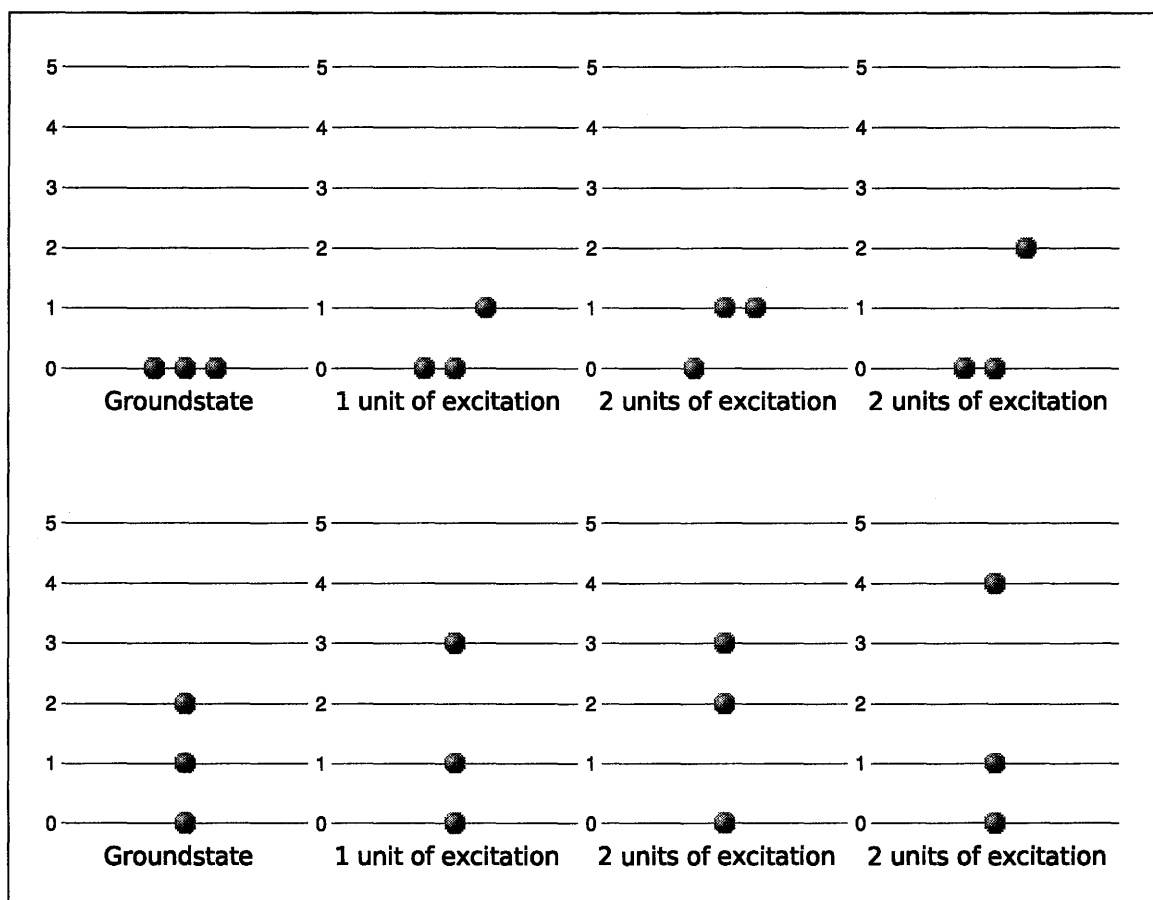


Figure 2.1: Excited particle states with a boson system on the top row and a fermion system on the bottom row. From left to right for each system i) The ground state of the system ii) A state with one particle excited iii) A state with two particles excited by one unit of energy iv) A state with one particle excited by two units of energy.

spectra to obtain the nuclear level densities of specific isotopes [7, 8], the nucleons can be modelled by a mean-field interaction and exponential growth in the level densities is observed.

A fit of Eq. (2.2) to the experimental data, with g_0 as an adjustable parameter, provides good agreement to the observed level densities, as shown in Figure 2.2. We can see deviations from this curve for low excitations. Because the formula for the density of states, given by Eq. (2.2) is an asymptotic result for high excitation energies, it should not be expected to hold for low excitations. To understand the nuclear level densities at low excitation energies and deviations away from the mean-field model of the nucleus, it is necessary to first provide the mean-field density of states in the low excitation energy regime.

Leboeuf uses the number-theoretic work of Rademacher [3] to provide a few low excitation energy corrections to the one species density of states [4, 5],

$$\begin{aligned} \ln(\hbar\omega\rho^{(1)}(E)) &= \sqrt{\frac{2\pi^2\frac{E}{\hbar\omega}}{3}} - \ln\left(\sqrt{48}\frac{E}{\hbar\omega}\right) \\ &\quad - \frac{\pi^2 + 72}{24\sqrt{6}\pi}\left(\frac{E}{\hbar\omega}\right)^{-\frac{1}{2}} - \left(\frac{3}{4\pi^2} - \frac{1}{24}\right)\left(\frac{E}{\hbar\omega}\right)^{-1} + O\left(\left(\frac{E}{\hbar\omega}\right)^{-\frac{3}{2}}\right), \end{aligned} \quad (2.3)$$

and the two species density of states [6],

$$\begin{aligned} \ln(\hbar\omega\rho^{(2)}(E)) &= 2\sqrt{\frac{\pi^2\frac{E}{\hbar\omega}}{3}} - \ln\left(\frac{12\left(\frac{E}{\hbar\omega}\right)^{\frac{5}{4}}}{3^{\frac{1}{4}}}\right) \\ &\quad - \left(\frac{\pi}{36} + \frac{15}{16\pi}\right)\sqrt{3}\left(\frac{E}{\hbar\omega}\right)^{-\frac{1}{2}} + \frac{\frac{35}{192} + \frac{\pi^2}{864}}{\frac{E}{\hbar\omega}} + O\left(\left(\frac{E}{\hbar\omega}\right)^{-\frac{3}{2}}\right). \end{aligned} \quad (2.4)$$

The goal of this chapter is to reproduce the low excitation energy corrections by a standard statistical technique rather than a number-theoretic technique. The

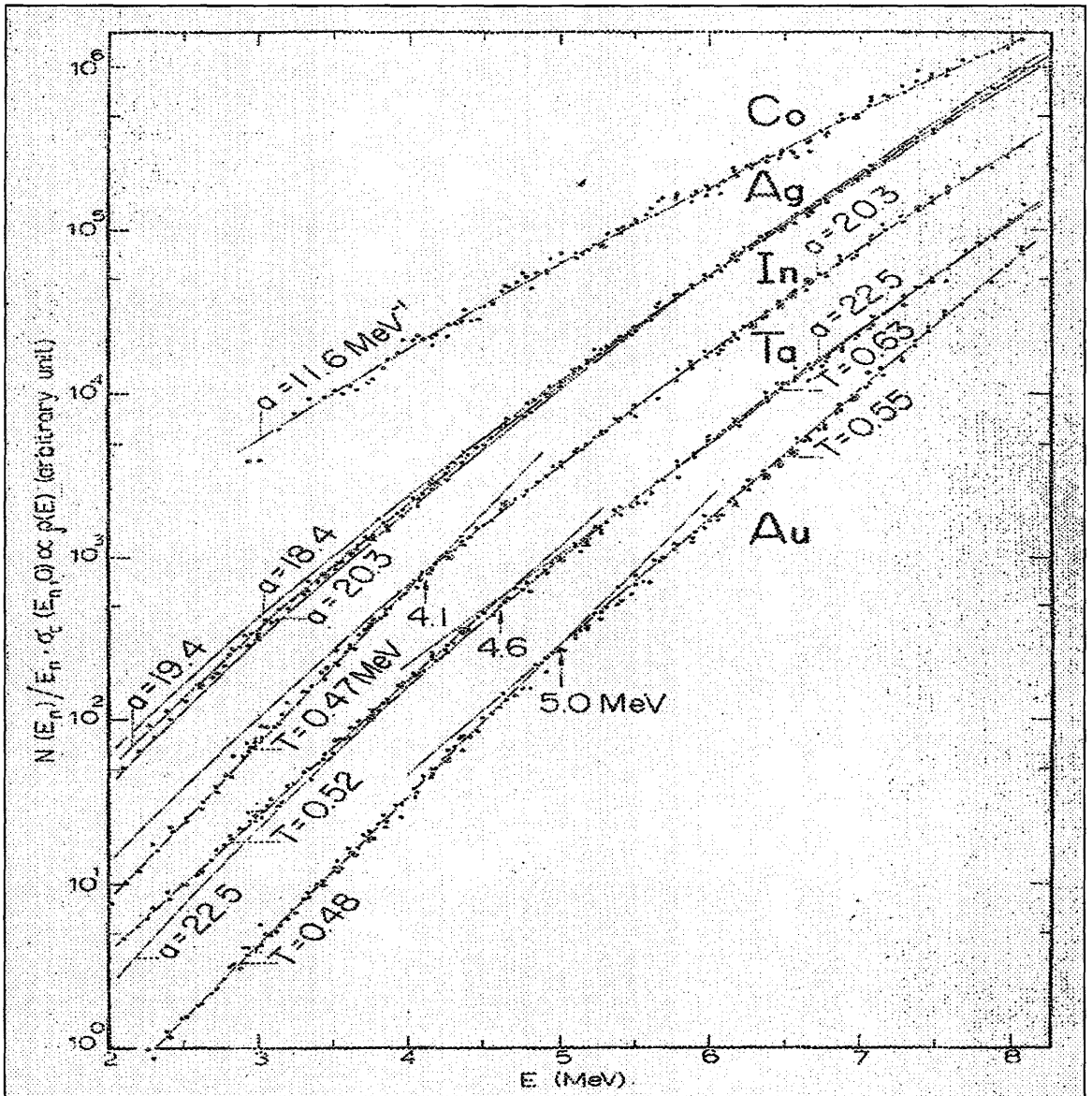


Figure 2.2: The experimental level densities of Co, Ag, In, Ta, Au. Note that $a = g_0$. The symbol T corresponds to the fitted temperature for the constant temperature model in which the level densities vary as $e^{\frac{E}{k_b T}}$. Data provided by K. Tsukada et al. [7]

process is quicker and we believe a statistical derivation of low excitation energy corrections can be applied to other systems, such as systems with energy degeneracy, whereas it would not be possible to obtain low excitation energy corrections by a number-theoretic technique.

2.3 Method

2.3.1 Alternate derivation to arrive at low excitation energy corrections for one species of particles

In order to arrive at the density of states, we start with some basic concepts. The exact quantum density of states,

$$\rho(\xi) = \sum_n \delta(\xi - \xi_n), \quad (2.5)$$

is given by a sum of Dirac delta functions over all possible energy configurations, ξ_n , of that system. By taking a Laplace transform of the quantum density of states, we obtain a partition function,

$$Z(\beta) = \int_0^\infty d\xi \rho(\xi) e^{\beta\xi} = \sum_n e^{-\beta\xi_n}. \quad (2.6)$$

The Laplace transform variable, β , can be identified as the conjugate to the energy and is the inverse temperature in units of the inverse Boltzmann constant. By an inverse Laplace transform of the partition function, we get back an expression for the density of states,

$$\rho(\xi) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} d\beta Z(\beta) e^{\beta\xi}. \quad (2.7)$$

We start with a canonical partition function,

$$Z(\beta) = \prod_{n=0}^{\infty} \frac{1}{1 - e^{-\beta\epsilon_n}}, \quad (2.8)$$

and valid as the number of particles goes to infinity, to arrive at the corrected density of states for one species of spinless particles in a nondegenerate harmonic trap. In a 1-D equispaced harmonic trap, the number of excited configurations for a many boson system and a many fermion system are equal. The single particle energy levels, $\epsilon_n = \hbar\omega n$, are indexed by the integer n . We set $\hbar\omega = 1$ for convenience. The total energy of the bosonic system, ξ , is equal to the excitation energy of the system, E , since the ground state energy has been set to zero.

The partition function is rewritten as $Z(\beta) = e^{\ln Z(\beta)}$ and $\ln Z(\beta)$ evaluated by an Euler-Maclaurin expansion. We collect all terms that appear in the exponent in Eq. (2.7) and define it as the entropy[11],

$$S(\beta) = \beta E + \ln Z(\beta) = \beta\left(E - \frac{1}{24}\right) + \frac{\pi^2}{6\beta} + \frac{1}{2} \ln \beta - \frac{1}{2} \ln(2\pi) + O(\beta^2). \quad (2.9)$$

It should be noted that retaining the shell correction $-\frac{\beta}{24}$ is essential in obtaining Leboeuf's density of states [4, 5]. Neglecting higher order β^2 terms in Eq. (2.9), we use a saddle-point condition to arrive at the density of states with the saddle-point condition defined by the familiar equation ,

$$\left. \frac{\partial S}{\partial \beta} \right|_{\beta_0} = E + \frac{\partial}{\partial \beta} \ln Z(\beta_0) = 0. \quad (2.10)$$

The previous equation has multiple roots in β , but we choose β_0 to be the positive, real root such that

$$\beta_0 = \frac{1}{12} \frac{-3 + \sqrt{9 + 24(E - \frac{1}{12})\pi^2}}{E - \frac{1}{12}}. \quad (2.11)$$

We expand $S(\beta)$ about β_0 using a Taylor series and expand the third and higher order β terms such that

$$\begin{aligned} e^{S(\beta)} &= e^{S^{(0)} + S^{(2)} \frac{(\beta - \beta_0)^2}{2!} + \sum_{j=3}^{\infty} S^{(j)} \frac{(\beta - \beta_0)^j}{j!}} \\ &= e^{S^{(0)}} e^{S^{(2)} \frac{(\beta - \beta_0)^2}{2!}} \left(1 + \sum_{k=1}^{\infty} \frac{(\sum_{j=3}^{\infty} S^{(j)} \frac{(\beta - \beta_0)^j}{j!})^k}{k!} \right), \end{aligned} \quad (2.12)$$

where $S^{(k)} = \frac{\partial^k S(\beta_0)}{\partial \beta^k} |_{\beta_0}$. Using the expansion in Eq. (2.12), we evaluate the density of states,

$$\rho(E) = \frac{e^{S^{(0)}}}{\sqrt{2\pi S^{(2)}}} \left(1 + \frac{S^{(4)}}{8(S^{(2)})^2} - \frac{S^{(6)} + 10S^{(3)}}{48(S^{(2)})^3} + O\left(\frac{1}{(S^{(2)})^4}\right) \right), \quad (2.13)$$

with the non-Gaussian part retained.

The first term for the density of states was obtained, for example, by Tran[11]. The first few saddle-point correction terms can be found in Hoare[12] and in Appendix A. We retain terms up to 12th order in the derivative of $S(\beta)$ with the reasoning stated in Appendix A.

The logarithm of the density of states is taken and then expanded about a large excitation, E , to reproduce Bethe's asymptotic terms in Eq. (1.1) along with Leboeuf's low excitation energy corrections[4, 5]. Ayoub's compressed formula[13] for the density of states is given as well with $\tilde{E} = E - \frac{1}{24}$.

The density of states,

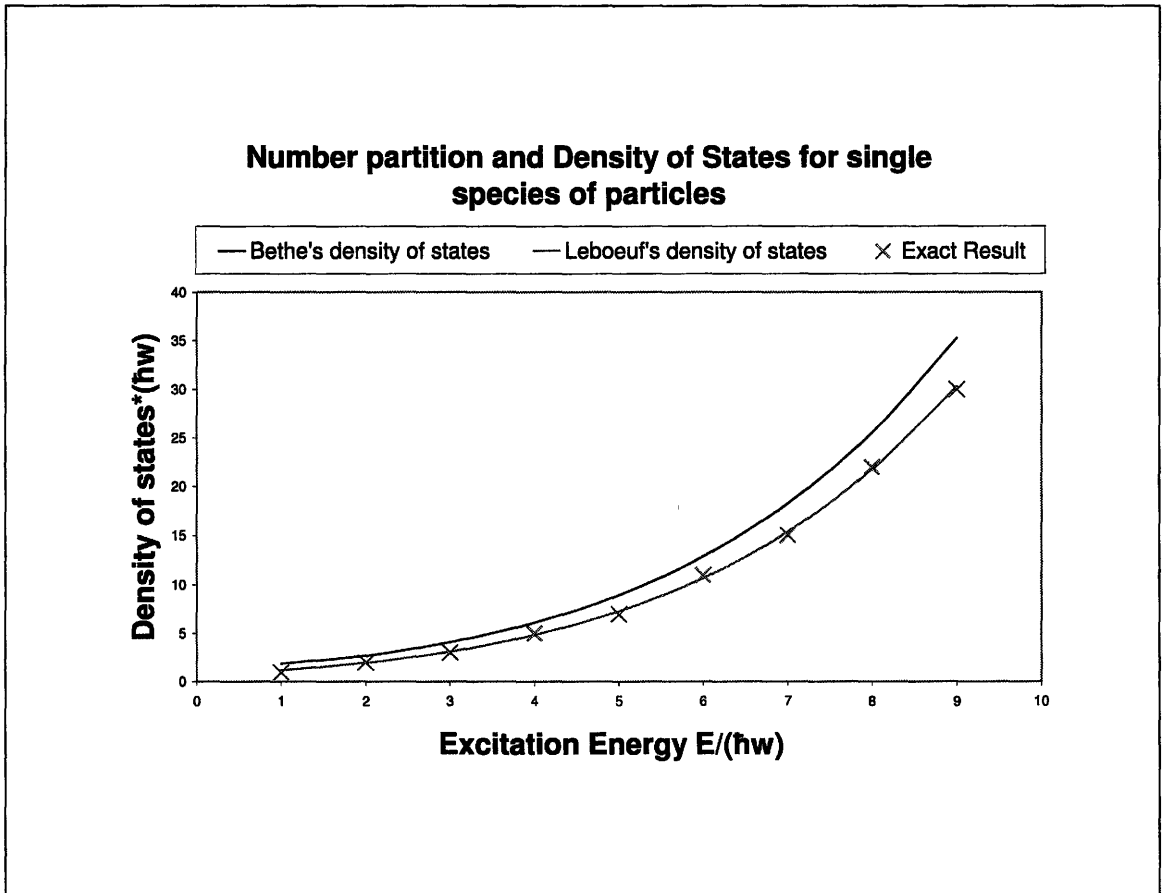


Figure 2.3: The density of states for one species of particles in a harmonic well. The top curve is Bethe's approximation and the lower curve is with Leboeuf's excitation energy corrections. Crosses represent the exact number of states $p(E)$.

$$\begin{aligned}
 \ln \rho^{(1)}(E) &= \sqrt{\frac{2\pi^2 E}{3}} - \ln(\sqrt{48E}) - \frac{\pi^2 + 72}{24\sqrt{6}\pi} E^{-\frac{1}{2}} - \left(\frac{3}{4\pi^2} - \frac{1}{24}\right) E^{-1} + O(E^{-\frac{3}{2}}) \\
 &= \frac{e^{\pi\sqrt{\frac{2E}{3}}}}{\sqrt{48E}} \left(1 - \frac{1}{\pi\sqrt{\frac{2E}{3}}}\right), \tag{2.14}
 \end{aligned}$$

is plotted against Bethe's asymptotic density of states and the exact number of states as shown in Figure 2.3.

2.3.2 Derivation for two species of particles

For two species of particles, such as a neutron and proton system, within the equispaced, nondegenerate spectra, the excitation energy can distribute itself over 1 set of particles or over both sets. This creates more possible excited configurations as shown in Figure 2.4. The exact number of states for n units of $\hbar\omega$ is

$$p^{(2)}(n) = \sum_{i=0}^n p(i)p(n-i). \tag{2.15}$$

Because we are dealing with two species of particles, the canonical partition we used in the previous section is not convenient and we need a Grand Canonical partition function. The quantum density of states,

$$\rho(\xi, N, P) = \sum_{i,n,p} \delta(N-n)\delta(P-p)\delta(\xi - \xi_i(n, p)), \tag{2.16}$$

is summed over all possible energy configurations, $\xi_i(n, p)$. We label one species as neutrons and label the number of neutrons by N and the other species as protons and label the number of protons by P . A triple Laplace transform of the density of states yields a Grand Canonical partition function,

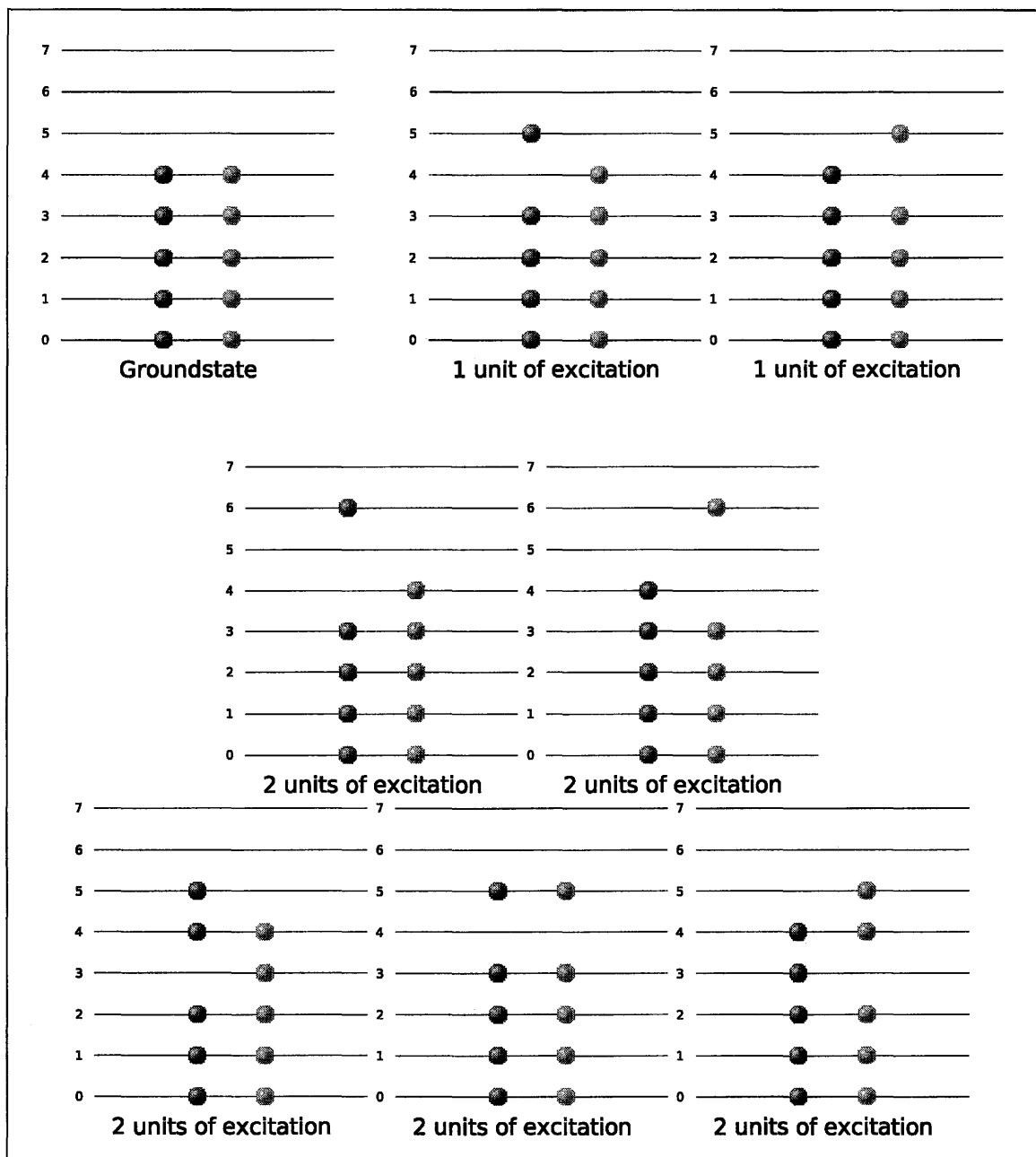


Figure 2.4: Two species of noninteracting particles in a harmonic oscillator well. (Top-right) The ground state of the system. (Top-left) Two states are possible for one unit of excitation. (Bottom) Five states are possible for two units of excitation.

$$\begin{aligned}
 Z_G^F(\beta, \alpha_N, \alpha_P) &= \int_0^\infty \int_0^{0\infty} \int_0^\infty d\xi dN dP \rho(\xi, N, P) e^{\alpha_P P + \alpha_N N - \beta \xi} \\
 &= \sum_{i,n,p} e^{\alpha_P p + \alpha_N n - \beta \xi_i(n,p)}. \tag{2.17}
 \end{aligned}$$

The variables conjugate to particle numbers P and N, α_P and α_N respectively, are defined as $\alpha_P = \beta \mu_P$ and μ_P the proton chemical potential, and $\alpha_N = \beta \mu_N$ and μ_N the neutron chemical potential. Inverse Laplace transforming the partition function gives us our density of states for the system,

$$\rho(P, N, E) = \frac{1}{(2\pi i)^3} \int_{-i\infty}^{i\infty} \int_{-i\infty}^{i\infty} \int_{-i\infty}^{i\infty} d\beta d\alpha_P d\alpha_N Z_G^F(\alpha_P, \alpha_N, \beta) e^{\beta \xi - \alpha_P P - \alpha_N N}. \tag{2.18}$$

We use a product definition of the Grand Canonical partition function,

$$Z_G^F(\alpha_P, \alpha_N, \beta) = \prod_{n=0}^{\infty} ((1 + e^{\alpha_P - \beta \epsilon_n})(1 + e^{\alpha_N - \beta \epsilon_n}))^{g(n)}, \tag{2.19}$$

for fermions[14]. The single particle energy levels are denoted by ϵ_n . The energy degeneracy is denoted by $g(n)$ and $g(n) = 1$ for a nondegenerate spectrum.

The total energy of the system is ξ with $\xi = \xi_0 + E$ and ξ_0 the ground state of the system associated with a fermi system. To correspond to the number of partitions with two sets of integers, the protons and neutrons are assumed to be spinless and noninteracting.

As previously, $\ln Z_G^F(\alpha_P, \alpha_N, \beta)$ is evaluated by an Euler-Maclaurin expansion which yields an expression,

$$S(\alpha_P, \alpha_N, \beta) = \beta \left(\xi + \frac{1}{6} \right) - \alpha_P P - \alpha_N N + \frac{\frac{\alpha_P^2}{2} + \frac{\alpha_N^2}{2} + \frac{\pi^2}{3}}{\beta}, \tag{2.20}$$

after neglecting cubic and higher order β terms and assuming the chemical potentials are large. Similar to an expression in Rosenzweig [15] but for two species of particles.

We evaluate the chemical potential integrals by setting the exact ground state to $\xi_0^{(i)} = i(i-1)/2$ for the i th species and then by completing the square on the variables α_i . We are left with a similar two species entropy condition,

$$S_2(\beta) = \beta\left(E - \frac{1}{12}\right) + \frac{\pi^2}{3\beta} + \ln \beta - \ln(2\pi), \quad (2.21)$$

as in Eq. (2.7) with the particle number information eliminated.

Proceeding in much the same way as in the previous subsection, we obtain a two species density of states,

$$\begin{aligned} \ln(\rho_2(E)) = & 2\sqrt{\frac{\pi^2 E}{3}} - \ln\left(\frac{12E^{\frac{5}{4}}}{3^{\frac{1}{4}}}\right) - \left(\frac{\pi}{36} + \frac{15}{16\pi}\right)\sqrt{3}E^{-\frac{1}{2}} \\ & + \frac{\frac{5}{48} - \frac{45}{64\pi^2}}{E} + O(E^{-\frac{3}{2}}). \end{aligned} \quad (2.22)$$

The first two terms are Bethe's asymptotic terms found in Eq. (1.2) and the $E^{-\frac{1}{2}}$ term matches Leboeuf's term. But the E^{-1} correction coefficient does not match Leboeuf's E^{-1} correction coefficient [6], $\frac{35}{192} + \frac{\pi^2}{864}$. However, a plot of Figure 2.5 shows the Gaussian integrated technique to achieve a slightly better fit than Leboeuf's number-theoretic technique to the actual density of states.

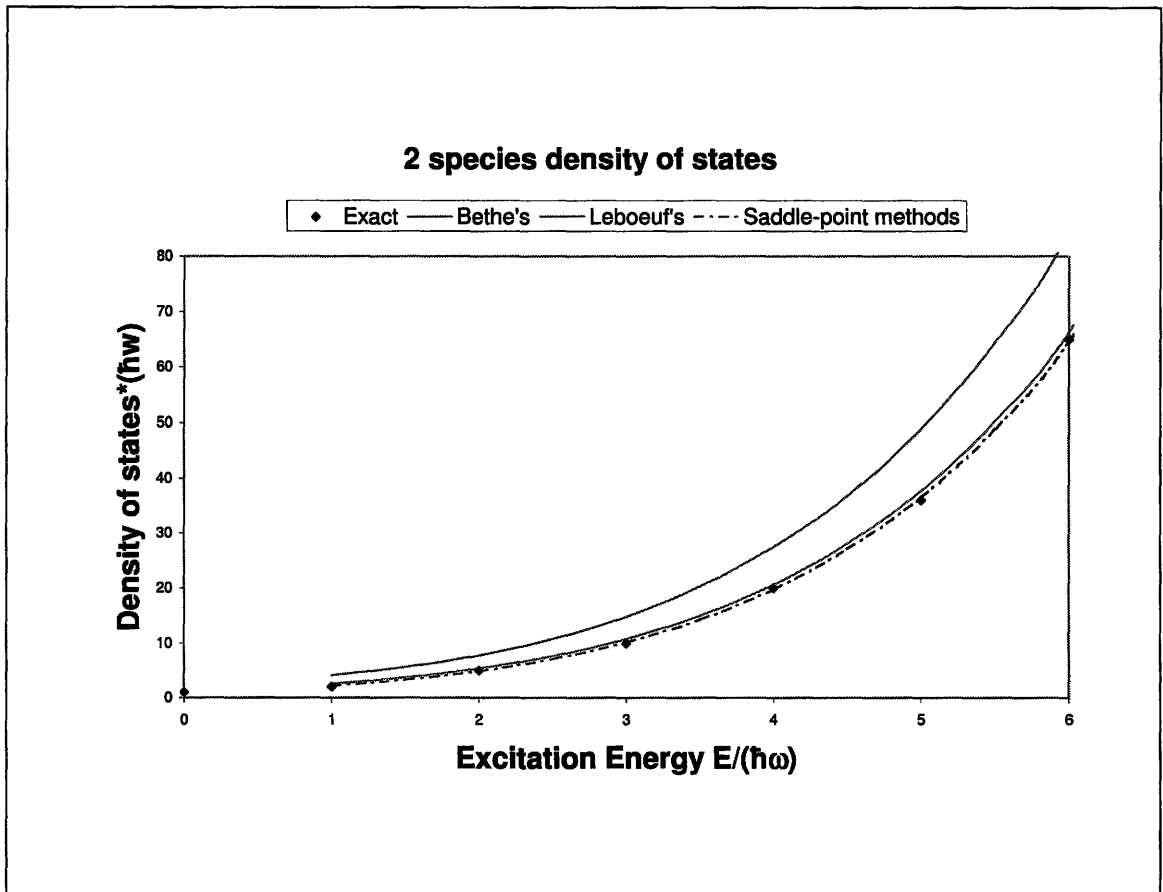


Figure 2.5: The density of states for two species of particles in a trapped harmonic well. The top curve is Bethe's approximation. Leboeuf's number-theoretic corrections are higher than the evaluation of the density of states by a saddle-point technique, which is represented by the dashed line. Diamonds represent the exact number of states for two sets of particles.

Chapter 3

Particles confined in degenerate spectrums

We now study systems of particles confined to a degenerate equispaced spectrum, the 3-D harmonic oscillator. In the previous chapter, it could be shown that the number of macrostates for bosons or fermions within an equispaced, nondegenerate spectrum was directly related to the number of partitions of an integer. This is not the case for bosons or fermions confined to in a degenerate spectrum. In 1-D, the number of macrostates was one for the system at the groundstate. The number of macrostates for a fermion system at the ground state energy can be shown to be $n(0) = {}_g C_p$ with g the energy degeneracy of the last filled shell and p the number of particles occupying the last filled shell. Four such states are shown in Figure 3

There is no quick method to calculate the number of excited states for a system of fermion particles within the degenerate, harmonic oscillator spectrum. Each excited microstate must be saved and compared with other possible microstates of the system to eliminate possible duplicate microstates being computed. We can arrive at a series

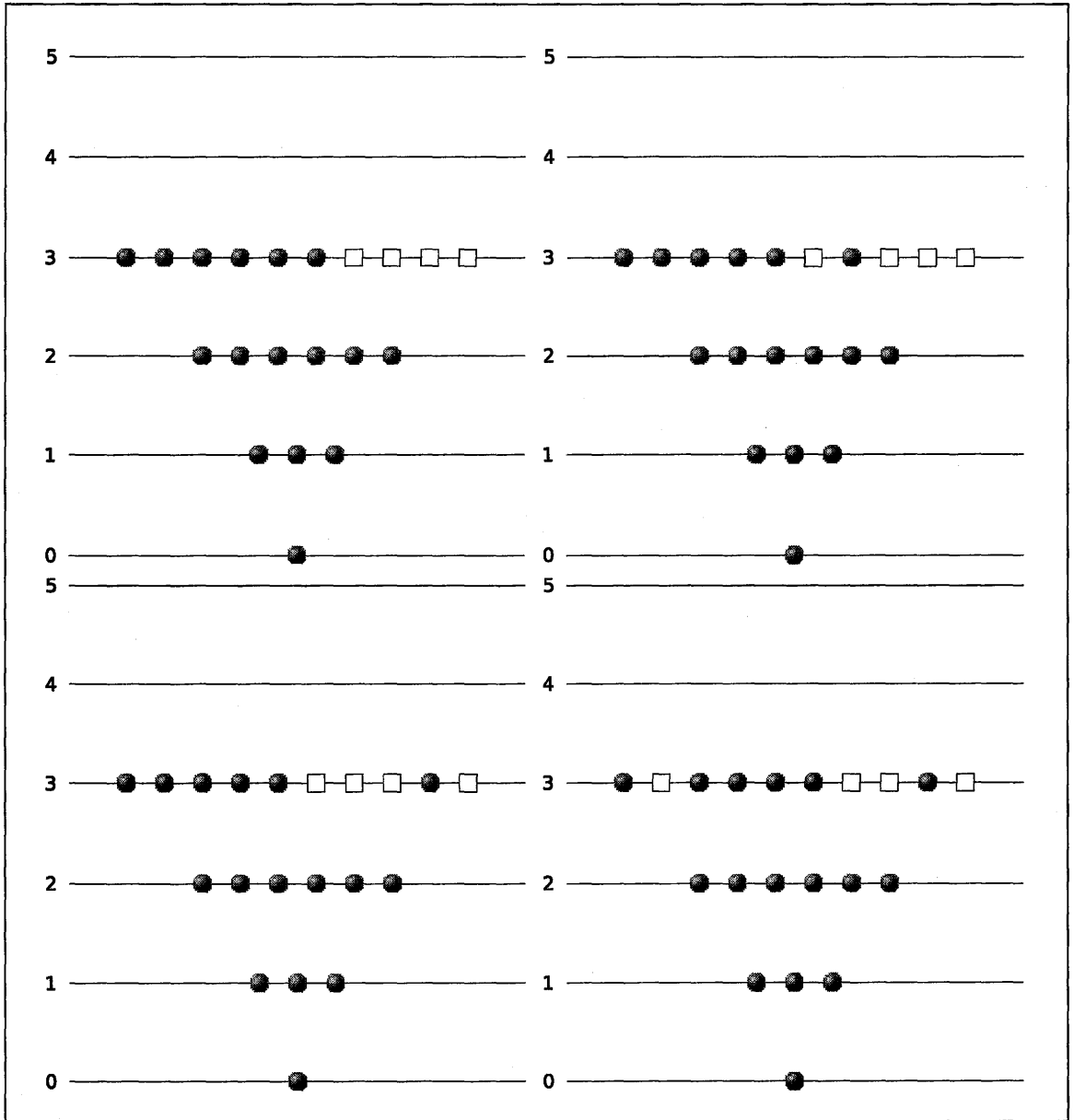


Figure 3.1: Four out of 210 possible microstate configurations are shown for a fermion system at the ground state energy.

expression for the density of states of the system and show that the density of states fluctuates at the magic numbers of the system, $P_i = \sum_{n=0}^i g(n)$, with the degeneracy of each level for the 3-D harmonic oscillator given by $g(n) = \frac{(n+1)(n+2)}{2}$.

The generation of the exact number of microstates for a system of boson particles is much easier. The number of excited microstates of this system is related to the number of repeating parts in a partition of integers and the degeneracy of the level for the integer value of the repeating part. The integer 3 can be expressed as $3 = 1+1+1$. Three particles are excited to the first excited state with the degeneracy of the level, $g(1) = 3$. There are ten possible microstate configurations and can be counted by obtaining the partitions of the number of particles in the level with the number of parts less than or equal to the degeneracy of the level. Table 3.1 gives the exact number of microstates for an excitation energy in integer units of the spacing of the levels, $\hbar\omega$.

The evidence for shell effects can be found in nuclear level densities for various elemental isotopes [8]. At the nuclear magic numbers, $\{2, 8, 20, 28, 50, 82, 126\}$, the fitting parameter g_o from Eq. (2.2) drops from the mean value. The major shell effect can be reproduced theoretically by insertion of orbital periods and other numerical constants. However, this chapter will show that it is possible to reproduce the major shell effects by the statistical approach with the oscillations contained in the low excitation energy corrections.

Table 3.1: Number of microstates for boson particles in a 3-D harmonic spectrum.

Integer	Number of Microstates
0	1
1	3
2	12
3	38
4	117
5	330
6	906
7	2367
8	6027
9	14873
10	35892

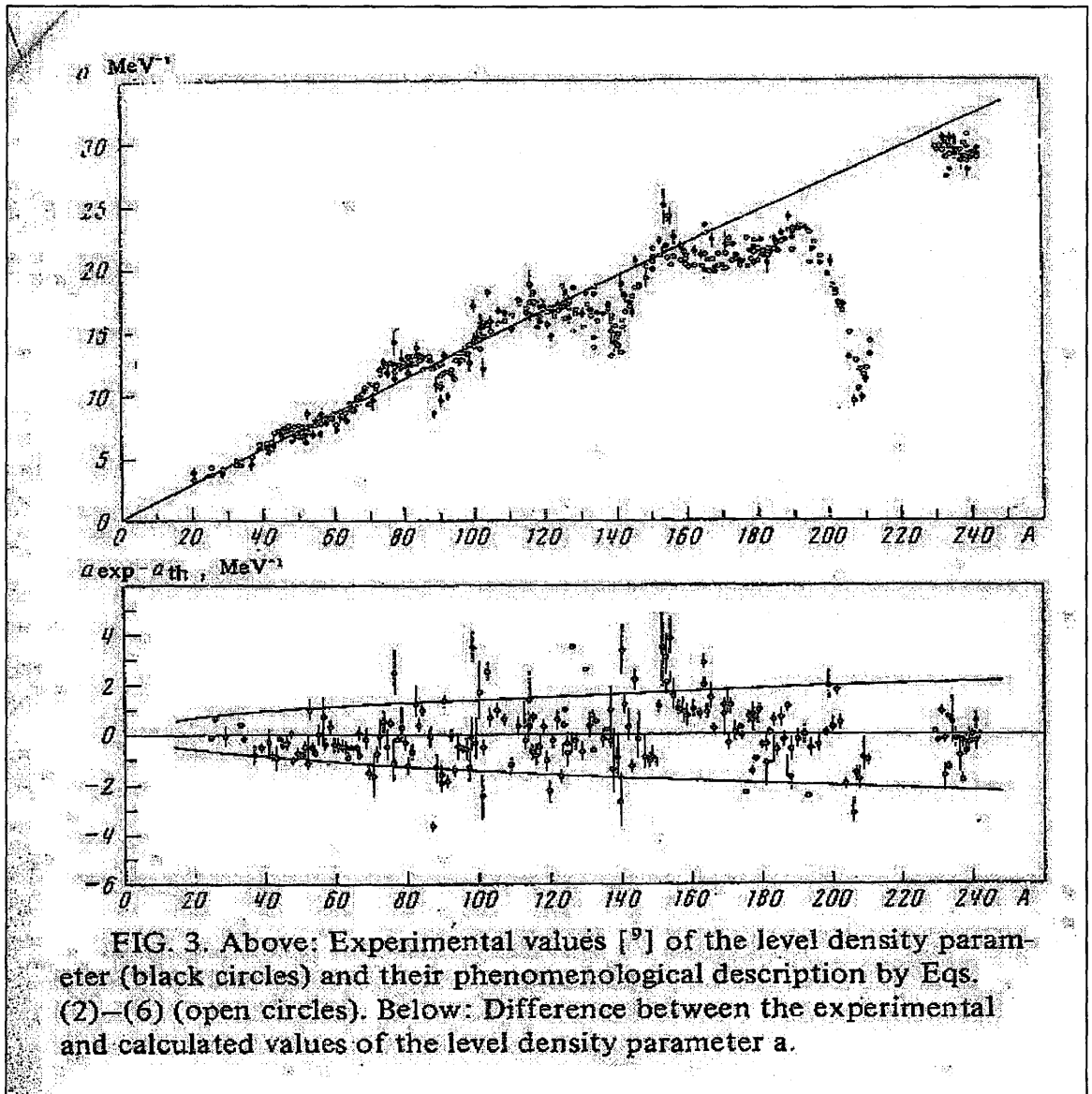


FIG. 3. Above: Experimental values ^[9] of the level density parameter (black circles) and their phenomenological description by Eqs. (2)–(6) (open circles). Below: Difference between the experimental and calculated values of the level density parameter a .

Figure 3.2: A plot of the single particle level density parameter, g_0 , for various nuclear elements. The fitting parameter, $a = g_0$, varies about the mean trend line of the particle number given by $\frac{A}{8}$.

3.1 Method

3.1.1 Derivation for systems of bosons

We start with a canonical formulation for the density of states. The canonical partition function is given as

$$Z(\beta) = B_N(x) \prod_{n=1}^{\infty} \frac{1}{(1-x^n)^{g(n)}}, \quad (3.1)$$

with $x = e^{-\beta\hbar\omega}$ and $B_N(x)$ a bosonic polynomial, with the polynomials to the 2-D harmonic oscillator found in Tran's thesis work [16] and the polynomials to the 3-D harmonic oscillator found in Schmidt and Schnack [17]. The energy degeneracy for the 3-D harmonic oscillator system is $g(n) = \frac{(n+1)(n+2)}{2}$. The single particle energy spacing is set to $\hbar\omega = 1$. The Euler-Maclaurin expansion is performed on the logarithm of the partition function, $Z(\beta)$, to obtain

$$\begin{aligned} \ln Z(\beta) = & \ln B_N(e^{-\beta}) - \frac{19}{480}\beta + \frac{\pi^4}{90\beta^3} + \frac{3\zeta(3)}{2\beta^2} \\ & + \frac{\pi^2}{6\beta} + \frac{5}{8} \ln \beta - \frac{1}{2} \ln(2\pi) + \frac{3}{2}\zeta(1, -1) + \frac{1}{2}\zeta(1, -2). \end{aligned} \quad (3.2)$$

with the single parameter zeta function the Riemann Zeta function and the double parameter zeta function to be the Hurwitz Zeta function, $\zeta(n, q) = \sum_{k=1}^{\infty} \frac{1}{(k+q)^n}$. We neglect $\ln B_N(e^{-\beta})$ from the partition function by the assumption that when the temperature is low, this term goes to zero and when the temperature is high, the value of the function is negligent compared to the dominant $\frac{\pi^4}{90\beta^3}$ temperature term.

Using the temperature saddle point condition, $\frac{\partial S}{\partial \beta}|_{\beta_0} = 0$, the solution to the saddle point condition, β_0 , is a solution to a quartic equation and not easily expressible. We use the standard expression for the saddle point density of states,

$$\rho(E) = \frac{e^{S^{(0)}}}{\sqrt{2\pi S^{(2)}}}, \quad (3.3)$$

as found in Tran [11], for example. The non-Gaussian correction terms are left out because of series convergence issues for small excitations. A plot of the non-Gaussian correction terms, given by Figure 3.3 and as they appear in Appendix A, shows convergence for large values of the excitation energy. It's possible that not enough non-Gaussian terms are being retained, for small excitation energies, to obtain an overall reasonable correction term. A large excitation energy series expansion also fails due to the amount of recursion necessary to evaluate the series expression. However, a plot of the density of states in Figure 3.4 shows considerable agreement to the exact number of bosonic microstates for a fixed excitation energy.

3.1.2 System of fermions

The main goal in this section is to show that the density of states can naturally explain the shell effects of half-filled levels and oscillation can be explained by the coefficients to the low excitation terms in the density of states calculations. Our method will closely follow Bohr & Mottelson [14]. We start with a Grand Canonical fermion partition function

$$Z_G^F(\alpha_N, \alpha_P, \beta) = \prod_{n=0}^{\infty} (1 + e^{\alpha_N - \beta\epsilon_n})(1 + e^{\alpha_P - \beta\epsilon_n})^{g(n)}, \quad (3.4)$$

valid as the number of particles grows large. We label one species of particles as neutrons and the other species as protons as defined in Chapter 2. The single particle energy levels are defined as $\epsilon_n = \hbar\omega(n + \frac{3}{2})$. The fermions are not assumed spinless this time and the energy degeneracy, $g(n) = (n + 1)(n + 2)$, accounts for

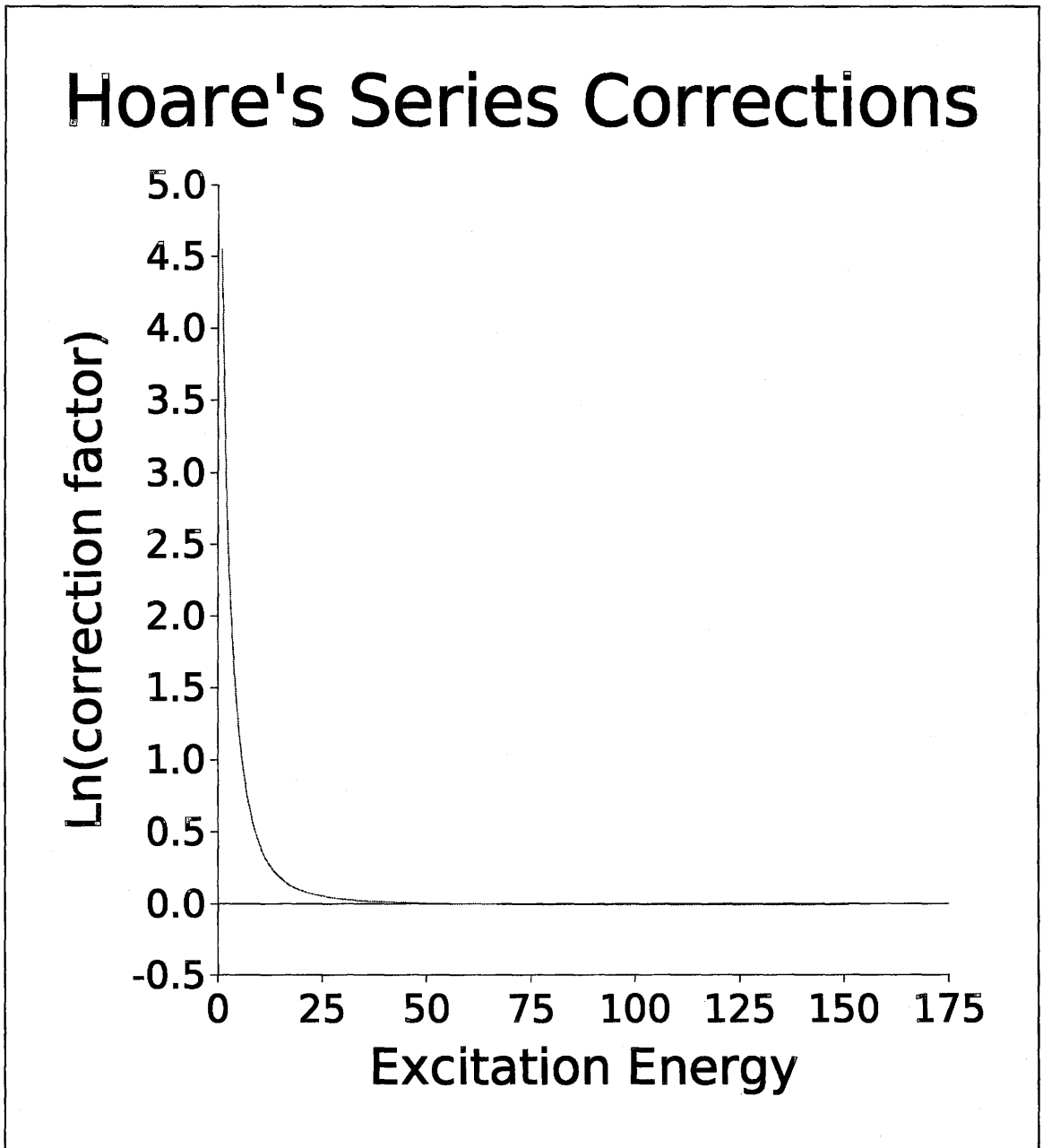


Figure 3.3: Hoare's non-Gaussian correction factors to the density of states. For large excitation values, the correction factors become negligent.

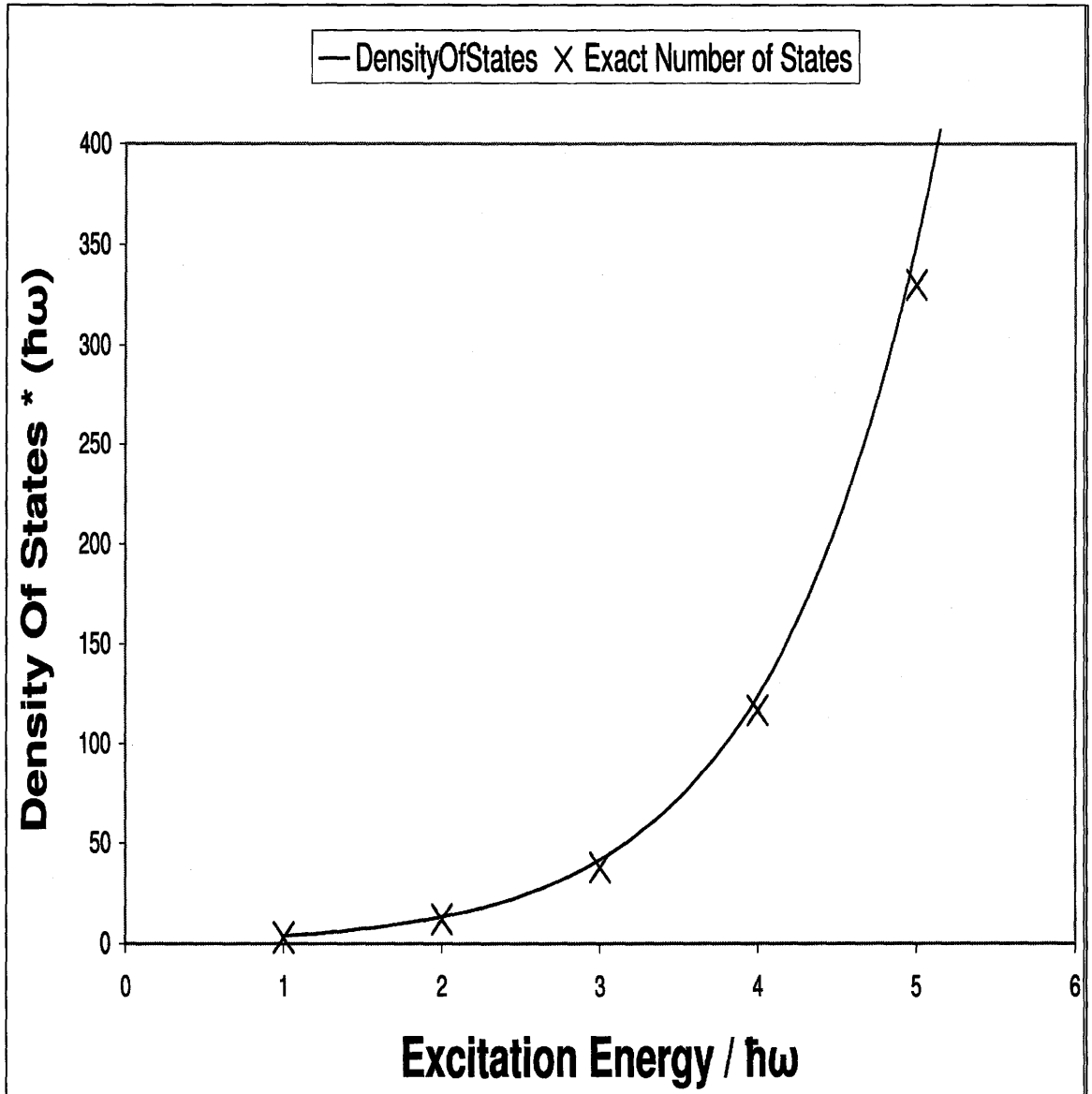


Figure 3.4: A plot of the density of states for one species of bosons residing in a degenerate harmonic well. Crosses represent the exact number of microstates for the given excitation energy.

this. We evaluate the entropy, $S(\alpha_N, \alpha_P, \beta) = \beta\xi - \alpha_N N - \alpha_P P + \ln Z(\alpha_N, \alpha_P, \beta)$, with the chemical potentials of the respective particles and temperature assumed to be large, specifically under the condition $\hbar\omega \ll \tau \ll \mu_{(i)}$, where τ is the temperature in units of the Boltzmann constant, k_b . This leads to defining the logarithm of the partition function, $\ln Z(\alpha_N, \alpha_P, \beta)$, as

$$\begin{aligned} \ln Z_G^F(\alpha_N, \alpha_P, \beta) &= \frac{17}{480}\beta + \left(\int_0^{\mu_P} + \int_0^{\mu_N} \right) (\alpha^{(i)} - \beta\epsilon)\tilde{g}(\epsilon) d\epsilon \\ &+ \frac{\pi^2}{6\beta}(\tilde{g}(\mu_P) + \tilde{g}(\mu_N)) + \frac{7\pi^4}{360\beta^3}(\tilde{g}''(\mu_P) + \tilde{g}''(\mu_N)), \end{aligned} \quad (3.5)$$

with $\tilde{g}(\epsilon)$ as the energy degeneracy as a function of the energy.

The shell correction, $\frac{17}{480}$, is specific to the 3-D spherical harmonic oscillator potential but other than this constant, (3.5) is still a general expression for a fermion system. We are left with a triple saddle-point condition to solve for the corrected density of states.

$$\left. \frac{\partial S(\alpha_P, \alpha_N, \beta)}{\partial \alpha_P} \right|_{\alpha_{N0}, \alpha_{P0}, \beta_0} = 0 \quad (3.6)$$

$$\left. \frac{\partial S(\alpha_P, \alpha_N, \beta)}{\partial \alpha_N} \right|_{\alpha_{N0}, \alpha_{P0}, \beta_0} = 0 \quad (3.7)$$

$$\left. \frac{\partial S(\alpha_P, \alpha_N, \beta)}{\partial \beta} \right|_{\alpha_{N0}, \alpha_{P0}, \beta_0} = 0 \quad (3.8)$$

There is no analytic solution for the chemical potentials and temperature so we approximate the chemical potential saddle-points further by defining $P = \int_0^{\frac{\alpha_{i0}}{\beta_0}} d\epsilon g(\epsilon)$ where the fermi energy is the chemical potential for the i th species. Our temperature independant saddle points for the chemical potentials are

$$\mu_{i0} = \frac{1}{2}(12P + \sqrt{-1 + 144P^2})^{\frac{1}{3}} + \frac{1}{2} \frac{1}{(12P + \sqrt{-1 + 144P^2})^{\frac{1}{3}}}. \quad (3.9)$$

This allows us to obtain a solution for the saddle point temperature as defined by the following reduced quartic equation,

$$\begin{aligned}
 \frac{\partial S(\alpha_P, \alpha_N, \beta)}{\partial \beta} \Big|_{\alpha_{N0}, \alpha_{P0}, \beta_0} &= E + \delta \xi_0^P + \delta \xi_0^N + \frac{17}{480} - \frac{\pi^2}{6\beta_0^2} (\tilde{g}(\mu_{P0}) + \tilde{g}(\mu_{N0})) \\
 &\quad - \frac{\pi^2}{6\beta_0} (\tilde{g}'(\mu_{P0}) \frac{\mu_{P0}}{\beta_0} - \tilde{g}'(\mu_{N0}) \frac{\mu_{N0}}{\beta_0}) \\
 &= E + \frac{17}{480} - \frac{\pi^2}{2} ((\mu_{N0})^2 + (\mu_{P0})^2 - \frac{1}{6}) \frac{1}{\beta_0^2} - \frac{7\pi^4}{90\beta_0^4} \\
 &= 0,
 \end{aligned} \tag{3.10}$$

and $\delta \xi_0^{(i)} = \xi_0^{(i)} - \tilde{\xi}_0^{(i)}$ the difference between the exact quantum mechanical zero-temperature groundstate $\xi_0^{(i)}$ and the smooth quantum mechanical groundstate $\tilde{\xi}_0^{(i)} = \int_0^{\mu_{i0}} d\epsilon \epsilon \tilde{g}(\epsilon)$.

With the given saddle-points, we expand $S(\alpha_P, \alpha_N, \beta)$ by a triple Taylor series about the saddle-points. The zeroth order derivative is taken outside of the integral, while the first order derivatives vanish under the saddle-point conditions. Our density of states then becomes

$$\begin{aligned}
 \rho(N, P, E) &= \frac{1}{(2\pi i)^3} \int_{a-i\infty}^{a+i\infty} \int_{b-i\infty}^{b+i\infty} \int_{c-i\infty}^{c+i\infty} d\beta d\alpha_N d\alpha_P e^{S(\alpha_N, \alpha_P, \beta)} \\
 &= \frac{e^{S(\alpha_{N0}, \alpha_{P0}, \beta_0)}}{(2\pi i)^3} \int_{a-i\infty}^{a+i\infty} \int_{b-i\infty}^{b+i\infty} \int_{c-i\infty}^{c+i\infty} d\beta d\alpha_N d\alpha_P \\
 &\quad e^{S^{(2)} + S^{(3)} + S^{(4)} + \dots},
 \end{aligned} \tag{3.11}$$

with the second order derivatives collected into the expression,

$$\begin{aligned}
 S^{(2)} = & \frac{\partial^2 S (\beta - \beta_0)^2}{\partial \beta^2 2!} + \frac{\partial^2 S (\alpha_P - \alpha_{P0})^2}{\partial \alpha_P^2 2!} + \frac{\partial^2 S (\alpha_N - \alpha_{N0})^2}{\partial \alpha_N^2 2!} \\
 & + \frac{\partial^2 S}{\partial \beta \partial \alpha_P} (\beta - \beta_0)(\alpha_P - \alpha_{P0}) + \frac{\partial^2 S}{\partial \beta \partial \alpha_N} (\beta - \beta_0)(\alpha_N - \alpha_{N0}) \\
 & + \frac{\partial^2 S}{\partial \alpha_P \partial \alpha_N} (\alpha_N - \alpha_{N0})(\alpha_P - \alpha_{P0}), \tag{3.12}
 \end{aligned}$$

all third order derivatives collected into $S^{(3)}$, etc. The integral is solved by completing the square on the second order terms defined by Eq. (3.12). The density of states can be expressed as

$$\rho(N, P, E) = \frac{e^{S(\alpha_{N0}, \alpha_{P0}, \beta_0)}}{\sqrt{D}} (1 + G^{(4)} + G^{(6)} + \dots), \tag{3.13}$$

where D is a determinant of second order entropy derivatives and can also be found in Bohr & Mottelson [14], and $G^{(k)}$ represents the Gaussian integrated k th order derivative terms, when $e^{S^{(3)}+S^{(4)}+\dots}$ is expanded as a Taylor series. Finally, performing a large one-particle level density series expansion on this density of states, we obtain the following density of states

$$\rho(N, P, E) \propto \frac{e^{\frac{4}{3}\sqrt{\eta E} + \frac{4}{3} \frac{(\delta \epsilon_0^P + \delta \epsilon_0^N + \frac{17}{480})}{2}} \sqrt{\frac{\eta}{E}}}{E^{\frac{5}{4}}}, \tag{3.14}$$

with $\eta = \pi^2 \left(\frac{\mu_{N0}^2 + \mu_{P0}^2}{2} - \frac{1}{12} \right)$ closely related to the single particle density at the fermi energy.

A plot of Eq. (3.14) in Figure 3.5 shows a lower density of states when the shells are completely filled compared to the high density of states when the shells are half-filled. We provide a 2-D plot of this density of states along the $P = 41$ line in Figure 3.6.

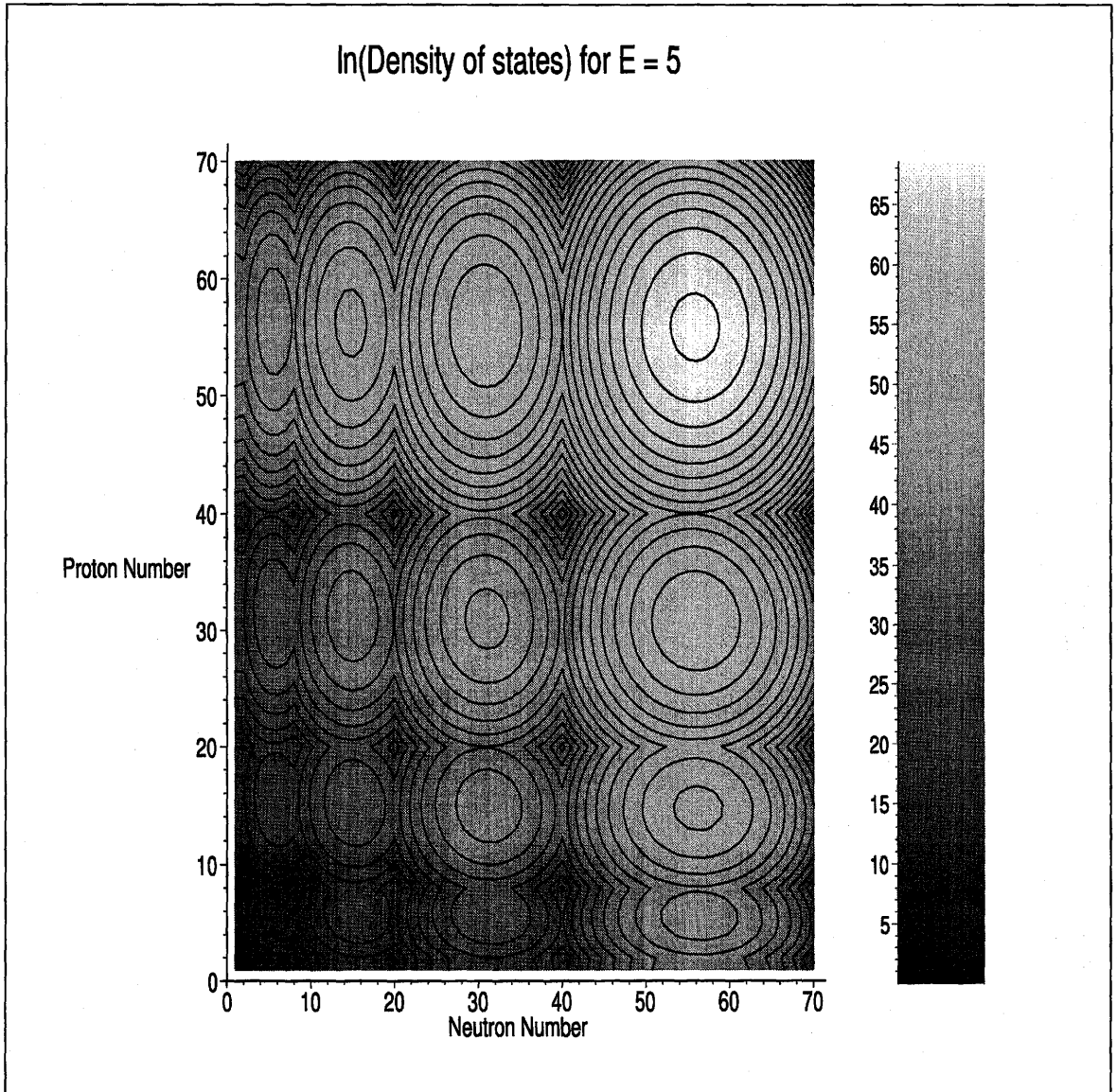


Figure 3.5: The density of states for two species of particles in a 3-D harmonic well. For a fixed excitation energy of 5 units of $\hbar\omega$ we can see oscillation structure at the harmonic oscillator magic numbers and we see growth in the density of states with increasing particle number.

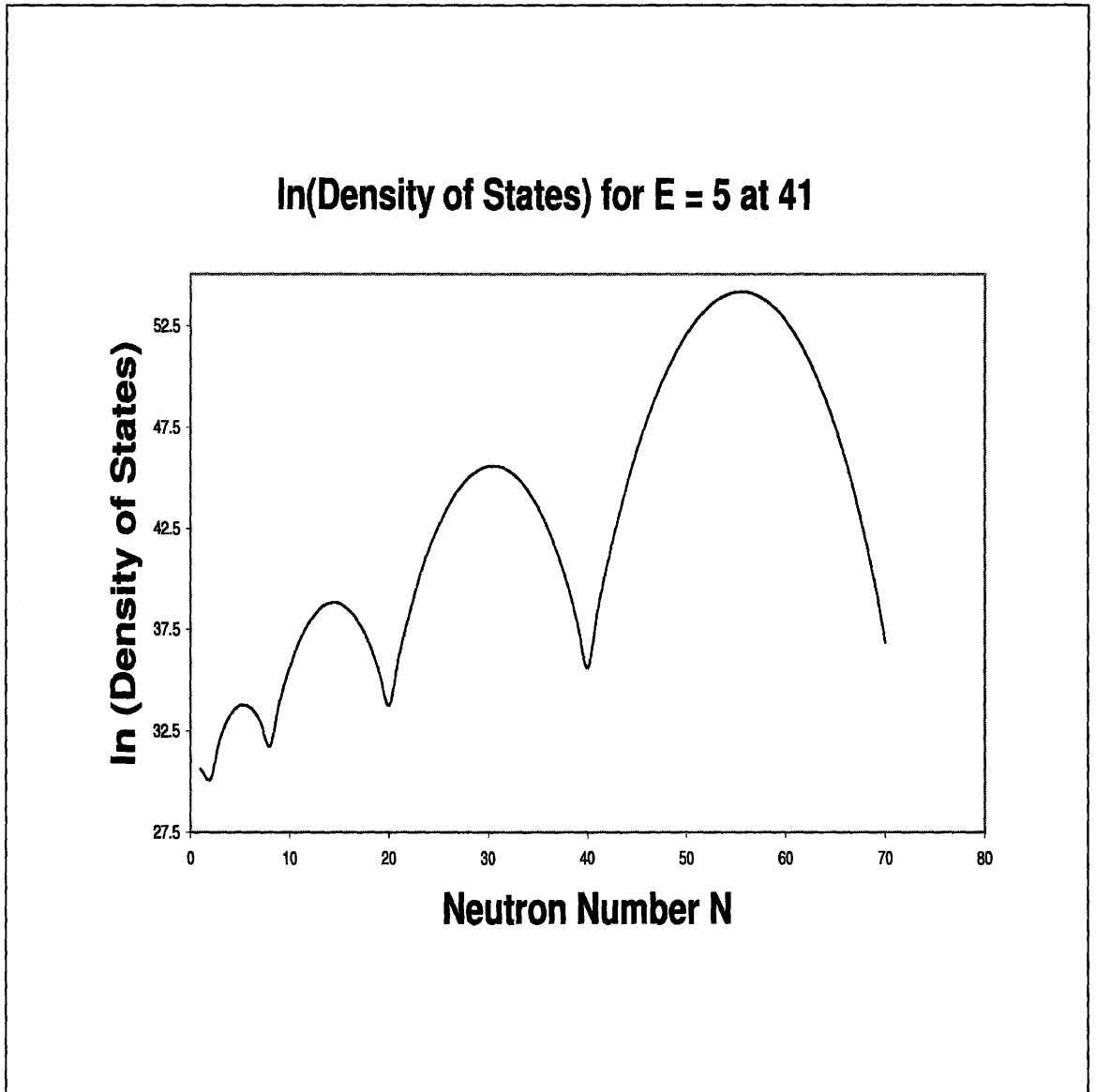


Figure 3.6: The logarithm of the density of states with fixed proton number $P = 41$, and varying neutron number only.

Chapter 4

Discussion

Working with the canonical partition, we are able to derive Leboeuf's low excitation energy corrections [4, 5] for particles confined within the equispaced, non-degenerate single-particle spectrum. A high temperature asymptotic expansion for the density of states, while incorporating non-Gaussian corrections, was valid. The hope was that a statistical derivation for the density of states for other systems would provide us with a correct series expansion for the density of states for other systems. Generalizing the saddle point technique to two species of fermion could provide us with the first of Leboeuf's low excitation energy corrections [6] but the coefficient to the second correction, under the saddle point technique, was an order of magnitude smaller than Leboeuf's.

Generalizing to a system with degeneracy, the saddle point does hold for a system of bosons. The difficulty in attempting to obtain an exact series expansion for the density of states is in the amount of recursion necessary to expand the quartic solution for the temperature. The non-Gaussian correction factors also appear divergent for low excitation energies with the possible explanation that not enough of the

correction factors have been retained.

The issue of a density of states phase transition in Bose-Einstein condensation was not addressed. The number of particles was very large and the critical temperature $T_c \propto N^{\frac{1}{3}} \hbar \omega$, such that the saddle point temperature was never above the critical temperature of the system.

Applying the saddle point technique to a system of fermions within a degenerate single particle spectrum does yield shell structure in the low excitation energy corrections, as a function of the particle numbers. As Rosenzweig [15] had predicted, the density of states is highest when the partially filled shell level is half filled and lowest when completely filled. The algorithm to generate the exact number of states was not developed, due to the necessity of linked list data structures and the number of levels that would need to be reproduced.

Appendix A

Non-Gaussian terms

$$h(y) = \mathcal{L}(f(x), y) = \frac{1}{(2\pi i)} \int_{c-i\infty}^{c+i\infty} dx e^{S(x)} \quad (\text{A.1})$$

We start with the inverse Laplace transform of any single variable function and c a real constant to the right of all singularities. The functions, $S(x)$ and $g(x)$, are defined as $S(x) = g(x) + yx$ and $g(x) = e^{\ln f(x)}$. In this paper, $S(x)$ is the entropy and $g(x)$ is the logarithm of the partition function. Taylor expanding $S(x)$ about a positive, real point of zero slope given by x_0 leaves us with

$$h(y) = \frac{e^{S^{(0)}}}{2\pi i} \int_{c-i\infty}^{c+i\infty} dx e^{S^{(2)} \frac{(x-x_0)^2}{2!}} e^{b(x)} \quad (\text{A.2})$$

$$b(x) = S^{(3)} \frac{(x-x_0)^3}{3!} + S^{(4)} \frac{(x-x_0)^4}{4!} + \dots \quad (\text{A.3})$$

We follow the notation as in in Chapter 2 and define $S^{(k)} = \frac{\partial}{\partial x} S(x)|_{x_0}$. The second exponential function, the non-Gaussian part $e^{b(x)}$, is expressed as its Maclaurin expansion. A variable substitution is made in order to evaluate the integral. The

constant c is set so that $c = x_0$ and define the integration variable u so that imaginary numbers are eliminated from the density of states, with $u = \frac{x-x_0}{i}$. Odd powers of u in the exponential expansion drop out when integrated and we collect similar even powers of u which leaves us with

$$h(y) = \frac{e^{S^{(0)}}}{2\pi} \int_{-\infty}^{\infty} du e^{-S^{(2)} \frac{u^2}{2}} (1 + S^{(4)} \frac{u^4}{4!} - (\frac{S^{(6)}}{6!} + \frac{S^{(3)}}{3!2!}) u^6 + \dots). \quad (\text{A.4})$$

We use the Gaussian integration relation $\int_{-\infty}^{\infty} dx x^{2n} e^{-ax^2} = \frac{(2n-1)!!}{2^n a^n} \sqrt{\frac{\pi}{a}}$ to obtain a final expression for

$$\begin{aligned} h(y) = & \frac{e^{S^{(0)}}}{\sqrt{2\pi S^{(2)}}} \left(1 + \frac{S^{(4)}}{8(S^{(2)})^2} - \frac{S^{(6)} + 10(S^{(3)})^2}{48(S^{(2)})^3} \right. \\ & + \frac{S^{(8)} + 56S^{(3)}S^{(5)} + 35(S^{(4)})^2}{384(S^{(2)})^4} \\ & - \frac{S^{(10)} + 120S^{(3)}S^{(7)} + 2100(S^{(3)})^2S^{(4)} + 126(S^{(5)})^2 + 210S^{(4)}S^{(6)}}{3840(S^{(2)})^5} \\ & + \frac{595S^{(4)}S^{(8)} + 462(S^{(6)})^2 + 27720S^{(3)}S^{(4)}S^{(5)} + 15400(S^{(3)})^4}{46080(S^{(2)})^6} \\ & + \frac{220S^{(3)}S^{(9)} + S^{(12)} + 792S^{(5)}S^{(7)} + 9240(S^{(3)})^2S^{(6)} + 5775(S^{(4)})^3}{46080(S^{(2)})^6} \\ & \left. + O\left(\frac{1}{(S^{(2)})^7}\right) \right) \end{aligned} \quad (\text{A.5})$$

up to 7th order in $\frac{1}{S^{(2)}}$.

For the equispaced nondegenerate harmonic oscillator, with the appropriate variable substitutions, a large excitation series expansion on $\frac{S^{(4)}}{(S^{(2)})^2}$ and $\frac{(S^{(3)})^2}{(S^{(2)})^3}$ yields terms of order $\sqrt{\frac{1}{E}}$. The terms, $\frac{S^{(6)}}{(S^{(2)})^3}$, $\frac{S^{(3)}S^{(5)}}{(S^{(2)})^4}$, $\frac{(S^{(4)})^2}{(S^{(2)})^4}$, $\frac{(S^{(3)})^2S^{(4)}}{(S^{(2)})^5}$, and $\frac{(S^{(3)})^4}{(S^{(2)})^6}$ yield terms of order $\frac{1}{E}$. The leading order on these terms does change with one species of particles or two species of particles.

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