NUCLEAR LEVEL DENSITY WITH INTERACTIONS

by

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ABSTRACT

A formalism is developed which can be used to calculate nuclear level densities with realistic interactions. The grand partition function is constructed and the level density is obtained by Laplace inversion. The formalism is a generalization of the technique used when the only residual interaction is the pairing force. It takes into account both Hartree-Fock and pairing-type effects. Illustrative examples are given in the specific case of Sn isotopes.

The formalism, as developed here, pertains to spherical nuclei. It can be generalized to include cases where, for example, shape transitions can occur. However, numerical calculations become difficult with generalized interactions. To study this effect, instead, a pairing plus quadrupole force is used. This effect may be important in Sn isotopes and can explain experimental data.

Exact model space calculations are also done to test the validity of the partition function approach for calculation of level densities.

RESUME

Nous présentons dans ce travail un formalisme, qui peut être utilisé pour calculer les densités de niveaux nucléaires avec des intéractions réalistes. La grande fonction de partition est construite et la densité de niveaux est obtenue par une inversion de Laplace. Ce formalisme qui trent compte à la fois des effets de type Couplage ainsi que ceux de type Hartree-Fock, est une généralisation de la technique utilisée quand la seule intéraction résiduelle est la force de couplage. Nous donnons quelques exemples type pour le problème spécifique des isotopes de l'étain.

La formalisme tel que développé ici, convient particulièrement aux noyaux sphériques, mais peut être généralisé pour inclure des cas où, par exemple, des changements de forme peuvent avoir lieu. Cependant les calculs numériques pour les intéractions généralisées deviennent trop élaborés; pour étudier ces cas on a eu recours à une force combinée "couplage plus quadrupole". Ces changements de formes peuvent être importantes pour les isotopes de l'étain et peuvent expliquer les données expérimentales.

Nous avons aussi obtenu des solutions exactes pour des modèles d'espace ce qui nous a permis de verifier la validité de l'approche de la fonction de partition pour le calcul des densités de niveaux.

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CHAPTER I

INTRODUCTION

The density of nuclear levels is one of the essential features of the nuclear spectrum at high excitation energies. Measurement of nuclear level density is necessary for the analysis of experimental data on the properties of highly excited states and also for understanding and analyzing complex nuclear reactions.

In theoretical studies of the nuclear level density, two distinct approaches are commonly employed; the spectroscopic approach for the low excitation energy, and the statistical mechanics approach for the high excitation energy.

The density of states of a nucleus depends strongly on the energy of excitation (with respect to the ground state) and on its mass. Near the ground state of light nuclei, the levels are about 1 MeV apart, while in heavy nuclei, they may be about 50 keV apart (except for the magic number of neutrons and protons). These may be observed in scattering experiments.† Thus at the low excitation energy, the levels are small in number, well separated and rather simple in structure. Spectroscopic approach is usually employed for the analysis of these low-lying excited levels and provides information regarding configurations, residual interactions, etc.

† E. Segre, Nuclei and Particles (Benjamin, New York, 1965).

The number of levels increases very rapidly with increasing excitation energy and the nature of the excitations becomes complicated. The existence of such complex levels is illustrated by the densely spaced, sharp resonances in the slow neutron capture reaction. The density of these levels is about 10^6 times greater than the average single particle level density (in a nucleus with A ~ 100), and their widths are also 10^6 times smaller than expected for a single particle excitation[1]. This evidence indicates that the neutron, on entering the nucleus, can share its energy with a large number of degrees of freedom of the target, and thus forms a highly complex configuration called the compound nucleus[2,3], which then decays to the final products. The spectroscopic approach is not so suitable for the analysis of this complex state of motion. Instead, the statistical approach may be used to obtain a more comprehensive description of the average behaviour of the compound nucleus and of its decay. Therefore, at the neutron binding energy and higher, it is appropriate to use the nuclear statistical model to study the experimental data on the properties of high excitations. The nuclear level density is the most fundamental quantity in the nuclear statistical model since it describes the statistical nuclear properties and can be inferred from reaction experiments.

Experimental data on nuclear level densities are obtained principally from slow neutron capture reaction. In

this experiment, the nuclear energy levels are observed at an energy just above the neutron binding energy and the level density is obtained by counting the number of resonances in a particular neutron energy interval. The levels excited by slow neutron resonance spectroscopy have only selected values of angular momentum and parity. For a doubly even target nucleus, s-wave neutron capture excites levels of a single spin and parity $\frac{1}{2}^+$ and therefore the level density $\rho(E, \frac{1}{2}, +)$ is measured. If the capturing nucleus is odd-even and has ground state spin and parity I^π, levels excited will have spin $I + \frac{1}{2}$ and $I - \frac{1}{2}$ and parity π. In that case, one measures $\rho(E, I + \frac{1}{2}, \pi) + \rho(E, I - \frac{1}{2}, \pi)$. In many calculations and in the ones done here one first calculates the density of states

$$\omega(E) = \Sigma(2I + 1)\,[\rho(E, I, +) + \rho(E, I, -)]$$

and deduces subsequently the level density $\rho(E, I, \pi)$ observed in experiment.

Numerous studies have been devoted for the derivation of formulae expressing the level density as a function of various constants of motions, e.g., excitation energy, number of particles (protons and neutrons), angular momentum, parity, etc. An analytic expression for the nuclear level density was first given by Bethe, usually referred to as the Bethe formula[4]. The derivation of this formula is based on a model of non-interacting fermions confined to the nuclear

volume[4-10]. The model is known as equidistant model as the single particle orbitals are assumed to be equally spaced. Due to its simple analytical results, the equidistant model has been widely used in data analysis although the Hamiltonian on which it is based is quite unrealistic and oversimplified. Because of the unrealistic Hamiltonian, the equidistant model does not predict the structure observed in level densities near closed shells. Also it cannot explain the differences in level densities of odd mass and even mass nuclei. The equidistant model has been modified in many ways by a number of authors. A pairing energy correction to the excitation energy[11-13], determined from experimentally obtained odd-even mass differences[13-18] has been introduced to account for the odd-even effect. A shell correction has been introduced in terms of an energy shift in the ground state[13,15]. A set of equally spaced levels of constant degeneracy[19,20], or a bunched single particle level spectrum[21,22] were used in order to simulate to some extent the effect of shell model degeneracies and bunching.

Bloch[23] developed a general method to include the shell model in level density calculations. More detailed and accurate theoretical information about level densities is obtained when one uses realistic single particle levels calculated from the shell model. However a realistic calculation of the level densities also needs the introduction of the residual interactions. This can be done in a simple way by

means of the pairing interaction. The superconductivity theory and the BCS Hamiltonian[24-26] have been applied in the evaluation of level densities. The application of the pairing Hamiltonian to excited nuclei has resulted in much improvement in the prediction of the low-energy behavior of the level densities. Numerical calculations of level densities have been performed on the basis of shell-model single-particle level scheme and the pairing Hamiltonian by either combinational method[27] or by means of the partition function method[28-34].

The combinatorial method consists in counting the number of different ways in which the nucleons can be distributed among the available single particle levels for a fixed energy of the system. Thus one may perform an exact counting of the levels. Since the value of level density is quite high especially for heavy nuclei, such calculation can be done only with large computers and are limited to low excitation energy. An improved method of direct counting of the number of states in the framework of the semi-microscopic nuclear model was given by Soloviev et al.[35]. However, the method does not obey a sum rule to be discussed in chapter II.

A rather new approach in the level density problem was initiated by French and collaborators[36]. The method is not limited to a simple pairing force and can be used for general interactions. Consider a large but finite space of M ($= \sum_a (2j_a + 1)$) single particle states. If there are N nucleons

in this space, then the level density is, to lowest order, approximated by

$$\omega(E) = \frac{d}{(2\pi F^2)^{\frac{1}{2}}} \exp[-(E - \bar{E})^2/2F^2] \qquad (I.1)$$

with

$$d = \binom{M}{N} ,$$

$$\bar{E} = \frac{1}{d} \sum_i \langle N, i|H|N, i\rangle ,$$

$$F^2 = \langle E^2\rangle - \bar{E}^2 ,$$

$$\langle E^2\rangle = \frac{1}{d} \sum_i \langle N, i|H^2|N, i\rangle .$$

Eq. (I.1) is the first term of a Gram-Charlier series[36] and can also be obtained[37] from standard techniques of statistical mechanics. Higher order corrections to Eq. (I.1) have also been given by French et al.

Although globally Eq. (I.1) fits exact model space calculations remarkably well, the method is not very suitable for comparing experimental data at 8-9 MeV excitation. The reasons are two-fold. Eq. (I.1) is an expansion about $\bar{E}$ and E is necessarily far removed from $\bar{E}$ (i.e., it is necessary to take enough single particle configurations). Secondly, to compare with experiment, it is necessary to transform $\rho(E)$ into $\rho(E_{exc.})$. This necessitates defining a ground state energy E_0 usually through

$$\int_{-\infty}^{E_0} \rho(E)\, dE = \frac{1}{2} .$$

The error in obtaining E_0 in this approximate way can lead to significant error in $\rho(E_{exc.})$. To compare with experimental data, it is therefore advantageous to have a method which directly gives $\rho(E_{exc.})$.

The method used in this work is based on the grand partition function approach. The method has been used for fermions in a one-body potential and also for fermions in a one-body field interacting with each other by a pure pairing force. We extend the method to more general interactions. We find that this is quite straightforward and practical calculations can be carried out. The formalism developed is applied to spherical nuclei (Sn isotopes) and the results are compared with those obtained in pure pairing force case and Hartree-Fock case. The objective is to examine whether such a formalism is at all feasible and whether it leads to any essential difference from previous work[28-34].

In the next chapter, we develop the mathematical formalism to calculate nuclear level densities with realistic interactions. For simplicity we restrict ourselves to spherical nuclei. In chapter III, we present and discuss the numerical results for Sn isotopes. We find that our calculation of level densities underestimates experimental results by unacceptable factors. In order to test the validity of

the grand partition function approach, exact calculations of level densities are done in a semi-realistic model space (chapter IV). It is found that the grand partition function is a reasonable approximation in the model space. Finally the question of whether Sn isotopes remain spherical at higher excitation energies is discussed. Variational calculations done in the specific case of Sn isotopes suggest that although these nuclei are spherical in the ground state (zero temperature), it is possible that they prefer deformation at finite but low temperature. This can lead to very large changes in the calculated values of level densities. In chapter V, we study this effect by considering a pairing plus quadrupole force.

CHAPTER II

MATHEMATICAL FORMALISM

It is well established that low energy spectra in spherical nuclei are strongly influenced by pairing correlation. Thus it is easier to talk in terms of quasi-particles (qp) rather than in terms of particles. A BCS calculation for low energy spectra can be routinely done even for a large number of particles in a large shell model space. But it is not necessary to assume a simple pairing force; realistic matrix elements can be used. The formalism was set up by Baranger[38] many years ago and has since been used by various authors[39-43] to investigate low energy spectra. Thus the ground state of an even nucleus is considered to be a BCS ground state and low-lying excited states are two qp states. Higher excited states are produced by four qp, six qp, etc.

The danger of using such a procedure to calculate level densities lies in overcounting. For definitiveness, consider the model space to have $2M[= \sum_a (2j_a + 1)]$ single particle states and a nucleus with 2m particles in the model space. The total number of states in this nucleus is then $\binom{2M}{2m}$. The counting procedure described above would yield for this nucleus one BCS ground state, $\binom{2M}{2}$ two qp states, $\binom{2M}{4}$ four qp states, $\binom{2M}{6}$ six qp states, etc. Therefore, we would get $\sum_{m=0}^{M} \binom{2M}{2m}$ states. Thus the total number of even qp states

equals the total number of states for all even systems; likewise, the total number of odd qp states equals the total number of states for all odd systems. Thus if we write

$$Z \alpha \prod_a (1 + e^{-\beta E_a})$$

where E_a's are qp energies, then Z cannot represent the canonical partition function for a single given nucleus; rather it must be related to the grand partition function.

A more serious objection is the following; usual BCS calculations minimize the ground state whereas, at neutron separation energies one is concerned with four to eight quasiparticle excitations. It would be better to have a theory which also minimizes excited states. As we will see, the grand partition function approach takes care of both these aspects. The objective then is to obtain the grand partition function as precisely as possible as a function of temperature and then to obtain the density of states in a given nucleus by "double" Laplace inversion. For completeness and for later use, we write down in the next section some well known quantities relating the density of states $\omega(E, N)$ in a given nucleus to the grand partition function Z. We begin the investigation of Z in Sec. II.2.

II.1 The density of states from the grand partition function

The statistical properties of a nucleus defined in terms of its number of particles and total energy are contained in the grand partition function:

$$Z(\alpha,\beta) = \sum_{i,N} e^{\alpha N} e^{-\beta E_i(N)} = \sum_{i,N} \exp[-\beta(E_i(N) - \lambda N)]$$

where β is the inverse of the temperature and $\alpha = \lambda\beta$ where λ is the chemical potential. Here α and β are two Lagrange multipliers associated with particle number and energy respectively.

In the framework of statistical mechanics, the density of states is the inverse Laplace transform of the grand partition function

$$\omega(E,N) = \frac{1}{(2\pi i)^2} \int_{-i\infty}^{i\infty}\int e^{\ell n Z(\alpha,\beta)}\, e^{-\alpha N}\, e^{\beta E}\, d\alpha d\beta \ .$$

The integral is evaluated with good approximation by the saddle-point method [for derivation, see Appendix I] and leads to

$$\omega(E,N) = \frac{1}{2\pi} \frac{e^S}{[D_{\alpha\alpha} D_{\beta\beta} - D_{\alpha\beta}^2]^{\frac{1}{2}}} \ , \qquad \text{(II.1)}$$

where S is the entropy of the system as defined in statistical mechanics

$$S = \ell nZ(\alpha_0,\beta_0) - \alpha_0 N + \beta_0 E \ . \qquad \text{(II.2)}$$

The constants α_0,β_0 are so chosen that

$$\left.\frac{\partial\ \ell nZ}{\partial\alpha}\right|_{\alpha_0,\beta_0} = N \ , \qquad \text{(II.3)}$$

$$\left.\frac{\partial\ \ell nZ}{\partial\beta}\right|_{\alpha_0,\beta_0} = -E \ . \qquad \text{(II.4)}$$

The quantities $D_{\alpha\alpha}$, $D_{\beta\beta}$ and $D_{\alpha\beta}$ are second derivatives:

$$D_{\alpha\alpha} = \left.\frac{\partial^2\ \ell nZ}{\partial\alpha^2}\right|_{\alpha_0,\beta_0} , \qquad \text{(II.5)}$$

$$D_{\beta\beta} = \left.\frac{\partial^2\ \ell nZ}{\partial\beta^2}\right|_{\alpha_0,\beta_0} , \qquad \text{(II.6)}$$

$$D_{\alpha\beta} = \left.\frac{\partial^2\ \ell nZ}{\partial\alpha\partial\beta}\right|_{\alpha_0,\beta_0} . \qquad \text{(II.7)}$$

II.2 Density of states in a pair-correlated nucleus.

We will first try to obtain the grand partition function for our system. To do this, it is necessary to extend Baranger's treatment[38] to include finite temperature. Since we deal with spherical nuclei, the single particle shell model states will have quantum numbers j_a, m_a. They may also have other quantum numbers like parity, ℓ, n, etc. These will

be collectively labeled by lower case latin subscripts, and the corresponding single particle creation and annihilation operators will be called, for example, $c_a^\dagger$ and c_a. They satisfy the usual Fermi anti-commutation relations

$$\{c_a^\dagger, c_b\} = \delta_{ab} \; ; \; \{c_a^\dagger, c_b^\dagger\} = \{c_a, c_b\} = 0 \; .$$

In association with the subscript a, we will use the capital latin subscript A which stands for all the quantum numbers except the magnetic quantum number m_a. The Hamiltonian $H - \lambda\hat{N}$ is given by

$$H - \lambda\hat{N} = \Sigma(\varepsilon_a - \lambda)\, c_a^\dagger c_a + \frac{1}{4} \Sigma\, V_{acbd}\, c_a^\dagger c_c^\dagger c_d c_b \qquad \text{(II.8)}$$

where ε_a's are shell model single particle energies and V_{acbd} is an antisymmetrized matrix element.

$$V_{acbd} = - V_{cabd} = - V_{acdb} = V_{cadb} \; .$$

In order to avoid excessive writing, we take the matrix elements to be real.

We now seek a transformation by which the Hamiltonian reduces to the form

$$H - \lambda\hat{N} \approx R + \Sigma\, E_a \alpha_a^\dagger \alpha_a \; . \qquad \text{(II.9)}$$

If such a reduction is possible, then the grand partition function will be obtained as

$$Z(\beta\lambda,\beta) = \mathrm{Tr}\, e^{-\beta(H-\lambda N)}$$

$$= e^{-\beta R} \prod (1 + e^{-\beta E_a}) \qquad \text{(II.10)}$$

Using the rules of grand canonical ensemble[44,45], the probability of occupation f_a is given by

$$f_a = \langle \alpha_a^\dagger \alpha_a \rangle = \frac{1}{1+e^{\beta E_a}} , \qquad \text{(II.11a)}$$

$$\langle \alpha_a^\dagger \alpha_b \rangle = \delta_{ab} f_a , \qquad \text{(II.11b)}$$

$$\langle \alpha_a^\dagger \alpha_b^\dagger \rangle = \langle \alpha_a \alpha_b \rangle = 0 , \qquad \text{(II.11c)}$$

where the notation $\langle\ \rangle$ implies an ensemble average. The reduction implied in Eq. (II.9) is attempted using the Bogoliubov-Valatin[25,46] transformation to quasi-particles.

$$\alpha_a = u_a c_a - s_a v_a c_{-a}^\dagger \qquad \text{(II.12a)}$$

$$\alpha_a^\dagger = u_a c_a^\dagger - s_a v_a c_{-a} \qquad \text{(II.12b)}$$

where

$$s_a = (-)^{j_a - m_a} \; ; \; u_a = u_A \; ; \; v_a = v_A .$$

$\alpha_a^\dagger$ and α_a are the quasi-particle creation and absorption operators respectively. $-a$ is obtained from a by changing the sign of the magnetic quantum number. u_a and v_a are real and for the transformation to be unitary and preserve the Fermion anticommutation rules

$$\{\alpha_a^\dagger, \alpha_b\} = \delta_{ab} \; ; \; \{\alpha_a^\dagger, \alpha_b^\dagger\} = \{\alpha_a, \alpha_b\} = 0 \; ,$$

u_a and v_a must satisfy

$$u_a^2 + v_a^2 = 1 \qquad \text{(II.13)}$$

The inverse of relations (II.12) are

$$c_a = u_a \alpha_a + s_a v_a \alpha_{-a}^\dagger \qquad \text{(II.14a)}$$

$$c_a^\dagger = u_a \alpha_a^\dagger + s_a v_a \alpha_{-a} \qquad \text{(II.14b)}$$

As in the usual BCS theory, we will rewrite $(H - \lambda \hat{N})$ as a sum of normal products using Wick's theorem:

$$c_a^\dagger c_b = :c_a^\dagger c_b: + \langle c_a c_b \rangle \qquad \text{(II.15a)}$$

$$\begin{aligned} c_a^\dagger c_c^\dagger c_d c_b = {} & \langle c_a^\dagger c_b \rangle \langle c_c^\dagger c_d \rangle - \langle c_a^\dagger c_d \rangle \langle c_c^\dagger c_b \rangle \\ & + \langle c_a^\dagger c_c^\dagger \rangle \langle c_d c_b \rangle \\ & + \langle c_a^\dagger c_b \rangle : c_c^\dagger c_d : + \langle c_c^\dagger c_d \rangle : c_a^\dagger c_b : \\ & - \langle c_a^\dagger c_d \rangle : c_c^\dagger c_b : - \langle c_c^\dagger c_b \rangle : c_a^\dagger c_d : \\ & + \langle c_a^\dagger c_c^\dagger \rangle : c_d c_b : + \langle c_d c_b \rangle : c_a^\dagger c_c^\dagger : \\ & + : c_a^\dagger c_c^\dagger c_d c_b : \end{aligned} \qquad \text{(II.15b)}$$

Since V_{acbd} has a lot of symmetries, we can group together terms which give identical results when summed over

all acbd. Then we may write

$$c_a^\dagger c_c^\dagger c_d c_b \to 2 \langle c_a^\dagger c_b \rangle \langle c_c^\dagger c_d \rangle + \langle c_a^\dagger c_c^\dagger \rangle \langle c_d c_b \rangle + 4 \langle c_c^\dagger c_d \rangle : c_a^\dagger c_b : + \langle c_a^\dagger c_c^\dagger \rangle : c_d c_b : + \langle c_d c_b \rangle : c_a^\dagger c_c^\dagger : : c_a^\dagger c_c^\dagger c_d c_b :$$

We can now rewrite Eq. (II.8) as

$$H - \lambda \hat{N} = A_0 + A_2 + A_4 \tag{II.16}$$

where the subscripts on the right-hand side of Eq. (II.16) refer to the number of qp operators in normal order:

$$A_0 = \Sigma\ (\varepsilon_a - \lambda) \langle c_a^\dagger c_a \rangle + \frac{1}{2} \Sigma\ V_{acbd} \langle c_a^\dagger c_b \rangle \langle c_c^\dagger c_d \rangle + \frac{1}{4} \Sigma\ V_{acbd} \langle c_a^\dagger c_c^\dagger \rangle \langle c_d c_b \rangle \tag{II.17a}$$

$$A_2 = \Sigma\ (\varepsilon_a - \lambda) : c_a^\dagger c_a : + \Sigma\ V_{acbd} \langle c_c^\dagger c_d \rangle : c_a^\dagger c_b : + \frac{1}{4} \Sigma\ V_{acbd} \langle c_a^\dagger c_c^\dagger \rangle : c_d c_b : + \frac{1}{4} \Sigma\ V_{acbd} \langle c_d c_b \rangle : c_a^\dagger c_c^\dagger : \tag{II.17b}$$

$$A_4 = \frac{1}{4} \Sigma\ V_{acbd} : c_a^\dagger c_c^\dagger c_d c_b : \tag{II.17c}$$

The only difference from the zero temperature calculation is that ensemble averages replace ground state expectation values. So as to be able to write down a simple expression

for the grand partition function, we will neglect A_4 in this section. We will return to its discussion in section II.4.

The right-hand side of Eq. (II.17a) can be evaluated by using Eqs. (II.14) and Eqs. (II.11). For example, we obtain

$$\langle c_a^\dagger c_b \rangle = \delta_{ab} [v_a^2 + (u_a^2 - v_a^2) f_a]$$

$$s_a \langle c_a^\dagger c_c^\dagger \rangle = s_a \langle c_c c_a \rangle = \delta_{a-c} u_a v_a (1-2f_a)$$

Let us now define two new quantities ρ_a and k_a:

$$\rho_a \equiv \langle c_a^\dagger c_a \rangle ,$$

$$k_a \equiv s_a \langle c_a^\dagger c_{-a}^\dagger \rangle = s_a \langle c_{-a} c_a \rangle .$$

We then have

$$\langle c_a^\dagger c_b \rangle = \delta_{ab} \frac{1}{2}[1 - (u_a^2 - v_a^2)(1-2f_a)] = \delta_{ab} \rho_a = \delta_{ab} \rho_A , \tag{II.18}$$

$$s_a \langle c_a^\dagger c_c^\dagger \rangle = s_a \langle c_c c_a \rangle = \delta_{a-c} u_a v_a (1-2f_a) = \delta_{a-c} k_a = \delta_{a-c} k_A . \tag{II.19}$$

Using Eqs. (II.18) and (II.19), Eq. (II.17a) reduces to

$$A_0 = \Sigma (\varepsilon_a - \lambda) \rho_a + \frac{1}{2} \Sigma V_{abab} \rho_a \rho_b + \frac{1}{4} \Sigma V_{a-ab-b} s_a s_b k_a k_b .$$

We now turn to A_2. We split it into four parts:

$$A_2 = A_2^{(1)} + A_2^{(2)} + A_2^{(3)} + A_2^{(4)} ,$$

with

$$A_2^{(1)} = \Sigma\ (\varepsilon_a - \lambda)\ :\ c_a^\dagger c_a\ : ,$$

$$A_2^{(2)} = \Sigma\ V_{acbc}\ \rho_c\ :\ c_a^\dagger c_b\ : ,$$

$$A_2^{(3)} = \frac{1}{4}\ \Sigma\ V_{a-abd}\ s_a k_a\ :\ c_d c_b\ : ,$$

$$A_2^{(4)} = \frac{1}{4}\ \Sigma\ V_{acb-b}\ s_b k_b\ :\ c_a^\dagger c_c^\dagger\ : ,$$

where we have used Eqs. (II.18) and (II.19). Let us now consider $A_2^{(2)}$.

$$A_2^{(2)} = \Sigma\ V_{j_a m_a j_c m_c j_b m_b j_c m_c}\ \rho_c\ :\ c_a^\dagger c_b\ :$$

Summing over m_c, we obtain $j_a = j_b$, $m_a = m_b$; otherwise the term is zero. If further, as in Ref. 38, we assume that among all our orbitals A, B ,..., a given combination of charge, parity, and j value occurs only once[†], then the above term can be written as

$$A_2^{(2)} = \Sigma\ V_{acac}\ \rho_c\ :\ c_a^\dagger c_a\ : .$$

[†]For a more general treatment, see Appendix II.

Following the same argument, we can write

$$A_2^{(3)} = \frac{1}{4} \Sigma V_{a-ab-b} s_a k_a : c_{-b} c_b : ,$$

and

$$A_2^{(4)} = \frac{1}{4} \Sigma V_{a-ab-b} s_b k_b : c_a^\dagger c_{-a}^\dagger : .$$

Let us now define

$$\mu_a = - \sum_c V_{acac} \rho_c , \tag{II.20}$$

$$\Delta_a = - \frac{1}{2} s_a \sum_b V_{a-ab-b} s_b k_b \tag{II.21}$$

and

$$\eta_a = \epsilon_a - \mu_a - \lambda . \tag{II.22}$$

We then have

$$A_2^{(1)} + A_2^{(2)} = \Sigma \eta_a : c_a^\dagger c_a : , \tag{II.23a}$$

$$A_2^{(4)} + A_2^{(3)} = - \frac{1}{2} \Sigma s_a \Delta_a [: c_a^\dagger c_{-a}^\dagger : + : c_{-a} c_a :] . \tag{II.23b}$$

Now from Eqs. (II.14),

$$c_a^\dagger c_a = u_a^2 \alpha_a^\dagger \alpha_a + s_a u_a v_a (\alpha_a^\dagger \alpha_{-a}^\dagger + \alpha_{-a} \alpha_a) + v_a^2 - v_a^2 \alpha_{-a}^\dagger \alpha_{-a} ,$$

$$s_a c_a^\dagger c_{-a}^\dagger = s_a (u_a^2 \alpha_a^\dagger \alpha_{-a}^\dagger - v_a^2 \alpha_{-a} \alpha_a)$$

$$+ u_a v_a (1 - \alpha_a^\dagger \alpha_a - \alpha_{-a}^\dagger \alpha_{-a}) ,$$

and

$$s_a c_{-a} c_a = s_a (u_a^2 \alpha_{-a} \alpha_a - v_a^2 \alpha_a^\dagger \alpha_{-a}^\dagger)$$

$$+ u_a v_a (1 - \alpha_a^\dagger \alpha_a - \alpha_{-a}^\dagger \alpha_{-a}) .$$

Let us now use Eq. (II.15a) and Eqs. (II.18) and (II.19) to obtain

$$: c_a^\dagger c_a : = u_a^2 \alpha_a^\dagger \alpha_a - v_a^2 \alpha_{-a}^\dagger \alpha_{-a}$$

$$+ s_a u_a v_a (\alpha_a^\dagger \alpha_{-a}^\dagger + \alpha_{-a} \alpha_a) - (u_a^2 - v_a^2) f_a ,$$

$$s_a : c_a^\dagger c_{-a}^\dagger : = s_a (u_a^2 \alpha_a^\dagger \alpha_{-a}^\dagger - v_a^2 \alpha_{-a} \alpha_a)$$

$$- u_a v_a (\alpha_a^\dagger \alpha_a + \alpha_{-a}^\dagger \alpha_{-a}) + 2 f_a u_a v_a ,$$

and

$$s_a : c_{-a} c_a : = s_a (u_a^2 \alpha_{-a} \alpha_a - v_a^2 \alpha_a^\dagger \alpha_{-a}^\dagger)$$

$$- u_a v_a (\alpha_a^\dagger \alpha_a + \alpha_{-a}^\dagger \alpha_{-a}) + 2 f_a u_a v_a .$$

Eqs. (II.23) then reduce to

$$A_2^{(1)} + A_2^{(2)} = \Sigma \eta_a [(u_a^2 - v_a^2) \alpha_a^\dagger \alpha_a$$

$$+ s_a u_a v_a (\alpha_a^\dagger \alpha_{-a}^\dagger + \alpha_{-a}\alpha_a) - (u_a^2 - v_a^2) f_a] \qquad \text{(II.24a)}$$

$$A_2^{(3)} + A_2^{(4)} = -\frac{1}{2} \Sigma s_a \Delta_a (u_a^2 - v_a^2)(\alpha_a^\dagger \alpha_{-a}^\dagger + \alpha_{-a}\alpha_a)$$

$$+ 2 \Sigma \Delta_a u_a v_a \alpha_a^\dagger \alpha_a - 2 \Sigma \Delta_a u_a v_a f_a \,. \qquad \text{(II.24b)}$$

Finally, using our definitions of μ, Δ, and η we obtain

$$A_0 = \Sigma(\varepsilon_a - \lambda)\, \rho_a - \frac{1}{2} \Sigma\, u_a \rho_a - \frac{1}{2} \Sigma\, \Delta_a k_a$$

$$= \Sigma\, \eta_a \rho_a + \frac{1}{2} \Sigma\, \mu_a \rho_a - \frac{1}{2} \Sigma\, \Delta_a k_a \qquad \text{(II.25)}$$

and from Eqs. (24),

$$A_2 = \Sigma [\eta_a (u_a^2 - v_a^2) + 2\Delta_a u_a v_a]\, \alpha_a^\dagger \alpha_a$$

$$+ \Sigma [\eta_a u_a v_a - \frac{1}{2} \Delta_a (u_a^2 - v_a^2)]\, s_a (\alpha_a^\dagger \alpha_{-a}^\dagger + \alpha_{-a}\alpha_a)$$

$$- \Sigma [\eta_a (u_a^2 - v_a^2) + 2\Delta_a u_a v_a]\, f_a \,. \qquad \text{(II.26)}$$

In order to obtain Eq. (II. 9), we require that u and v satisfy the equation

$$\eta_a u_a v_a - \frac{1}{2} \Delta_a (u_a^2 - v_a^2) = 0$$

which together with Eq. (II. 13) gives

$$2u_a v_a = \Delta_a / E_a \;;\; u_a^2 - v_a^2 = \eta_a / E_a \;; \qquad \text{(II.27)}$$

with

$$E_a = (\eta_a^2 + \Delta_a^2)^{\frac{1}{2}} \qquad \text{(II.28a)}$$

$$= \eta_a(u_a^2 - v_a^2) + 2\Delta_a u_a v_a \qquad \text{(II.28b)}$$

Eq. (II.26) then reduces to

$$A_2 = \Sigma\, E_a \alpha_a^\dagger \alpha_a - \Sigma\, E_a f_a$$

Also, substituting Eqs. (II.27) into Eqs. (II.18) and (II.19), we get

$$\rho_a = \frac{1}{2}\left[1 - \frac{\eta_a}{E_a}(1 - 2f_a)\right] \qquad \text{(II.29)}$$

$$k_a = \frac{\Delta_a}{2E_a}(1 - 2f_a) \qquad \text{(II.30)}$$

where

$$f_a = 1/(1 + e^{\beta E_a}) .$$

We are now ready for the reduction implied in Eq. (II.9).

$$H - \lambda\hat{N} \approx R + \Sigma\, E_a \alpha_a^\dagger \alpha_a ,$$

where R is given by the c-number terms of A_0 and A_2 :

$$R = \Sigma\, \eta_a \rho_a + \frac{1}{2}\Sigma\, \mu_a \rho_a - \frac{1}{2}\Sigma\, \Delta_a k_a - \Sigma\, E_a f_a$$

$$= \frac{1}{2} \Sigma \eta_a [1 - \frac{\eta_a}{E_a} (1 - 2f_a)] + \frac{1}{2} \Sigma \mu_a \rho_a$$

$$- \Sigma \frac{\Delta_a^2}{2E_a} (1 - 2f_a) + \frac{1}{2} \Sigma \Delta_a k_a - \Sigma E_a f_a$$

$$= \frac{1}{2} \Sigma (\eta_a - E_a) + \frac{1}{2} \Sigma \mu_a \rho_a + \frac{1}{2} \Sigma \Delta_a k_a \qquad \text{(II.31)}$$

II.3 The grand partition function and related statistical quantities.

We finally obtain an approximate expression for the grand partition function from Eqs. (II.10) and (II.31):

$$Z = \exp[-\frac{1}{2} \beta \Sigma (\eta_a - E_a + \mu_a \rho_a + \Delta_a k_a)] \prod_a (1 + e^{-\beta E_a}) \qquad \text{(II.32)}$$

By letting $\mu_a \to 0$, one obtains the grand partition function of the pure BCS case (Section II.7); by letting $\Delta_a \to 0$ one obtains the Hartree-Fock case (Appendix II). There is a self-consistency condition implied in Eqs. (II.29) and (II.30) and Eqs. (II.20) and (II.21); ρ_a and k_a depend upon μ_a and Δ_a which in turn depend upon ρ_a and k_a. The emergence of non-zero f_a is the only new feature from the formalism of Ref. 38. In solving the self-consistent equations numerically, this extra feature causes little extra work.

We now need the derivatives of $\ell n Z$ and an expression for entropy [Eq. (II.2) to Eq. (II.7)]. After some algebra

(Appendix III) one obtains

$$N = \frac{\partial \ \ell nZ}{\partial \alpha} = \Sigma \ \rho_a \ , \qquad \text{(II.33)}$$

$$-E = \frac{\partial \ \ell nZ}{\partial \beta}$$

$$= - \Sigma \ \epsilon_a \rho_a + \frac{1}{2} \Sigma \ \mu_a \rho_a + \frac{1}{2} \Sigma \ \Delta_a k_a \ . \qquad \text{(II.34)}$$

$$S = \beta \ \Sigma \ E_a f_a + \Sigma \ \ell n [1 + e^{-\beta E_a}] \qquad \text{(II.35)}$$

Equations (II.33) and (II.34) determine the values of α_0, β_0. The needed second derivatives are

$$\frac{\partial^2 \ \ell nZ}{\partial \alpha^2} = \Sigma \frac{\partial \rho_a}{\partial \alpha} \ , \qquad \text{(II.36)}$$

$$\frac{\partial^2 \ \ell nZ}{\partial \beta^2} = - \Sigma \ \epsilon_a \frac{\partial \rho_a}{\partial \beta} + \Sigma \ \mu_a \frac{\partial \rho_a}{\partial \beta} + \Sigma \ \Delta_a \frac{\partial k_a}{\partial \beta} \ , \qquad \text{(II.37)}$$

where we have used (Appendix III)

$$\frac{1}{2} \frac{\partial}{\partial \beta} \Sigma \ \mu_a \rho_a = \Sigma \ \mu_a \frac{\partial \rho_a}{\partial \beta}$$

and

$$\frac{1}{2} \frac{\partial}{\partial \beta} \Sigma \ \Delta_a k_a = \Sigma \ \Delta_a \frac{\partial k_a}{\partial \beta} \ .$$

We also get

$$\frac{\partial^2 \ \ell nZ}{\partial \alpha \partial \beta} = - \Sigma \ \epsilon_a \frac{\partial \rho_a}{\partial \alpha} + \Sigma \ \mu_a \frac{\partial \rho_a}{\partial \alpha} + \Sigma \ \Delta_a \frac{\partial k_a}{\partial \alpha} \ , \qquad \text{(II.38)}$$

or equivalently,

$$\frac{\partial^2 \ell n Z}{\partial \beta \partial \alpha} = \Sigma \frac{\partial \rho_a}{\partial \beta} . \qquad \text{(II.39)}$$

Thus in order to evaluate the second derivatives, we need the values of $\partial \rho_a/\partial \alpha$, $\partial \rho_a/\partial \beta$, $\partial k_a/\partial \alpha$, and $\partial k_a/\partial \beta$. We will now proceed to illustrate how these can be obtained.

From Eqs. (II.29) and (II.30) by direct differentiation (Appendix IV), we obtain

$$\frac{\partial \rho_a}{\partial \alpha} = (Y_a \Delta_a^2 + X_a \eta_a^2)(\beta \frac{\partial \mu_a}{\partial \alpha} + 1)$$

$$- \beta \eta_a (X_a + Y_a) \Delta_a \frac{\partial \Delta_a}{\partial \alpha} , \qquad \text{(II.40)}$$

$$\frac{\partial k_a}{\partial \alpha} = - \eta_a (X_a - Y_a) \Delta_a (\beta \frac{\partial \mu_a}{\partial \alpha} + 1)$$

$$+ \beta (Y_a \eta_a^2 + X_a \Delta_a^2) \frac{\partial \Delta_a}{\partial \alpha} , \qquad \text{(II.41)}$$

where we have defined

$$X_a = f_a (1 - f_a)/E_a^2$$

$$Y_a = (1 - 2f_a)/(2\beta E_a^3) .$$

Equations (II.40) and (II.41) cannot yet be used to solve for $\partial \rho_a/\partial \alpha$ and $\partial k_a/\partial \alpha$ as these contain the unknowns $\partial \mu_a/\partial \alpha$ and $\partial \Delta_a/\partial \alpha$. However, these unknowns can be expressed in terms of $\partial \rho_a/\partial \alpha$ and $\partial k_a/\partial \alpha$. From Eqs. (II.20) and (II.21)

$$\frac{\partial \mu_a}{\partial \alpha} = - \Sigma V_{acac} \frac{\partial \rho_c}{\partial \alpha} , \tag{II.42}$$

$$\frac{\partial \Delta_a}{\partial \alpha} = - \frac{1}{2} s_a \Sigma V_{a-ab-b} s_b \frac{\partial k_b}{\partial \alpha} . \tag{II.43}$$

Substituting Eqs. (II.42) and (II.43) in Eqs. (II.40) and (II.41), we obtain a set of coupled linear equations for $\partial \rho_a / \partial \alpha$ and $\partial k_a / \partial \alpha$:

$$\frac{\partial \rho_a}{\partial \alpha} + \beta (Y_a \Delta_a^2 + X_a \eta_a^2) \Sigma V_{acac} \frac{\partial \rho_c}{\partial \alpha}$$

$$- \frac{1}{2} \beta \eta_a (X_a - Y_a) s_a \Delta_a \Sigma V_{a-ab-b} s_b \frac{\partial k_b}{\partial \alpha}$$

$$= Y_a \Delta_a^2 + X_a \eta_a^2 ,$$

and

$$- \beta \eta_a (X_a - Y_a) \Delta_a \Sigma V_{acac} \frac{\partial \rho_c}{\partial \alpha} + \frac{\partial k_a}{\partial \alpha}$$

$$+ \frac{1}{2} \beta (Y_a \eta_a^2 + X_a \Delta_a^2) s_a \Sigma V_{a-ab-b} s_b \frac{\partial k_b}{\partial \alpha}$$

$$= - \eta_a (X_a - Y_a) \Delta_a .$$

In matrix form, we may write

$$\begin{pmatrix} P & Q \\ R & S \end{pmatrix} \begin{pmatrix} \frac{\partial \rho}{\partial \alpha} \\ \frac{\partial k}{\partial \alpha} \end{pmatrix} = \begin{pmatrix} Y\Delta^2 + X\eta^2 \\ - \eta (X - Y) \Delta \end{pmatrix} , \tag{II.44}$$

with

$$P_{AB} = \delta_{AB} - \beta(Y_A\Delta_A^2 + X_A\eta_A^2)\ 2[(j_B + \tfrac{1}{2})/(j_A + \tfrac{1}{2})]^{\frac{1}{2}}\ F(AABBO),$$

$$Q_{AB} = \beta\eta_A(X_A - Y_A)\ \Delta_A[(j_B + \tfrac{1}{2})/(j_A + \tfrac{1}{2})]^{\frac{1}{2}}\ G(AABBO),$$

$$R_{AB} = \beta\eta_A(X_A - Y_A)\ \Delta_A\ 2[(j_B + \tfrac{1}{2})/(j_A + \tfrac{1}{2})]^{\frac{1}{2}}\ F(AABBO),$$

$$S_{AB} = \delta_{AB} - \beta(Y_A\eta_A^2 + X_A\Delta_A^2)\ [(j_B + \tfrac{1}{2})/(j_A + \tfrac{1}{2})]^{\frac{1}{2}}\ G(AABBO),$$

where we have used the spherical symmetry of our problem to do the summation over the magnetic quantum numbers (Appendix V):

$$\sum_{m_b} V_{abab} = -2[(j_B + \tfrac{1}{2})/(j_A + \tfrac{1}{2})]^{\frac{1}{2}}\ F(AABBO),$$

$$s_a \sum_{m_b} s_b\, V_{a-ab-b} = -2[(j_B + \tfrac{1}{2})/(j_A + \tfrac{1}{2})]^{\frac{1}{2}}\ G(AABBO).$$

The F and G are the coupled matrix elements of the potential as defined by Baranger[38]. The dimensionality of the matrix in Eq. (II.44) is 2n where n is the number of j shells in the active space. It is possible to write the matrix equation in a much more symmetric form; this is done in Appendix VI.

A similar procedure for $\partial\rho/\partial\beta$ and $\partial k/\partial\beta$ (Appendix IV) leads to

$$\begin{pmatrix} P & Q \\ R & S \end{pmatrix}\begin{pmatrix} \frac{\partial\rho}{\partial\beta} \\ \frac{\partial k}{\partial\beta} \end{pmatrix} = \begin{pmatrix} -\lambda Y\Delta^2 - \eta X(E^2+\eta\lambda) \\ \Delta E^2 X + \Delta(X - Y)\eta\lambda \end{pmatrix} \qquad (II.45)$$

Thus only one matrix inversion is required to get all the second derivatives.

II.4 Introduction of an Auxiliary Hamiltonian.

The grand partition function of the previous section is, of course, approximate as the term $\hat{A}_4$ of Eq. (II.16) was dropped in obtaining it. Neglecting this term is dangerous in the nuclear case as the following argument will show. From the fundamental definition of the partition function (Section II.1), $\partial^2 \ell nZ/\partial\alpha^2$ and $\partial^2 \ell nZ/\partial\beta^2$ are fluctuations and as such, must be positive definite:

$$\frac{\partial^2 \ell nZ}{\partial\alpha^2} = \langle N^2\rangle - \langle N\rangle^2 > 0 ,$$

$$\frac{\partial^2 \ell nZ}{\partial\beta^2} = \langle E^2\rangle - \langle E\rangle^2 > 0 .$$

On the other hand, with our approximation [Eq. (II.36)],

$$\frac{\partial^2 \ell nZ}{\partial\alpha^2} = \frac{\partial}{\partial\alpha} \Sigma \rho_a = \frac{\partial}{\partial\alpha} \langle N\rangle = \frac{1}{\beta} \frac{\partial\langle N\rangle}{\partial\lambda} . \qquad \text{(II.46)}$$

There is no guarantee that the right hand side of Eq. (II.46) will turn out to be positive. Nuclear forces are saturating which means λ stays more or less constant as particles are added. This suggests that the right-hand side of Eq. (II.46) is as likely to be positive as negative if realistic matrix elements are used. The cause of this trouble is that as more

and more particles are added, the single particle energies $\varepsilon_a - \mu_a$ decrease and eventually drop below the essentially constant Fermi energy. This problem could disappear in some schematic models (such as the pairing plus quadrupole model) in which the single particle energies stay more or less constant and the Fermi level rises with increasing number of particles.

Fortunately, we are not interested in the grand partition function per se, rather, in the density of states in a given nucleus and at a given excitation energy. Thus we are allowed to add to the actual Hamiltonian another two-body interaction provided it does not change the excitation spectrum in a given nucleus. Therefore we replace

$$\frac{1}{4} V_{acbd} \, c_a^\dagger c_c^\dagger c_d c_b$$

by

$$\frac{1}{4} (V_{acbd} - M \delta_{ab} \delta_{cd} + M \delta_{ad} \delta_{cb}) \, c_a^\dagger c_c^\dagger c_d c_b \, .$$

This amounts to adding a term $-\frac{1}{2} M(\hat{N}^2 - \hat{N})$ to the Hamiltonean. The idea is try to cancel optimally the A_4 term due to V_{acbd} by the A_4 term due to M. The choice of M is dictated by the condition that [Eq. (II.40)]

$$\Sigma \, (Y_a \Delta_a^2 + X_a \eta_a^2) \, \frac{\partial \mu_a}{\partial \alpha} = 0$$

but the following choice is also adequately accurate:

$$M = \overline{V_{abab}} \ ,$$

where the averaging is done over the orbitals near the Fermi level. In terms of the F matrix, we may write

$$M = \frac{\sum_{ab} V_{abab}}{\sum_{ab} 1}$$

$$= \frac{-2 \sum_{AB} [(j_B + \frac{1}{2})/(j_A + \frac{1}{2})]^{\frac{1}{2}} (2j_A + 1) F(AABBO)}{\sum_{AB} (2j_A + 1)(2j_B + 1)}$$

$$= -\frac{\sum_{AB} [(j_A + \frac{1}{2})(j_B + \frac{1}{2})]^{\frac{1}{2}} F(AABBO)}{\sum_{AB} (j_A + \frac{1}{2})(j_B + \frac{1}{2})}$$

The coupled matrix elements F and G will now be different from their original values. They will be given as (Appendix VII):

$$F^{new}(AABBO) = F(AABBO) + M[(j_A + \tfrac{1}{2})(j_B + \tfrac{1}{2})]^{\frac{1}{2}} - \delta_{AB} \frac{M}{2}$$

$$G^{new}(AABBO) = G(AABBO) + \delta_{AB} M$$

II.5 Extension to two kinds of particles.

The formalism developed so far deals with a single kind of particles; but actually the nucleus is composed of two kinds of particles, neutrons and protons. The calculation of the density of states may be generalized for two kinds of particles by introducing a new Lagrange multiplier for the new kind of particles. The grand partition function will now depend on three parameters so that we are able to specify the average values of the energy E, the neutron number N_n and the proton number N_p:

$$Z(\alpha_n,\alpha_p,\beta) = \sum_{N_p,N_n,i} \exp[\alpha_p N_p + \alpha_n N_n - \beta E_i(N_p, N_n)]$$

As before, we take the Laplace inverse of Z to get the density of states

$$\omega(E,N_n,N_p) = \frac{1}{(2\pi i)^3} \int_{-i\infty}^{i\infty}\int\int \exp[\ln Z(\alpha_p,\alpha_n,\beta) - \alpha_p N_p - \alpha_n N_n + \beta E]\, d\alpha_p\, d\alpha_n\, d\beta.$$

In the saddle point approximation (Appendix I), this leads to

$$\omega(E,N_n,N_p) = \frac{1}{(2\pi)^{3/2}} \frac{e^S}{\sqrt{D}}$$

Here the entropy S is

$$S = \ell nZ(\alpha_{p0}, \alpha_{n0}, \beta_0) - \alpha_{p0} N_p - \alpha_{n0} N_n + \beta_0 E$$

and the constants α_{p0}, α_{n0}, and β_0 are so chosen that

$$\left.\frac{\partial\, \ell nZ}{\partial \alpha_p}\right|_{\alpha_{p0},\alpha_{n0},\beta_0} = N_p \ ,$$

$$\left.\frac{\partial\, \ell nZ}{\partial \alpha_n}\right|_{\alpha_{p0},\alpha_{n0},\beta_0} = N_n \ ,$$

$$\left.\frac{\partial\, \ell nZ}{\partial \beta}\right|_{\alpha_{p0},\alpha_{n0},\beta_0} = -E \ .$$

The quantity D is a determinant of second derivatives evaluated at α_{p0}, α_{no}, and β_0 :

$$D = \begin{vmatrix} \dfrac{\partial^2 \ell nZ}{\partial \alpha_p^2} & \dfrac{\partial^2 \ell nZ}{\partial \alpha_n \partial \alpha_p} & \dfrac{\partial^2 \ell nZ}{\partial \beta \partial \alpha_p} \\ \dfrac{\partial^2 \ell nZ}{\partial \alpha_p \partial \alpha_n} & \dfrac{\partial^2 \ell nZ}{\partial \alpha_n^2} & \dfrac{\partial^2 \ell nZ}{\partial \beta \partial \alpha_n} \\ \dfrac{\partial^2 \ell nZ}{\partial \alpha_p \partial \beta} & \dfrac{\partial^2 \ell nZ}{\partial \alpha_n \partial \beta} & \dfrac{\partial^2 \ell nZ}{\partial \beta^2} \end{vmatrix}$$

Extension of the formalism of the three previous sections to two kinds of particles is straightforward. We assume that pairing correlation exists between similar particles only. We introduce an extra index which may stand for either neutron or proton. Thus the generalization of Eqs. (II.20)

and (II.21) are

$$\mu_a(i) = -\sum_{c,j} V^{ij}_{acac}\, \rho_c(j) ,$$

$$\Delta_a(i) = -\frac{1}{2}\, s_a \sum_b V^{ii}_{a-ab-b}\, s_b k_b(i) .$$

The generalizations of Eqs. (II.33), (II.34), and (II.35) are given as (Appendix VIII):

$$N_i = \frac{\partial\, \ell n Z}{\partial \alpha_i} = \sum_a \rho_a(i) ,$$

$$-E = \frac{\partial\, \ell n Z}{\partial \beta} = -\sum_{a,i} \varepsilon_a(i)\, \rho_a(i) + \frac{1}{2} \sum_{a,i} \mu_a(i)\, \rho_a(i) + \frac{1}{2} \sum_{a,i} \Delta_a(i)\, k_a(i) ,$$

$$S = \beta \sum_{a,i} E_a(i) / (1 + e^{\beta E_a(i)}) + \sum_{a,i} \ell n [1 + e^{-\beta E_a(i)}] .$$

Similarly Eqs. (II.40) and (II.41) become

$$\frac{\partial \rho_a(j)}{\partial \alpha_i} = [Y_a(j)\, \Delta_a^2(j) + X_a(j)\, \eta_a^2(j)] \left(\beta \frac{\partial \mu_a(j)}{\partial \alpha_i} + \delta_{ij}\right) - \beta \eta_a(j) [X_a(j) - Y_a(j)]\, \Delta_a(j) \frac{\partial \Delta_a(j)}{\partial \alpha_i} ,$$

$$\frac{\partial k_a(j)}{\partial \alpha_i} = -\eta_a(j) [X_a(j) - Y_a(j)]\, \Delta_a(j) \left[\beta \frac{\partial \mu_a(j)}{\partial \alpha_i} + \delta_{ij}\right] + \beta [Y_a(j)\, \eta_a^2(j) + X_a(j)\, \Delta_a^2(j)] \frac{\partial \Delta_a(j)}{\partial \alpha_i} .$$

The generalizations of Eqs. (II.44) and (II.45) which are needed for the derivatives of ρ_a and k_a are given in Appendix IX. Following the same argument as in section II.4, one needs in general three constants, M_{nn}, M_{np}, and M_{pp} given as

$$M_{ij} = \overline{V^{ij}_{abab}}$$

II.6 Level density for a particular angular momentum.

The density of states derived in the previous sections is obviously

$$\omega(E) = \sum_I (2I + 1)\, \rho(E, I)$$

where $\rho(E, I)$ is the density of levels of a given angular momentum I (both parities included). $\omega(E)$ includes levels degenerate in M, the z-projection of the angular momentum I. We can also write

$$\omega(E) = \sum_M \rho(E, M) ,$$

then

$$\rho(E, I) = \rho(E, M = I) - \rho(E, M = I + 1) \qquad \text{(II.47)}$$

For our grand canonical ensemble, we have $\langle M \rangle = 0$ and making a Gaussian approximation, we write

$$\rho(E, M) = \omega(E) \frac{1}{(2\pi\sigma^2)^{\frac{1}{2}}} e^{-M^2/2\sigma^2} \qquad \text{(II.48)}$$

where σ^2 is called the spin cut-off parameter and is given by

$$\sigma^2 = \langle M^2 \rangle - \langle M \rangle^2 = \langle M^2 \rangle \qquad \text{(II.49)}$$

The quantity $\langle M^2 \rangle$ is the ensemble average of the operators J_Z^2. Now

$$J_Z^2 = \Sigma (J_Z)_{ab} \, c_a^\dagger c_b \; \Sigma (J_Z)_{cd} \, c_c^\dagger c_d$$

$$= \Sigma (J_Z^2)_{ad} \, c_a^\dagger c_d + \Sigma (J_Z)_{ab} \, (J_Z)_{cd} \, c_a^\dagger c_c^\dagger c_d c_b \, .$$

The first term is a one-body operator. In our basis, it is diagonal and gives $\Sigma \, m_a^2 \, f_a$. The second term is a two-body operator. It gives

$$\Sigma (J_Z)_{aa} \, (J_Z)_{cc} \, f_a f_c - \Sigma (J_Z)_{ac} \, (J_Z)_{ca} \, f_a f_c$$

$$= - \Sigma \, m_a^2 \, f_a^2 \, .$$

Together one obtains

$$\langle M^2 \rangle = \Sigma \, m_a^2 \, f_a (1 - f_a) \qquad \text{(II.50)}$$

In the present work, $\omega(E)$ was first calculated and

$\rho(E, I)$ was then obtained from Eqs. (II.47) - (II.50).

A formally exact expression for $\rho(E, N, M)$ may also be written down.

$$\rho(E,N,M) = \frac{1}{(2\pi i)^3} \int\int\int_{-i\infty}^{i\infty} e^{\ell n Z(\alpha,\nu,\beta)} e^{-\alpha N} e^{-\nu M} \times e^{\beta E} d\alpha d\nu d\beta$$

where ν is a Lagrange multiplier associated with M. The grand partition function $Z(\alpha,\nu,\beta)$ is to be obtained by solving for the Hamiltonian $H - \lambda N - \gamma M$ ($\nu = \beta\gamma$). The saddle point approximation gives

$$\rho(E,N,M) = \frac{1}{(2\pi)^{3/2}} \frac{e^S}{\sqrt{D}}$$

where

$$S = \ell n Z(\alpha_0,\nu_0,\beta_0) - \alpha_0 N - \nu_0 M + \beta_0 E$$

and as before α_0, ν_0 and β_0 are so chosen that

$$\left.\frac{\partial\, \ell n Z}{\partial \alpha}\right|_{\alpha_0,\nu_0,\beta_0} = N ,$$

$$\left.\frac{\partial\, \ell n Z}{\partial \nu}\right|_{\alpha_0,\nu_0,\beta_0} = M ,$$

$$\left.\frac{\partial\, \ell n Z}{\partial \beta}\right|_{\alpha_0,\nu_0,\beta_0} = -E ,$$

and D is a 3x3 determinant of second derivatives of ℓnZ evaluated at α_0, ν_0 and β_0.

The Hamiltonian $H - \lambda\hat{N} - \gamma\hat{M}$ is given by

$$H - \lambda\hat{N} - \gamma\hat{M} = \Sigma(\varepsilon_a - \lambda - \gamma m_a)\, c_a^\dagger c_a + \frac{1}{4}\Sigma\, V_{acbd}\, c_a^\dagger c_c^\dagger c_d c_b .$$

Using the Bogoliubov-Valatin transformation to quasi-particles, the above Hamiltonian can be diagonalized to the form

$$H - \lambda\hat{N} - \gamma\hat{M} \approx \frac{1}{2}\Sigma(\eta_a - E_a + \mu_a\rho_a + \Delta_a k_a) + \Sigma(E_a - \gamma m_a)\, \alpha_a^\dagger \alpha_a .$$

Therefore the grand partition function will be obtained as

$$Z(\beta\lambda, \beta\gamma, \beta) = \exp\left[-\frac{1}{2}\beta\Sigma(\eta_a - E_a + \mu_a\rho_a + \Delta_a k_a)\right] \prod_a \left[1 + e^{-\beta(E_a - \gamma m_a)}\right].$$

The quasi-particle occupation probability f_a will now be given by

$$f_a = \langle \alpha_a^\dagger \alpha_a \rangle = 1/(1 + e^{\beta(E_a - \gamma m_a)}) .$$

Since -a is obtained from a by changing the sign of the magnetic quantum number, we may write

$$f_{-a} = \langle \alpha_{-a}^\dagger \alpha_{-a} \rangle = 1/(1 + e^{\beta(E_a + \gamma m_a)}) .$$

Also,

$$\langle c_a^\dagger c_b \rangle = \delta_{ab} [v_a^2 + f_a u_a^2 - f_{-a} v_a^2]$$

$$= \delta_{ab} [v_a^2 - f_a v_a^2 + f_{-a} u_a^2]$$

$$= \delta_{ab} \rho_a = \delta_{ab} \rho_{-a} .$$

Similarly,

$$s_a \langle c_a^\dagger c_c^\dagger \rangle = s_a \langle c_c c_a \rangle = \delta_{a-c} u_a v_a (1 - f_a - f_{-a})$$

$$= \delta_{a-c} k_a = \delta_{a-c} k_{-a} .$$

Therefore f_a now depends upon m_a and hence ρ_a and k_a also depend upon m_a although ρ_a and k_a are independent of the sign of m_a.

The expressions for N and E are same as before [Eqs. (II.33) and (II.34)] and

$$M = \frac{\partial \ \ell n Z}{\partial \nu} = \Sigma \ m_a \ f_a ,$$

$$S = \beta \ \Sigma \ \frac{E_a - \gamma m_a}{1 + \exp [\beta (E_a - \gamma m_a)]} + \Sigma \ \ell n [1 + \exp(-\beta (E_a - \gamma m_a))] .$$

We also obtain

$$\frac{\partial^2 \ \ell n Z}{\partial \nu^2} = \Sigma \ m_a^2 \ f_a (1 - f_a) + \beta \ \Sigma \ m_a \ f_a (1 - f_a)$$

$$\times \left[\frac{\eta_a}{E_a} \frac{\partial \mu_a}{\partial \nu} - \frac{\Delta_a}{E_a} \frac{\partial \Delta_a}{\partial \nu} \right] ,$$

$$\frac{\partial^2 \ln Z}{\partial \nu \partial \alpha} = \Sigma \frac{\partial \rho_a}{\partial \nu} ,$$

$$\frac{\partial^2 \ln Z}{\partial \nu \partial \beta} = - \Sigma \epsilon_a \frac{\partial \rho_a}{\partial \nu} + \Sigma \mu_a \frac{\partial \rho_a}{\partial \nu} + \Sigma \Delta_a \frac{\partial k_a}{\partial \nu} .$$

Other second derivatives will have same expressions as given in Eqs. (II.36) - (II.39).

Since ρ_a and k_a now depend upon magnetic quantum numbers, the summation over magnetic quantum numbers in Eqs. (II.42) and (II.43) (See also Appendix V) can no more be done formally. Thus the dimensions of the matrix to be inverted [Eq. (II.44)] is much bigger and hence the calculation of level density becomes too long and laborious.

To compare with experiment, only level densities of low spin states are needed. This means only low values of M are required. In such cases, the Gaussian approximation is quite valid as will be shown in later sections.

Finally, experimental data are available for the level density with a definite parity π. If one assumes that the number of levels of each parity are equal, then the level density for a single parity will be given as

$$\rho(E,I,\pi) = \frac{1}{2} \rho(E,I) .$$

II.7 Reduction to the simple pairing force problem.

Most calculations for level densities employ a pure pairing force

$$G(ABCDO) = \delta_{AB}\,\delta_{CD}\,[(j_A + \tfrac{1}{2})(j_C + \tfrac{1}{2})]^{\frac{1}{2}}\, g$$

where g is a constant. The Hartree-Fock contribution coming from a pairing force is small and this is neglected. Previously we had

$$\Delta_A = \sum_B [(j_B + \tfrac{1}{2})/(j_A + \tfrac{1}{2})]^{\frac{1}{2}}\, G(AABBO)\, k_B \qquad \text{(II.51)}$$

Therefore for a simple pairing force, the gap parameter will be

$$\Delta_A = g \sum_B (j_B + \tfrac{1}{2})\, k_B \equiv \Delta. \qquad \text{(II.52)}$$

Let us now use Eq. (II.31) in Eq. (II.52)

$$\Delta = \frac{1}{2}\, g \sum_a k_a$$

$$= \frac{1}{2}\, g\, \Delta \sum \frac{1 - 2f_a}{2E_a},$$

from which we obtain the gap equation

$$\frac{2}{g} = \sum_a \frac{1 - 2f_a}{2E_a} \qquad \text{(II.53)}$$

Neglecting μ_a in Eq. (II.32), we obtain the grand partition function of the pure BCS case:

$$Z = \exp[-\frac{1}{2}\beta \Sigma (\epsilon_a - \lambda - E_a) - \beta \Delta^2/g] \prod_a (1 + e^{-\beta E_a})$$

where the quasi-particle energy E_a is now given as

$$E_a = [(\epsilon_a - \lambda)^2 + \Delta^2]^{\frac{1}{2}} .$$

The derivatives of ℓnZ are

$$N = \frac{\partial \ell nZ}{\partial \alpha} = \Sigma \rho_a \qquad \text{(II.54)}$$

$$-E = \frac{\partial \ell nZ}{\partial \beta}$$

$$= -\Sigma \epsilon_a \rho_a + \Delta^2/g \qquad \text{(II.55)}$$

The single-particle occupation probability ρ_a is now given by

$$\rho_a = \frac{1}{2}[1 - \frac{\epsilon_a - \lambda}{E_a}(1 - 2f_a)] \qquad \text{(II.56)}$$

The entropy will have the same expression as before (Eq. (II.35))

$$S = \beta \Sigma E_a f_a + \Sigma \ell n[1 + e^{-\beta E_a}] .$$

The second derivatives of ℓnZ are

$$\frac{\partial^2 \ell n Z}{\partial \alpha^2} = \Sigma \frac{\partial \rho_a}{\partial \alpha} , \qquad \text{(II.57a)}$$

$$\frac{\partial^2 \ell n Z}{\partial \beta^2} = - \Sigma \varepsilon_a \frac{\partial \rho_a}{\partial \beta} + \frac{2\Delta}{g} \frac{\partial \Delta}{\partial \beta} , \qquad \text{(II.57b)}$$

$$\frac{\partial^2 \ell n Z}{\partial \alpha \partial \beta} = - \Sigma \varepsilon_a \frac{\partial \rho_a}{\partial \alpha} + \frac{2\Delta}{g} \frac{\partial \Delta}{\partial \alpha} , \qquad \text{(II.57c)}$$

$$\frac{\partial^2 \ell n Z}{\partial \beta \partial \alpha} = \Sigma \frac{\partial \rho_a}{\partial \beta} . \qquad \text{(II.57d)}$$

The derivatives of ρ_a are obtained from Eq. (II.56) by direct differentiation:

$$\frac{\partial \rho_a}{\partial \alpha} = \Delta^2 Y_a + (\varepsilon_a - \lambda)^2 X_a - \beta(\varepsilon_a - \lambda)(X_a - Y_a) \Delta \frac{\partial \Delta}{\partial \alpha} ,$$

$$\frac{\partial \rho_a}{\partial \beta} = -\lambda \Delta^2 Y_a - (\varepsilon_a - \lambda) X_a [E_a^2 + (\varepsilon_a - \lambda) \lambda]$$

$$- \beta(\varepsilon_a - \lambda)(X_a - Y_a) \Delta \frac{\partial \Delta}{\partial \beta} ,$$

where X_a and Y_a are as defined in section II.3.

The gap equation (II.53) defines Δ as an implicit function of α and β and the partial derivative of Δ can be calculated from it explicitly:

$$\frac{\partial \Delta}{\partial \alpha} = \frac{\Sigma (\varepsilon_a - \lambda)(X_a - Y_a)}{\beta \Delta \Sigma (X_a - Y_a)} ,$$

$$\frac{\partial \Delta}{\partial \beta} = \frac{1}{\beta \Delta \Sigma (X_a - Y_a)} [\lambda \Sigma (\varepsilon_a - \lambda) Y_a - \Delta^2 \Sigma X_a$$

$$- \Sigma \varepsilon_a (\varepsilon_a - \lambda) X_a] .$$

Since the gap equation is true only for non-zero Δ, therefore above derivatives should be set equal to zero whenever $\Delta = 0$.

CHAPTER III

CALCULATIONS

Numerical calculations of the state and level densities have been performed for a realistic set of single particle levels and a general two-body interaction using the theory of the previous sections. The specific nuclei chosen are ^{116}Sn, ^{118}Sn and ^{120}Sn. The twelve active orbitals for both protons and neutrons and their single-particle energies are given in table 1. The inert core is assumed to be the nucleus ^{56}Ni. The single particle energies are taken from Lee and Hara[42,47]. The residual interaction is derived from the nucleon-nucleon interaction of Kahana, Lee and Scott[48]. The G and F matrix elements of the residual interaction are given in table 2. With these single-particle energies and two-body matrix elements, a very reasonable description for low energy spectra is obtained[42,47]. To obtain nuclear level densities at about 9 MeV excitation, it is probably necessary to take into account a few higher shells. However the effects of the truncation are studied later.

The constants M_{nn}, M_{np} and M_{pp} were chosen to be

$$M_{nn} = M_{pp} = - \frac{\sum_{AB} [(j_A+\frac{1}{2})(j_B+\frac{1}{2})]^{\frac{1}{2}} F^{nn}(AABBO)}{\sum_{AB} (j_A+\frac{1}{2})(j_B+\frac{1}{2})}$$

$$= - 0.174 \text{ MeV} ,$$

$$M_{np} = - \frac{\sum_{AB} [(j_A+\frac{1}{2})(j_B+\frac{1}{2})]^{\frac{1}{2}} F^{np}(AABBO)}{\sum_{AB} (j_A+\frac{1}{2})(j_B+\frac{1}{2})}$$

$$= - 0.380 \text{ MeV} .$$

The G and F matrix elements of the potential, after the introduction of the auxiliary Hamiltonian are given in table 3.

At zero temperature, the occupation probability f_a is zero and therefore, the zero-temperature calculation for the ground state of a given even-even nucleus were done by the usual BCS iteration method. There are no pairing correlations on the proton side . Z = 50 being a closed shell, the protons have a large energy gap (~ 5 MeV) between the occupied $0g_{9/2}$ orbital and the empty $1d_{5/2}$ orbital and therefore show no pairing correlations. The single particle energies of ^{116}Sn, ^{118}Sn and ^{120}Sn corrected for the self-energies μ_a are given in table 4.

The following procedure works well in performing a temperature dependent BCS calculation. For a given temperature and a given nucleus, we guess values for ρ_A and k_A. They provide trial values for μ_A and Δ_A:

$$\mu_A(i) = 2 \sum_{B,j} [(j_B+\tfrac{1}{2})/(j_A+\tfrac{1}{2})]^{\frac{1}{2}} F^{ij}(AABBO)\ \rho_B(j) ,$$

$$\Delta_A(i) = \sum_B [(j_B+\tfrac{1}{2})/(j_A+\tfrac{1}{2})]^{\frac{1}{2}} \; G(AABBO) \; k_B(i) \; .$$

The chemical potential is then fixed by demanding that

$$N_i = \sum_A (j_A+\tfrac{1}{2}) \left[1 - \frac{\varepsilon_A(i) - \mu_A(i) - \lambda_i}{[(\varepsilon_A(i)-\mu_A(i)-\lambda_i)^2 + \Delta_A(i)^2]^{\frac{1}{2}}}\right.$$

$$\left. \times \left(1 - \frac{2}{\exp\{\beta[(\varepsilon_A(i) - \mu_A(i) - \lambda_i)^2 + \Delta_A^2]^{\frac{1}{2}}\} + 1}\right)\right] .$$

One can now recalculate ρ_A and k_A from Eqs. (II.29) and (II.30). The procedure is then repeated until self-consistency is achieved.

Calculations of state and level densities were performed for a given sequence of temperatures. The values of ρ_A and k_A at a certain temperature were used to obtain the trial values of μ_A and Δ_A for the next higher temperature. As expected, the pairing correlations Δ_A for neutrons dropped as a function of temperature.

The excitation energy corresponding to the given temperature is

$$E^*(T) = E(T) - E(0) \; ,$$

where $E(T)$ is the energy at temperature T and $E(0)$ is the energy for $T = 0$.

TABLE 1. Single-particle energies in MeV. The nucleus ^{56}Ni is taken to be the closed shell.

Orbit	Protons	Neutrons
$1p_{3/2}$	7.64	7.11
$0f_{5/2}$	9.14	8.03
$1p_{1/2}$	9.90	8.52
$0g_{9/2}$	8.12	8.83
$1d_{5/2}$	10.00	9.46
$0g_{7/2}$	11.83	11.97
$2s_{1/2}$	9.99	9.11
$1d_{3/2}$	10.47	11.00
$0h_{11/2}$	10.66	11.66
$0h_{9/2}$	14.96	13.24
$1f_{7/2}$	12.50	12.31
$0i_{13/2}$	14.92	14.66

TABLE 2. The G and F matrix-elements of the residual interaction of Kahana, Lee and Scott[48].

	$1p_{3/2}$	$0f_{5/2}$	$1p_{1/2}$	$0g_{9/2}$	$1d_{5/2}$	$0g_{7/2}$	$2s_{1/2}$	$1d_{3/2}$	$0h_{11/2}$	$0h_{9/2}$	$1f_{7/2}$	$0i_{13/2}$
G(AABBO)	0.900	0.515	1.022	0.523	0.516	0.608	0.126	0.699	0.504	0.611	0.163	0.418
	0.515	0.392	0.211	1.641	0.494	0.280	0.171	0.080	1.278	0.175	0.606	0.914
	1.022	0.211	0.177	0.518	0.654	0.264	0.089	0.141	0.515	0.258	0.239	0.444
	0.523	1.641	0.518	0.581	0.315	1.724	0.202	0.495	0.422	1.557	0.141	0.276
	0.516	0.494	0.654	0.315	0.607	0.517	0.303	1.033	0.374	0.597	0.385	0.375
	0.608	0.280	0.264	1.724	0.517	0.195	0.181	0.155	1.551	0.107	0.481	1.259
	0.126	0.171	0.089	0.202	0.303	0.181	0.840	0.247	0.238	0.217	0.363	0.262
	0.699	0.080	0.141	0.495	1.033	0.155	0.247	0.185	0.565	0.203	0.761	0.567
	0.504	1.278	0.515	0.422	0.374	1.551	0.238	0.565	0.315	1.594	0.196	0.201
	0.611	0.175	0.258	1.557	0.597	0.107	0.217	0.203	1.594	0.024	0.499	1.453
	0.163	0.606	0.239	0.141	0.385	0.481	0.363	0.761	0.196	0.499	0.398	0.242
	0.418	0.914	0.444	0.276	0.375	1.259	0.262	0.587	0.201	1.453	0.242	0.108
F^{nn}(AABBO)	0.702	0.549	0.672	0.548	0.632	0.567	0.509	0.476	0.504	0.525	0.541	0.464
	0.549	0.342	0.266	1.522	0.598	0.308	0.254	0.258	1.390	0.261	0.684	1.184
= F^{pp}(AABBO)	0.672	0.266	0.089	0.494	0.728	0.272	0.136	0.119	0.469	0.243	0.567	0.442
	0.548	1.522	0.494	0.755	0.548	1.517	0.317	0.651	0.694	1.341	0.514	0.654
	0.632	0.598	0.728	0.548	0.582	0.615	0.436	0.787	0.511	0.635	0.540	0.473
	0.567	0.308	0.272	1.517	0.615	0.296	0.255	0.288	1.553	0.266	0.637	1.456
	0.509	0.254	0.136	0.317	0.436	0.255	0.420	0.261	0.303	0.266	0.370	0.293
	0.476	0.258	0.119	0.651	0.787	0.288	0.261	0.147	0.600	0.292	0.855	0.580
	0.504	1.390	0.469	0.694	0.511	1.553	0.303	0.600	0.646	1.524	0.497	0.609
	0.525	0.261	0.243	1.341	0.635	0.266	0.266	0.292	1.524	0.250	0.656	1.569
	0.541	0.684	0.567	0.514	0.540	0.637	0.370	0.855	0.497	0.656	0.490	0.465
	0.464	1.184	0.442	0.654	0.473	1.456	0.293	0.580	0.609	1.569	0.465	0.558
F^{np}(AABBO)	1.764	1.150	1.581	1.275	1.409	1.198	0.888	1.313	1.188	1.161	0.999	1.049
	1.150	1.409	0.702	2.914	1.233	1.318	0.560	0.756	2.432	1.141	1.395	1.911
	1.581	0.702	0.510	1.029	1.322	0.715	0.501	0.555	0.975	0.667	0.863	0.873
	1.275	2.914	1.029	2.143	1.227	3.030	0.661	1.212	1.946	2.703	1.170	1.700
	1.409	1.233	1.322	1.227	1.521	1.209	0.856	1.726	1.199	1.254	1.282	1.131
	1.198	1.318	0.715	3.030	1.209	1.347	0.557	0.787	2.840	1.264	1.237	2.469
	0.888	0.560	0.501	0.661	0.856	0.557	1.248	0.600	0.661	0.577	0.802	0.655
	1.313	0.756	0.555	1.212	1.726	0.787	0.600	0.709	1.183	0.796	1.530	1.159
	1.188	2.432	0.975	1.946	1.199	2.840	0.661	1.183	1.933	2.860	1.139	1.785
	1.161	1.141	0.667	2.703	1.254	1.261	0.577	0.796	2.860	1.259	1.222	2.761
	0.999	1.395	0.863	1.170	1.282	1.237	0.802	1.530	1.139	1.222	1.331	1.108
	1.049	1.911	0.873	1.700	1.131	2.469	0.655	1.159	1.785	2.761	1.108	1.739

TABLE 3. The new G and F matrix elements of the residual interaction after the introduction of the auxiliary Hamiltonian (section II.4).

	$1p_{3/2}$	$0f_{5/2}$	$1p_{1/2}$	$0g_{9/2}$	$1d_{5/2}$	$0g_{7/2}$	$2s_{1/2}$	$1d_{3/2}$	$0h_{11/2}$	$0h_{9/2}$	$1f_{7/2}$	$0i_{13/2}$
G(AABBO)	0.726	0.515	1.022	0.523	0.516	0.608	0.126	0.699	0.504	0.611	0.163	0.418
	0.515	0.218	0.211	1.641	0.494	0.280	0.171	0.080	1.278	0.175	0.606	0.914
	1.022	0.211	0.603	0.518	0.654	0.264	0.089	0.141	0.515	0.258	0.239	0.444
	0.523	1.641	0.518	0.407	0.315	1.724	0.202	0.495	0.422	1.557	0.141	0.276
	0.516	0.494	0.654	0.315	0.433	0.517	0.303	1.033	0.374	0.597	0.385	0.375
	0.608	0.280	0.264	1.724	0.517	0.021	0.181	0.155	1.551	0.107	0.481	1.259
	0.126	0.171	0.089	0.202	0.303	0.181	0.666	0.247	0.238	0.217	0.363	0.262
	0.699	0.080	0.141	0.495	1.033	0.155	0.247	0.012	0.565	0.203	0.761	0.567
	0.504	1.278	0.515	0.422	0.374	1.551	0.238	0.565	0.141	1.594	0.196	0.201
	0.611	0.175	0.258	1.557	0.597	0.107	0.217	0.203	1.594	-0.150	0.499	1.453
	0.163	0.606	0.239	0.141	0.385	0.481	0.363	0.761	0.196	0.499	0.225	0.242
	0.418	0.914	0.444	0.276	0.375	1.259	0.262	0.587	0.201	1.453	0.242	-0.066
F^{nn}(AABBO)	0.442	0.123	0.426	-0.001	0.206	0.075	0.263	0.128	-0.098	-0.025	0.050	-0.186
	0.123	-0.092	-0.035	0.850	0.077	-0.294	-0.046	-0.168	0.653	-0.412	0.082	0.387
= F^{pp}(AABBO)	0.426	-0.035	0.002	0.105	0.427	-0.076	-0.038	-0.127	0.044	-0.146	0.220	-0.017
	-0.001	0.850	0.105	-0.027	-0.124	0.741	-0.071	0.101	-0.257	0.473	-0.263	-0.374
	0.206	0.077	0.427	-0.124	0.147	0.013	0.135	0.362	-0.226	-0.036	-0.062	-0.323
	0.075	-0.294	-0.076	0.741	0.013	-0.312	-0.092	-0.203	0.701	-0.511	-0.058	0.537
	0.263	-0.046	-0.038	-0.071	0.135	-0.092	0.333	0.016	-0.122	-0.123	0.023	-0.167
	0.128	-0.168	-0.127	0.101	0.362	-0.203	0.016	-0.113	-0.002	-0.258	0.363	-0.070
	-0.098	0.653	0.044	-0.257	-0.226	0.701	-0.122	-0.002	-0.310	0.572	-0.354	-0.517
	-0.025	-0.412	-0.146	0.473	-0.038	-0.511	-0.123	-0.258	0.572	-0.531	-0.121	0.541
	0.050	0.082	0.220	-0.263	-0.062	-0.058	0.023	0.363	-0.354	-0.121	-0.118	-0.454
	-0.186	0.387	-0.017	-0.374	-0.323	0.537	-0.167	-0.070	-0.517	0.541	-0.454	-0.571
F^{np}(AABBO)	1.005	0.220	1.044	0.073	0.479	0.123	0.351	0.554	-0.129	-0.041	-0.076	-0.373
	0.220	0.269	0.044	1.442	0.093	0.001	-0.098	-0.175	0.820	-0.331	0.078	0.170
	1.044	0.044	0.130	0.179	0.664	-0.045	0.121	0.018	0.045	-0.182	0.104	-0.132
	0.073	1.442	0.179	-0.243	-0.245	1.330	-0.188	0.011	-0.135	0.804	-0.529	-0.548
	0.479	0.093	0.664	-0.245	0.381	-0.107	0.198	0.795	-0.413	-0.217	-0.035	-0.610
	0.123	0.001	-0.045	1.330	-0.107	-0.173	-0.203	-0.287	0.979	-0.438	-0.283	0.458
	0.351	-0.098	0.121	-0.188	0.198	-0.203	0.869	0.063	-0.270	-0.272	0.042	-0.350
	0.554	-0.175	0.018	0.011	0.795	-0.287	0.063	-0.051	-0.133	-0.405	0.455	-0.263
	-0.129	0.820	0.045	-0.135	-0.413	0.979	-0.270	-0.133	-0.346	0.779	-0.723	-0.678
	-0.041	-0.331	-0.182	0.804	-0.217	-0.438	-0.272	-0.405	0.779	-0.640	-0.477	0.513
	-0.076	0.078	0.104	-0.529	-0.035	-0.283	0.042	0.455	-0.723	-0.477	-0.189	-0.902
	-0.373	0.170	-0.132	-0.548	-0.610	0.458	-0.350	-0.263	-0.678	0.513	-0.902	-0.921

TABLE 4. Values of $\varepsilon_a - \mu_a$ in MeV at zero temperature for ^{116}Sn, ^{118}Sn and ^{120}Sn. The fermi level is denoted by λ.

Orbit	^{116}Sn		^{118}Sn		^{120}Sn	
	Proton	Neutron (λ=8.98)	Proton	Neutron (λ=9.31)	Proton	Neutron (λ=9.62)
$1p_{3/2}$	-0.12	0.24	-0.26	0.19	-0.37	0.16
$0f_{5/2}$	1.95	1.39	1.81	1.32	1.64	1.22
$1p_{1/2}$	2.16	1.86	2.07	1.85	2.00	1.86
$0g_{9/2}$	2.49	3.78	2.38	3.74	2.31	3.72
$1d_{5/2}$	7.58	7.32	7.55	7.30	7.54	7.29
$0g_{7/2}$	7.85	8.00	7.75	7.95	7.61	7.86
$2s_{1/2}$	8.80	8.40	8.77	8.39	8.81	8.42
$1d_{3/2}$	8.75	9.99	8.78	10.01	8.83	10.04
$0h_{11/2}$	9.07	10.05	9.07	10.04	9.09	10.05
$0h_{9/2}$	14.85	12.91	14.85	12.91	14.80	12.89
$1f_{7/2}$	14.38	13.74	14.51	13.78	14.64	13.82
$0i_{13/2}$	17.09	16.20	17.20	16.25	17.32	16.31

III.1 Results

Figure 1 shows the energy dependence of the density of states for the nuclei ^{116}Sn, ^{118}Sn and ^{120}Sn. For even Sn-isotopes, the experimentally measured quantity is

$$\rho = \rho(E,\ I = 0,\ +) + \rho(E,\ I = 1,\ +).$$

In figure 2, ρ for ^{116}Sn, ^{118}Sn and ^{120}Sn are plotted against excitation energy. The experimental values of ρ for each of the three nuclei at neutron separation energies[49] are also shown in the figure. It is seen that our calculation underestimates the level densities by a factor of thirty or worse. Discrepancies of the order of 100 for these isotopes have been mentioned in the literature before[31].

For the nucleus ^{116}Sn, calculations were also done assuming no pairing correlation to exist. Figure 3 compares the state densities for ^{116}Sn calculated with and without pairing. It is seen that the density of states is much higher if no pairing correlation is assumed to exist.

Simple pairing force calculations (Section II.7) were also performed for the three Sn isotopes to determine if there were significant deviations from our calculation with realistic matrix elements. To do this comparison, we obtained the quantities $\epsilon_a - \mu_a$ from our zero temperature calculations (Table 4). With these fixed, a pairing force calculation was done in which the value of g_n was varied. (Since there is no pairing on the proton side, the value of g_p is immaterial).

For a value of g_n = 0.1495 MeV, the pairing force calculation for ^{116}Sn gives a density of states which is indistinguishable from our calculation except at and near the critical temperature (Fig. 4). The density of states obtained from the pairing force calculation has an abrupt rise at the critical temperature. This is due to the fact that in a pairing force calculation, the gap parameter Δ decreases with temperature until, at and above a critical temperature, $\Delta = 0$ and the pairing correlation disappears altogether (Fig. 5). The value of $D_{\beta\beta}$ (Eqs. (II.1) and (II.6)) decreases suddenly at this temperature resulting in a sudden increase in the density of states. In our calculation with realistic matrix elements, the gap parameter Δ_A has different values for different orbitals and therefore all of them do not vanish at the same temperature although they do vanish within a small range of temperature.

Pairing force calculations were also performed for the nuclei ^{118}Sn and ^{120}Sn taking the same value of g_n. The density of states for these nuclei were found to be almost identical to that obtained for ^{116}Sn. On the other hand, our calculation with realistic matrix elements gave different state densities for these three nuclei (Fig. 1).

Calculations done in this chapter show that it is possible to incorporate realistic interactions in computing nuclear level density. However, our results thus far have grossly underestimated the experimental data. The reasons

for this are explored in the following chapters. It is tempting to put the blame on the matrix elements used. However, this is unlikely to be the reason as Lee[42,47] fits low energy data quite well. Another possibility is that the grand partition function approach is very inaccurate or that not enough number of configurations have been included in the model space. We investigate these possibilities in the next chapter. The third possibility is the most interesting one. In our calculations we assumed that Sn isotopes are spherical in the ground state (zero temperature) as well as at finite temperature. The question of possibility of shape change at finite temperature is dealt with in chapter V; the resulting change in level density is quite profound.

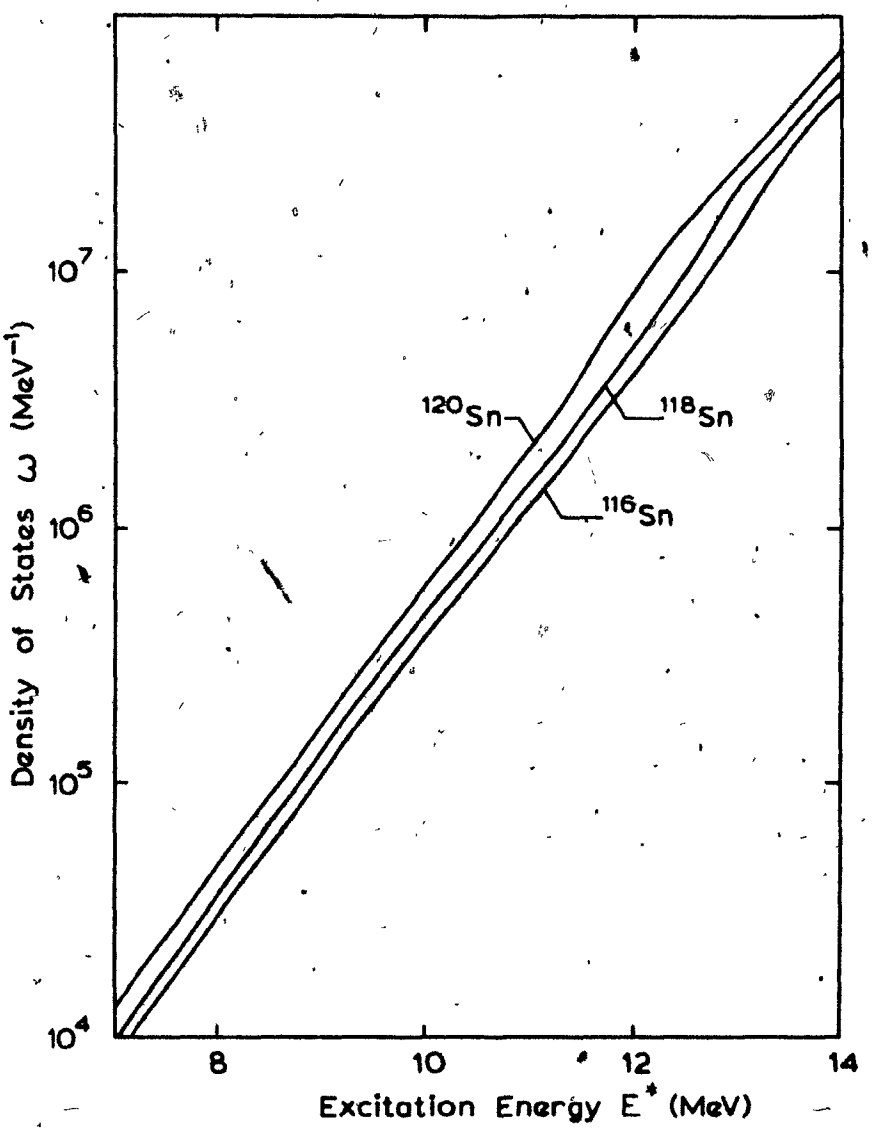

FIGURE 1. The energy dependence of the density of states for the nuclei (a) ^{116}Sn, (b) ^{118}Sn and (c) ^{120}Sn; ω includes a sum over states of both parities and all spins and all magnetic substates.

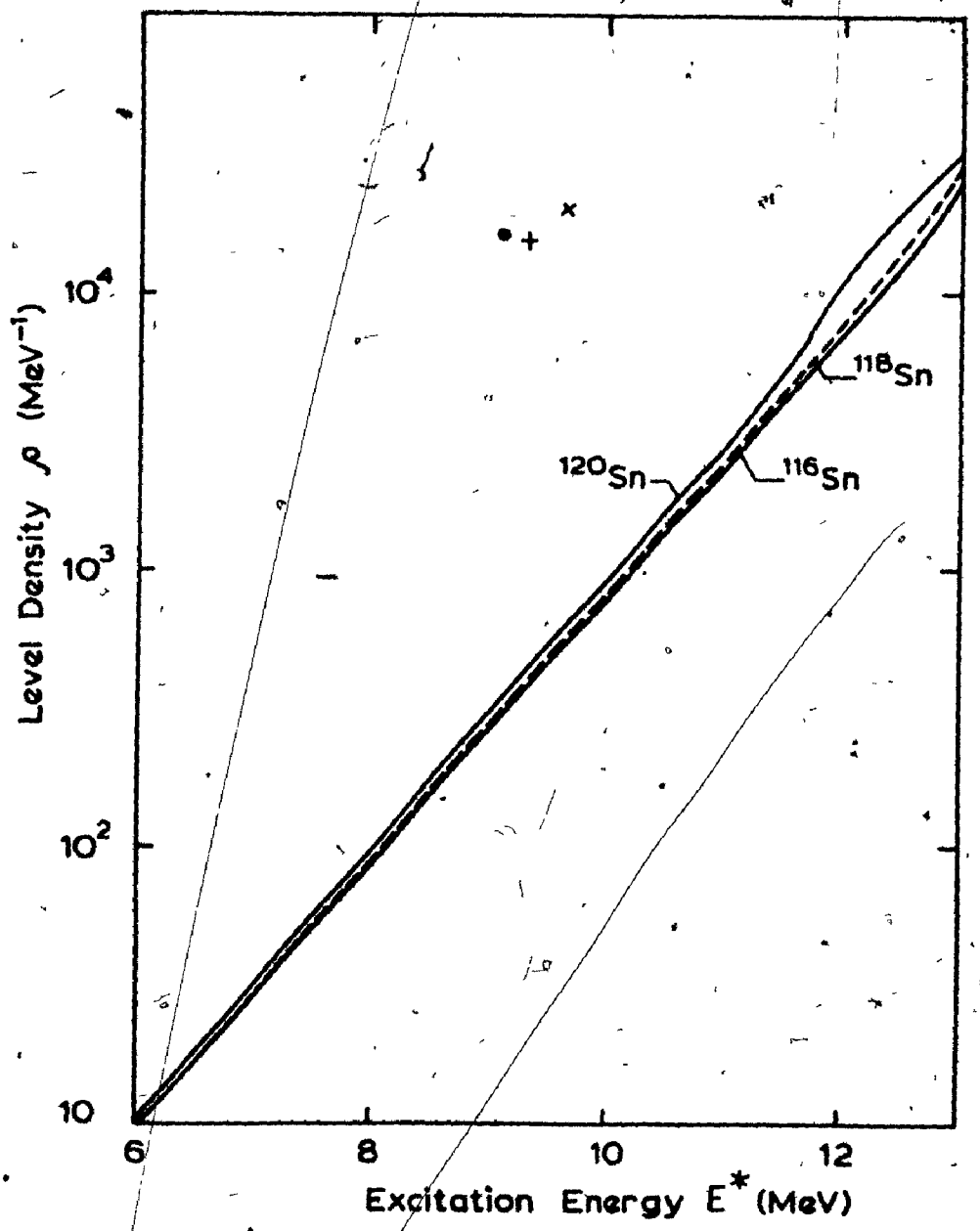

FIGURE 2. The level densities for the nuclei (a) ^{116}Sn, (b) ^{118}Sn and (c) ^{120}Sn; ρ is a sum over the levels of spins 0^+ and 1^+ with only one magnetic substate included for each spin. The experimental values of ρ for these nuclei are denoted by the symbols x, + and o respectively[49].

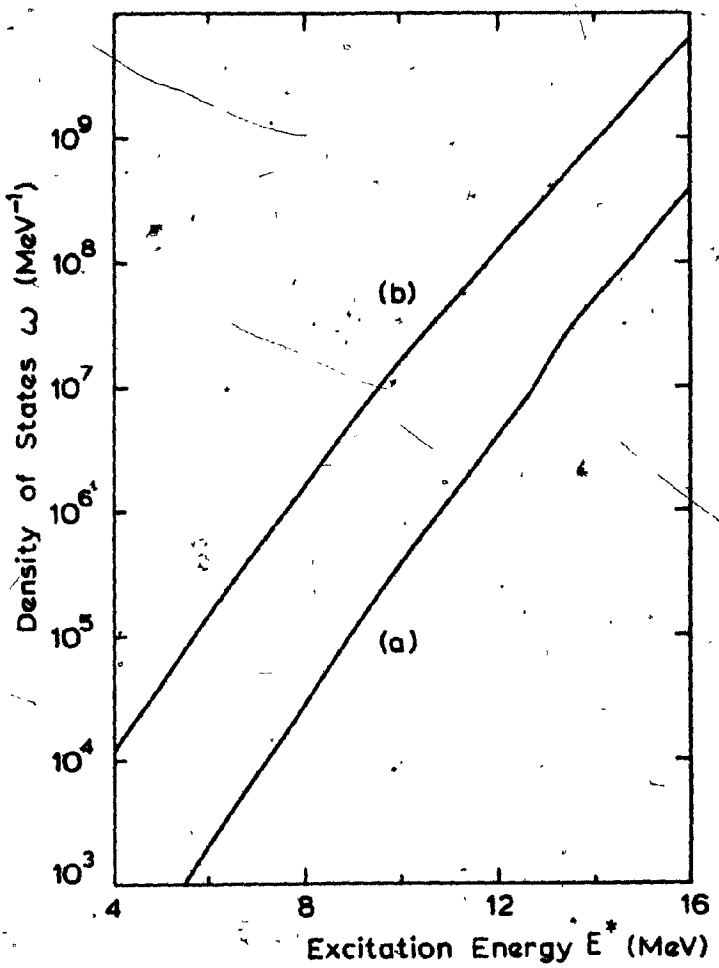

FIGURE 3. Comparison of the calculated density of states for the nucleus ^{116}Sn; (a) with pairing and (b) without pairing.

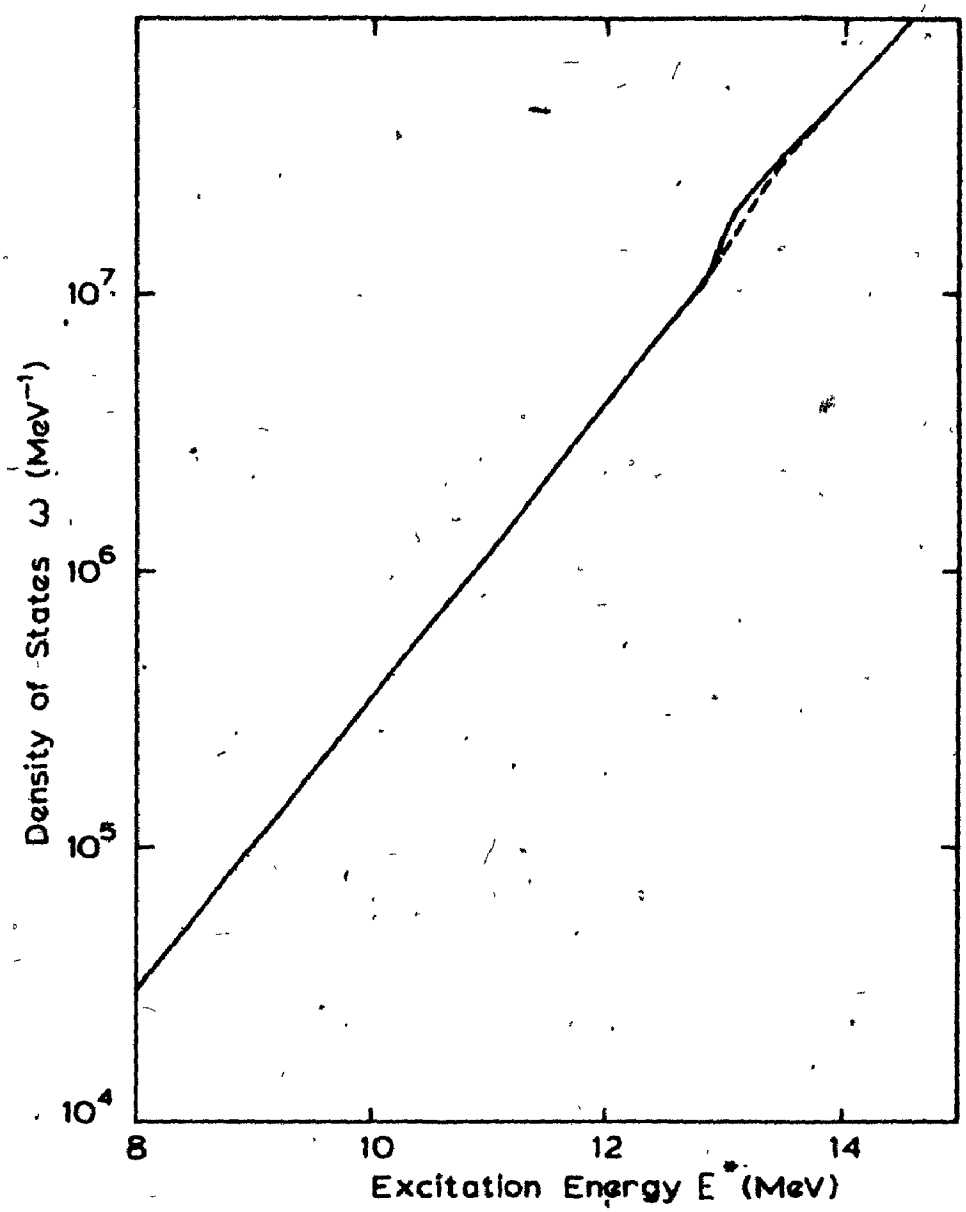

FIGURE 4. Density of states for the nucleus ^{116}Sn obtained from a pure pairing force calculation with $g_n = 0.1495$ MeV. The dashed line represents the calculation with realistic matrix elements and is the same as in Figure 1(a).

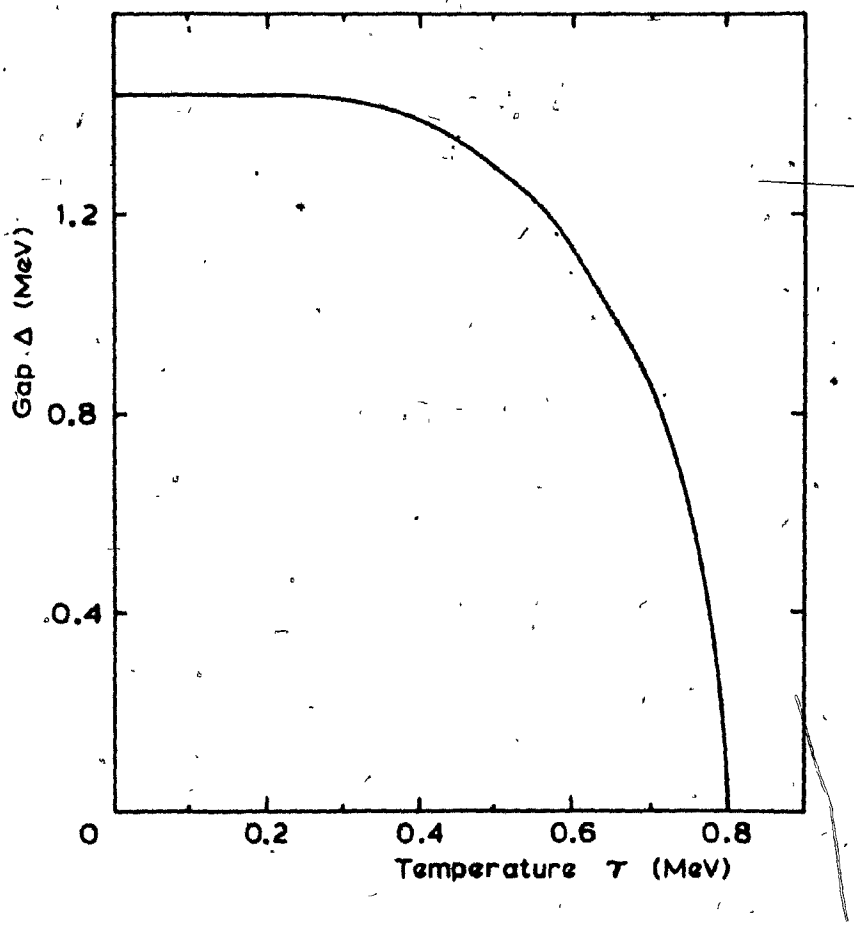

FIGURE 5. The temperature dependence of the gap parameter Δ for the nucleus ^{116}Sn. The pairing constant g_n is taken to be 0.1495 MeV.

CHAPTER IV

IV.1 Accuracy of the grand partition function approach.

The purpose of the work done in this chapter is to obtain some idea of the accuracy in a grand partition function approach. For the calculations in this chapter, we take a pure pairing force.

The model space for which exact calculations are to be done must be semi-realistic. A completely realistic valence space is too large to handle exactly. Exact calculations, therefore, were done in a moderately large space.

The two nuclei studied are ^{116}Sn and ^{117}Sn. These are regarded as 16 and 17 neutrons in the orbitals $1d_{5/2}$, $0g_{7/2}$, $2s_{1/2}$, $0h_{11/2}$ and $1d_{3/2}$. The single particle energies for neutrons are taken from Kisslinger and Sorensen[52] and are listed in Table 5. The pairing force strength is $g = 23/A$ MeV. The exact diagonizations were done using Kerman's quasi-spin formalism[52]. In spite of the simplification that this formalism provides, some of the matrices were quite large. The largest matrix in the case of ^{116}Sn was 110x110. The code for doing exact calculations with a pairing force was developed by B.C. Smith[50].

The results of matrix diagonalization are shown in the form of histograms in Figs. 6 and 7. Exact level densities obtained from a pure pairing force exhibit significant fluctuations. Some of these fluctuations are not real but rather

result from the simple nature of the pairing force which leads to many degeneracies. It is desirable to smooth these fluctuations in order to compare with results from approximate grand partition function method which provides a smoothed density. We smooth the exact level density by using the saddle-point method. This requires the following steps. From the exact eigenvalues one can obtain

$$Z_c(\beta) = \Sigma\, e^{-\beta E_i} .$$

The exact density is related to Z_c by

$$\rho(E) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} Z_c(\beta)\, e^{\beta E}\, d\beta .$$

The integral is evaluated by the saddle-point method and leads to

$$\rho(E) = \exp[\ell n\ Z_c(\beta_0) + \beta_0\, E] / [2\pi(\langle E^2\rangle - E^2)]^{\frac{1}{2}} ,$$

where

$$E = \Sigma\, E_i\, e^{-\beta_0 E_i} / Z_c(\beta_0) ,$$

$$\langle E^2\rangle = \Sigma\, E_i^2\, e^{-\beta E_i} / Z_c(\beta_0) .$$

In the present context, the main feature of the saddle-point method is that it converts a discrete density into a smooth one.

The smoothed densities obtained from the exact calculations are given in Table 6.

Using the same set of single-particle energies and the same pairing force, level densities for ^{116}Sn and ^{117}Sn were also calculated by the approximate grand partition function method (Section II.7). These level densities are compared with smoothed exact densities in Figs. 8 and 9. The approximate method is correct to within a factor of two. One feature of the approximate calculation is that it underestimates the level density below the critical temperature and overestimates it above the critical temperature.

If we now compare the exact model space calculation with experimental data[49], we find that we underestimate the experimental densities by a factor of 25 in both ^{116}Sn and ^{117}Sn. The first remedy that comes to mind is to increase the valence space. In this increased space (see Table 7), exact calculations are not possible. We use the approximate grand partition function method of Section II.7 since it was a reasonable approximation in the model space. (For the level density of odd-particle system, see Appendix X). When increasing the valence space, the value of the pairing constant g has to be decreased such that the gap Δ at zero temperature remains unchanged. The results of the larger space calculations for ^{116}Sn are shown in Fig. 10. There is no significant improvement in the results from our previous calculation with realistic matrix elements. It is possible

to obtain the correct experimental data by further reducing the value of g by more than 20%. However, this reduces the value of Δ to unacceptably low values.

TABLE 5. Neutron shell model energies for exact calculation in model space.

Orbital	Energy (MeV)
$1d_{5/2}$	0
$0g_{7/2}$	0.8
$2s_{1/2}$	1.3
$0h_{11/2}$	2.5
$1d_{3/2}$	2.8

TABLE 6. The smoothed state density $\omega(E)$ and smoothed level density $\rho(E,I,\pi)$ for ^{116}Sn and ^{117}Sn resulting from an exact calculation in the model space.

Excitation Energy	^{116}Sn		^{117}Sn	
(MeV)	$\omega(E)$ (MeV^{-1})	$\rho(E,0^+)+\rho(E,1^+)$ (MeV^{-1})	$\omega(E)$ (MeV^{-1})	$\rho(E,\frac{1}{2}^+)$ (MeV^{-1})
5	3×10^3	-	2×10^4	-
6	1.3×10^4	-	7×10^4	-
7	4.7×10^4	1×10^2	2.3×10^5	2×10^2
8	1.4×10^5	3×10^2	6.5×10^5	4×10^2
9	4.2×10^5	6×10^2	1.6×10^6	9×10^2
10	1.1×10^6	1×10^3	3.7×10^6	2×10^3
11	2.6×10^6	3×10^3	7.5×10^6	4×10^3
12	5.4×10^6	6×10^3	1.4×10^7	7×10^3
13	1.0×10^7	1.1×10^4	2.3×10^7	1.0×10^4
14	1.9×10^7	1.8×10^4	3.4×10^7	1.6×10^4
15	3.0×10^7	3×10^4	4.8×10^7	2.1×10^4

TABLE 7. Shell model energies used in full space calculations. These energies were calculated for a spherical Woods-Saxon potential well[a]. The energy scale for the neutrons has been shifted so that the $1d_{5/2}$ orbital has zero energy.

Orbital	Energy (MeV)	
	Proton	Neutron
$0f_{7/2}$	-15.695	-
$0f_{5/2}$	-11.224	-
$1p_{3/2}$	-10.759	-
$1p_{1/2}$	- 9.637	-
$0g_{9/2}$	- 7.701	-4.66
$1d_{5/2}$	- 2.508	0.0
$0g_{7/2}$	- 2.489	0.8
$2s_{1/2}$	- 0.669	1.3
$1d_{3/2}$	- 0.750	2.8
$0h_{11/2}$	-	2.5
$1f_{7/2}$	-	7.68
$2p_{3/2}$	-	8.92
$2p_{1/2}$	-	9.63
$1f_{5/2}$	-	10.24
$0h_{9/2}$	-	10.28

(a) N.B. de Takacsy, private communication, 1977.

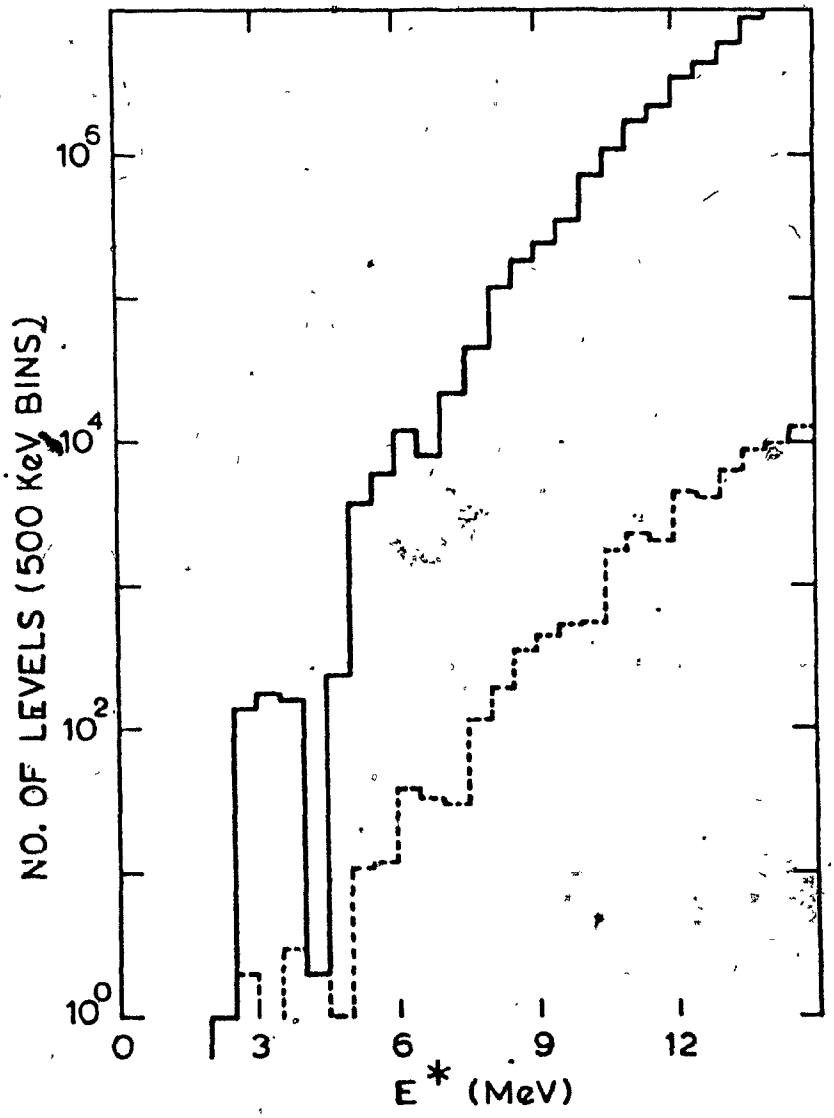

FIGURE 6. Histogram of energy levels for ^{116}Sn. The solid line represents the state density ω. The dashed line represents the level density ρ. It is a sum over the levels of spin 0^+ and 1^+ with only one magnetic substate included for each spin.

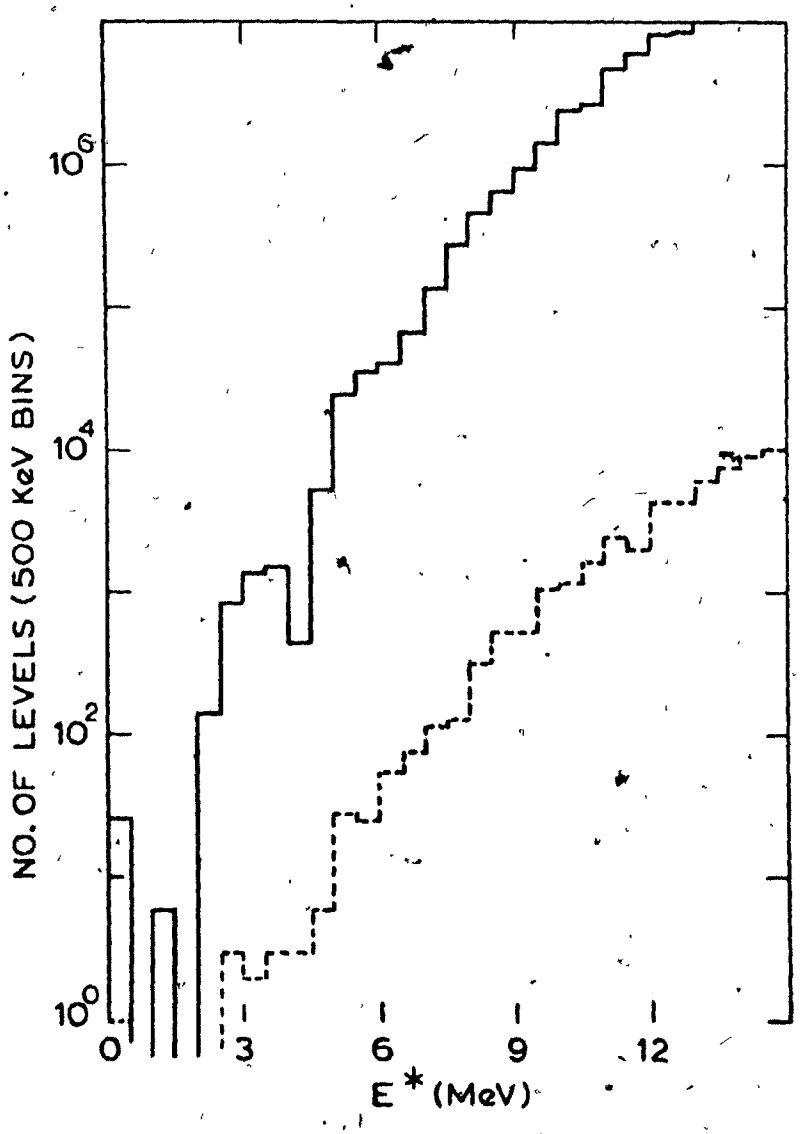

FIGURE 7. Histogram of energy levels for ^{117}Sn. The solid line represents the state density ω. The dashed line represents the level density ρ for spin $\frac{1^+}{2}$.

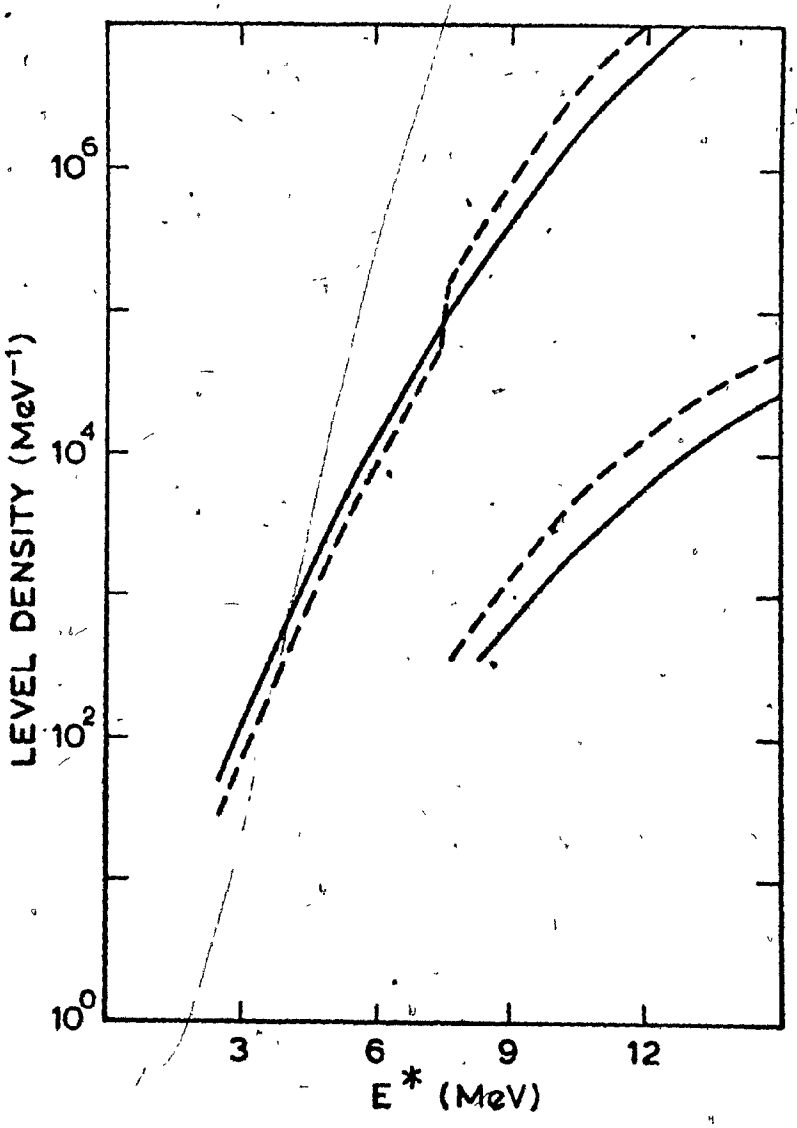

FIGURE 8. State density and level density for ^{116}Sn. The solid lines represent the densities obtained by smoothing the exact results by the saddle-point method. They correspond to the histograms in Figure 6. The dashed lines represent the approximate densities obtained from the grand partition function method.

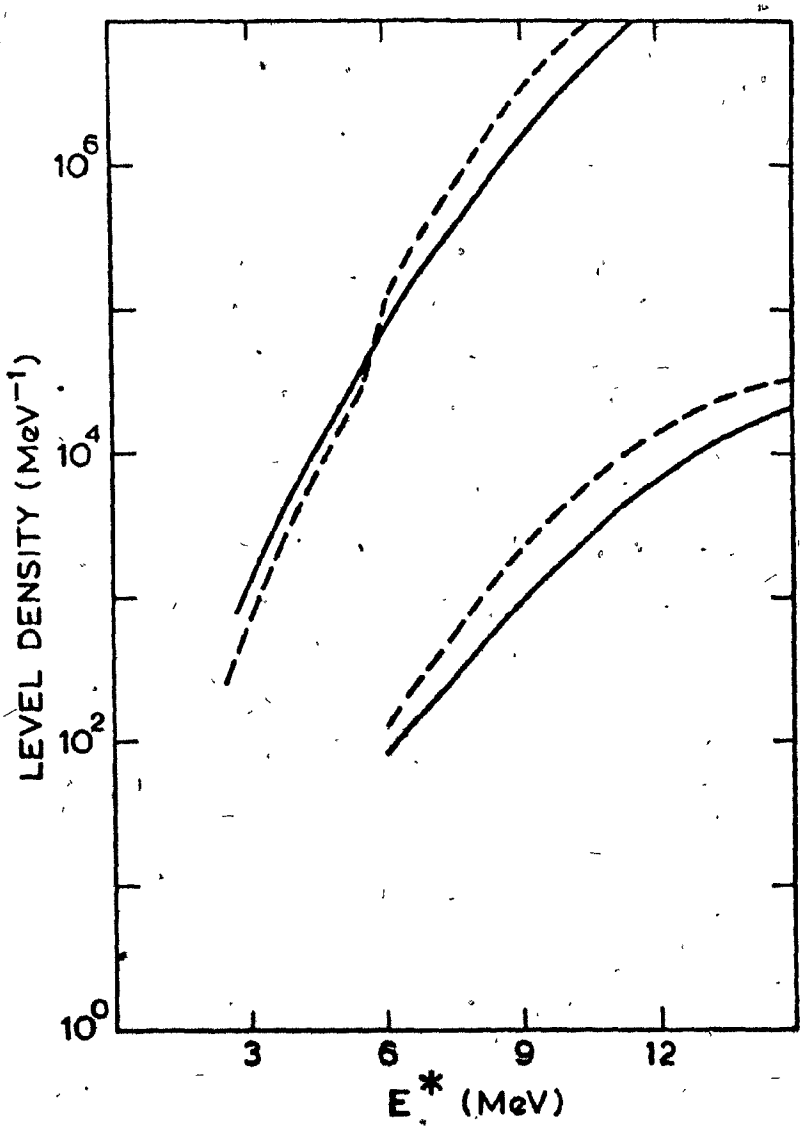

FIGURE 9. State density and level density for ^{117}Sn as described in caption to Figure 8.

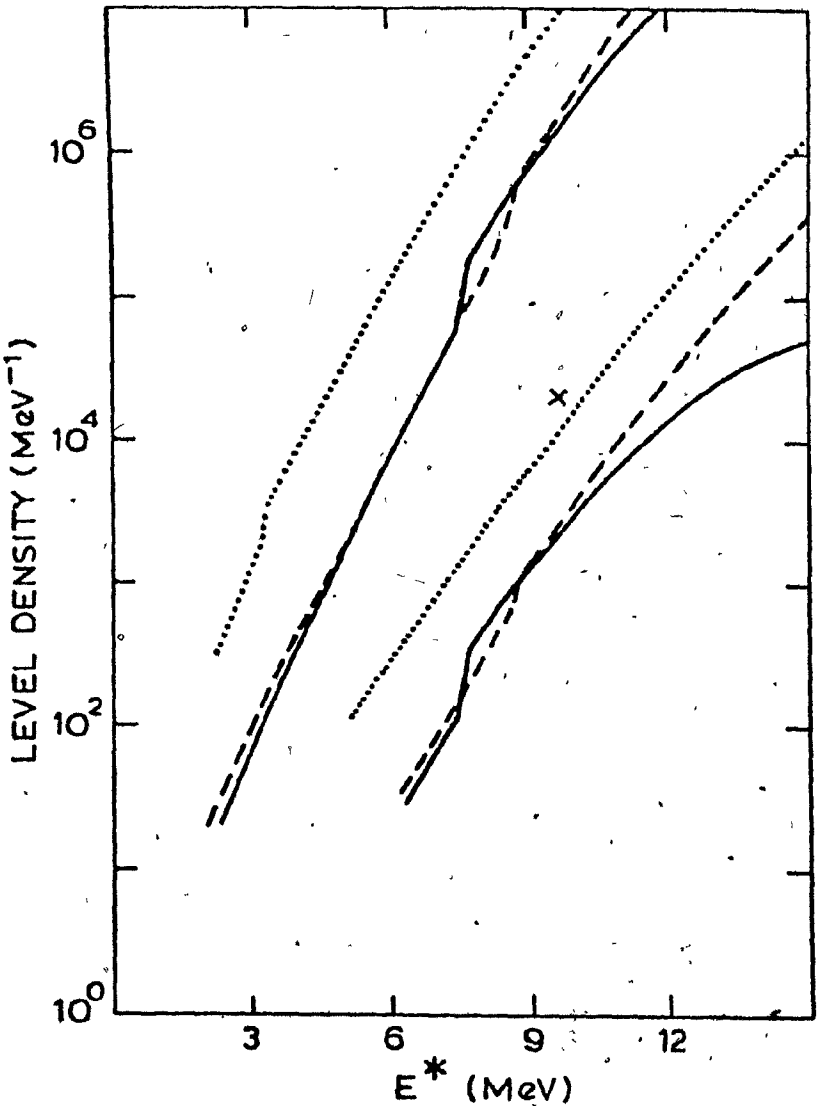

FIGURE 10. State density and level density for ^{116}Sn resulting from the grand partition function method. The solid lines are the same as the dotted lines in Figure 8 and result from a calculation in the semi-realistic space defined in Table 5. The dashed lines give the results for the full space (Table 7). The dotted lines are obtained by repeating the full space calculation but with the pairing force reduced by 20%. This gives closer agreement with the experimental value indicated by x. Unfortunately this reduces the pairing gap Δ from 1.234 MeV to the unrealistically low value of 0.714 MeV.

IV.2 Discussion

We thus reach the conclusion that provided one takes realistic single particle energies and reasonable values of the pairing force, the spherical model will grossly underestimate level densities in Sn isotopes. Indeed, in fitting nuclear level density data over a wide range of the nuclear periodic table, Dossing and Jensen[31] also found a similar discrepancy for Sn isotopes. One reason for this failure may be the following interesting possibility. As is well established, the Sn isotopes are spherical in the ground state. The formalism developed here, assumes, as most other calculations do, that nuclei which are spherical in the ground state, remain so at higher excitation energy. If however a large number of excited intrinsic states at about 8 MeV in these nuclei are deformed, then rotational states built upon these deformed intrinsic states will lead to a large increase in level density. Such increase can be as high as a factor of forty[31,34] in the well deformed region.

It is well-known that the major features of the residual interaction can be simulated by two forces--the pairing force and the quadrupole force. So long as the nucleus remains spherical, the quadrupole force makes no contribution to the energy of the system. The deformation of a nucleus is the result of two competing effects: the pairing force

which tends to make nuclei spherical and the quadrupole force which favors deformation. In Sn isotopes, at zero temperature the pairing force dominates and a spherical shape is favored. However, as mentioned earlier, the pairing effect decreases with increasing temperature and Δ drops in value as a function of temperature. But if the effect of pairing force is reduced, what keeps the nucleus from deforming? Of course, finite temperature tends to wash out the effects of the quadrupole force as well; however, it is a matter of differential effects that one has to study. This can be investigated by adding the quadrupole force to the pairing Hamiltonian and calculating the energy surface against deformation at zero temperature (ground state) as well as at finite temperature (excited states). At zero temperature, the shape is spherical; at finite but still low temperature, the pairing effect is weakened and the quadrupole force may take over, giving preference to a deformed shape over the spherical one. Provided nuclei do favor deformation, it is clear that a different formalism should be used to calculate level density at the appropriate excitation energy.

The formalism developed in chapter II to calculate the level densities for spherical nuclei may be generalized to include cases where shape transitions can occur. However, numerical calculations become difficult with generalized interactions. Therefore, to study the effect of deformation on nuclear level densities, we are constrained to use a

pairing plus quadrupole force instead of the general two-body interaction.

Quite apart from the question of level density, the possibility of deformation at finite temperature in a nucleus which is spherical in its ground state is interesting in itself.

CHAPTER V

V.1 Pairing plus quadrupole force at finite temperature.

We take the quadrupole force to be

$$V(1,2) = -\chi r_1^2 . r_2^2 \sum_{\mu} Y_{2\mu}(1)\, Y^*_{2\mu}(2) \qquad (V.1)$$

The other part of the residual interaction is the pairing force. At zero temperature, the energy vs. axially symmetric deformation can be studied[53,54] by the following procedure.

(1) Diagonalize the one-body Hamiltonian

$$H = H_0 - Dr^2 Y_{20} \qquad (V.2)$$

to obtain eigenvalues ε_a. Here H_0 is the shell model part and D is a parameter. If we equate $D = m\omega^2\beta_2$, where ω is the appropriate oscillator frequency, then β_2 is closely related to the quadrupole deformation parameter of the Nilsson model.

(2) The pairing force problem is now solved on these deformed orbitals. This means one solves the number equation and the gap equation:

$$N = \sum_{a>0} \left(1 - \frac{\varepsilon_a - \lambda}{E_a}\right) , \qquad (V.3)$$

$$\frac{2}{g} = \sum_{a>0} \frac{1}{E_a} , \qquad (V.4)$$

where

$$E_a = [(\epsilon_a - \lambda)^2 + \Delta^2]^{\frac{1}{2}} . \qquad (V.5)$$

The energy of the system as a function of deformation is given by

$$E(\beta_2) = \sum_{a>0} (H_0)_{aa} \left[1 - \frac{\epsilon_a - \lambda}{E_a}\right] - \frac{1}{2} \chi Q_0^2 - \Delta^2/g , \qquad (V.6)$$

where

$$Q_0 = \sum_{a>0} \langle a | r^2 Y_{20} | a \rangle \left(1 - \frac{\epsilon_a - \lambda}{E_a}\right) . \qquad (V.7)$$

An extremum in energy is obtained whenever $D = \chi Q_0$.

The generalization of this procedure to a given finite temperature $\tau \left(= \frac{1}{\beta} \right)$ leads to the following steps.

1′) Same as (1).

2′) One solves

$$N = \sum_{a>0} \left[1 - \frac{\epsilon_a - \lambda}{E_a} (1 - 2f_a)\right] , \qquad (V.8)$$

$$\frac{2}{g} = \sum_{a>0} \frac{1}{E_a} (1 - 2f_a) , \qquad (V.9)$$

where as before

$$E_a = [(\epsilon_a - \lambda)^2 + \Delta_a^2]^{\frac{1}{2}} ,$$

and

$$f_a = 1/(1 + e^{\beta E_a}) .$$

The energy of the system as a function of deformation is given by

$$E(\beta_2) = \sum_{a>0} (H_0)_{aa} [1 - \frac{\varepsilon_a - \lambda}{E_a} (1-2f_a)] - \frac{1}{2} \chi Q_0^2 - \Delta^2/g , \qquad (V.10)$$

where

$$Q_0 = \sum_{a>0} \langle a | r^2 Y_{20} | a \rangle [1 - \frac{\varepsilon_a - \lambda}{E_a} (1-2f_a)] . \qquad (V.11)$$

The free energy is given by

$$F = E - \tau S$$

where the entropy S is

$$S = -2 \sum_{a>0} [f_a \ln f_a + (1-f_a) \ln(1-f_a)] . \qquad (V.12)$$

The condition $D = \chi Q_0$ gives an extremum in F[55]. If there are more than one self-consistent solutions, then the one which gives the minimum value of F should be chosen.

The results of such variational calculations done on the nucleus ^{116}Sn are shown in Fig. 11. The various shell model single particle energies used for this calculation are

same as given in Table 7 (chapter IV). The results unfortunately are sensitive to the relative value of g and X. The results shown in Fig. 11 are for fixed g_n = 0.16 MeV. This gives Δ_n = 1.3 MeV in ^{116}Sn in the spherical zero temperature limit. Since Δ_p = 0, the value of g_p is immaterial. The value of X lies between the values of Ref. 53 and Ref. 54. Effects of small variations in the value of X on the free energy curve are shown. We find that shape transition can indeed occur. At zero temperature, the free energy is equivalent to the energy of the system and it minimizes at zero deformation. Yet at finite temperature, the free energy may minimize at non-zero deformation although the variation of free energy with deformation is not great. If one now takes this deformation as the proper static deformation and performs a standard rotational model calculation for level density, very large differences from the values in sections (III.1) and (IV.1) are found.

Although the free energy against deformation curves are relatively flat, the energy against deformation curves vary more rapidly. They also tend to favor larger deformations.

V.2 Level density using the rotational model.

The rotational model formulae for level density[30,31,34] are quite straightforward. Assuming a deformation β_2 = - 0.104 (the free energy was minimum at this value of deformation at temperature τ = 0.743 MeV and the corresponding excitation

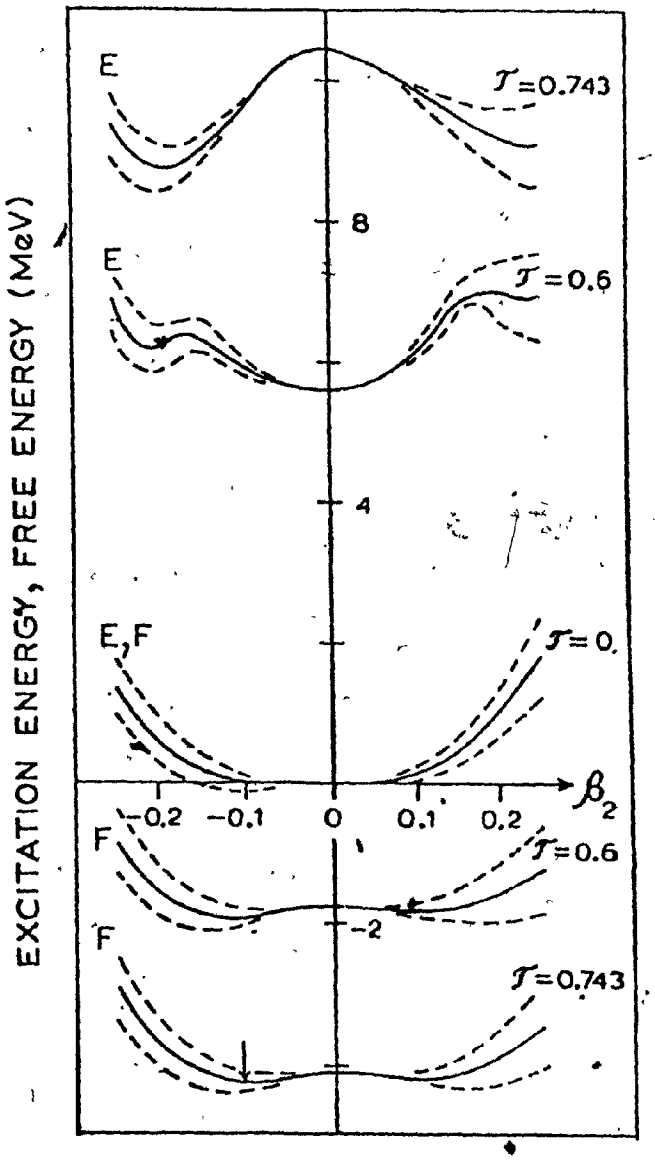

FIGURE 11. Potential energy surface and Helmholtz free energy surface as a function of quadrupole deformation for ^{116}Sn at various temperatures τ. The unit of τ is MeV. The solid lines correspond to a quadrupole strength $\chi = 0.0966\ (m\omega/\hbar)^2$ MeV with $\hbar\omega = 41.2\ A^{-1/3}$. The dotted lines give the results for χ altered by ±3%. The arrow indicates the minimum of F for $\tau = 0.743$ MeV.

energy was 9.51 MeV) we calculate $\omega_{intr.}(E)$ from which $\rho_{intr.}(E,\Omega)$ is obtained:

$$\rho_{intr}(E,\Omega) = (2\pi\sigma^2)^{-\frac{1}{2}} \omega_{intr}(E)\ e^{-\Omega^2/2\sigma^2}, \qquad (V.13)$$

where $\rho_{intr}(E,\Omega)$ is the level density for many particle states each of which has magnetic quantum number Ω and

$$\sigma^2 = 2 \sum_{k>0} k^2 f_k(1-f_k) \qquad (V.14)$$

In Eq. (V.14) k is the megnetic quantum number for each Nilsson-type oribital. Now

$$\rho(E,I) = \sum_{\Omega>0}^{I} \rho_{intr}\ [E - E_{rot}(\Omega,I),\ \Omega] \qquad (V.15)$$

and the rotational model prescribes

$$E_{rot}(\Omega,I) = \frac{\hbar^2}{2\mathcal{I}_\perp}\ [I(I+1) - \Omega^2] \qquad (V.16)$$

where $\mathcal{I}_\perp$ is the moment of inertia about an axis perpendicular to the symmetry axis. Combining Eq. (V.15) and (V.16) and with the usual approximation, one finally obtains

$$\rho(E,I,+) \simeq \frac{1}{2} \sum_{\Omega\geq 0} \rho_{intr}(E,\Omega)\ \exp\left[-\frac{\beta\hbar^2}{2\mathcal{I}_\perp}\ \{I(I+1) - \Omega^2\}\right] \qquad (V.17)$$

The rigid body moment of inertia is used in this calculation. Because only level densities for I = 0 and I = 1 are needed to compare with experimental data, the calculated value for level density is insensitive to the choice of $\mathcal{I}_\perp$. Reducing $\mathcal{I}_\perp$ by a factor of two changes the calculated level density by a few per cent.

The method outlined in this section gave $\rho(E,0,+) + \rho(E,1,+) = 6\times10^4$ MeV^{-1} for ^{116}Sn at the neutron separation energy. The experimental value is $(2\pm.8)\times10^4$ MeV^{-1} [49]. The spherical model (section IV.1) gives 2×10^3 MeV^{-1}. The neutron separation energy is 9.56 MeV. At this energy, with our forces the gap Δ_n has already gone to zero. We know from the exact model calculation in section IV.1 that above the critical temperature the grand partition function method overestimates the exact level densities. Looked in this light, the deformed model is in much better agreement with experiment than the spherical model.

V.3 Conclusion.

The present work had two main objectives. One was to obtain the level densities for spherical nuclei with realistic interactions.

The second motivation for this work arose as a byproduct of this study above. It was found that it is not possible to achieve agreement with the experimental data in Sn isotopes using a spherical model. If one considers the quadrupole

force in addition to the pairing force, quite interesting features emerge. In the cases investigated, the nucleus (^{116}Sn) is spherical in the ground state, yet it is more proper to think of it as being deformed when considering 8-9 MeV excitations. While this is an idealized model, it is more valid than a simple spherical model for level densities. It will be very interesting to verify if similar results are obtained with more realistic interactions.

APPENDIX I

THE SADDLE-POINT METHOD[56]

Let us consider an integral of the type

$$I = \left(\frac{1}{2\pi i}\right)^n \int_{-i\infty}^{i\infty} d\alpha_1 \ldots \int_{-i\infty}^{i\infty} d\alpha_n \exp[f(\alpha_1, \ldots, \alpha_n)]$$

where f is a real function of $\alpha_1, \ldots, \alpha_n$. In evaluating this expression, we will assume that the integrand is a rapidly varying function of $\alpha_1, \ldots, \alpha_n$. Thus, the main contribution to the integral comes from a small region around the point $(\alpha_{10}, \alpha_{20}, \ldots, \alpha_{n0})$, where the integrand is stationary. This point is called the saddle point. The conditions that determine this saddle point are

$$\left.\frac{\partial f}{\partial \alpha_i}\right|_{\alpha_{i0}} = 0 \quad , \quad i = 1, \ldots, n. \tag{AI.1}$$

Let us therefore assume that we can choose the paths of integration so that they go through this point. Expanding the exponent f in the integrand in a Taylor series around the point $(\alpha_{10}, \ldots, \alpha_{n0})$ determined by the conditions (AI.1), we obtain

$$f(\alpha_1, \ldots, \alpha_n) = f(\alpha_{10}, \ldots, \alpha_{n0}) + \frac{1}{2} \sum_{i,j} (\alpha_i - \alpha_{i0}) \times (\alpha_j - \alpha_{j0}) \left.\frac{\partial^2 f}{\partial \alpha_i \, \partial \alpha_j}\right|_0 + \ldots$$

Let us write

$$\alpha_i - \alpha_{i0} = x_i \ ,$$

$$\left.\frac{\partial^2 f}{\partial\alpha_i \partial\alpha_j}\right|_0 = f_{ij} \ .$$

Then, up to second order,

$$f(\alpha_1 , \ldots , \alpha_n) = f(\alpha_{10} , \ldots , \alpha_{n0}) + \frac{1}{2} \sum_{i,j} x_i x_j f_{ij} \ .$$

Now, by a linear orthogonal transformation

$$x_i = \sum_m C_{im} y_m \qquad \text{(AI.2)}$$

the quadratic form $\sum_{i,j} x_i x_j f_{ij}$ can be diagonalized to $\sum_i y_i^2 F_i$ where F_i are the eigen-values of the matrix f_{ij}. Then

$$I = \exp[f(\alpha_{10} , \ldots , \alpha_{n0})] \left(\frac{1}{2\pi i}\right)^n \int_{-i\infty}^{i\infty} dx_1 \ldots \int_{-i\infty}^{i\infty} dx_n$$

$$\times \exp\left(\frac{1}{2} \sum_{i,j} x_i x_j f_{ij}\right)$$

$$= \exp[f(\alpha_{10} , \ldots , \alpha_{n0})] \left(\frac{1}{2\pi i}\right)^n \int_{-i\infty}^{i\infty} dy_1 \ldots \int_{-i\infty}^{i\infty} dy_n$$

$$\times \exp\left(\frac{1}{2} \sum y_i^2 F_i\right) \frac{\partial(x_1 \ldots x_n)}{\partial(y_1 \ldots y_n)} \ ,$$

where $\frac{\partial(x_1 \ldots x_n)}{\partial(y_1 \ldots y_n)}$ is the Jacobian of the transformation from x_i to y_i and is equal to the determinant of the matrix $\partial x_i / \partial y_j$

which by (AI.2) is $\det|C_{ij}| = 1$, since the transformation is orthogonal.

Let us now write

$$y_k = iz_k$$

and obtain a Gaussian integral

$$I = \frac{1}{(2\pi)^n} \exp[f(\alpha_{10}, \ldots, \alpha_{n0})] \int_{-\infty}^{\infty} dz_1 \ldots \int_{-\infty}^{\infty} dz_n \times \exp\left(-\frac{1}{2} \Sigma F_i z_i^2\right)$$

$$= \frac{1}{(2\pi)^n} \exp[f(\alpha_{10}, \ldots, \alpha_{n0})] \frac{(2\pi)^{n/2}}{(F_1 F_2 \ldots F_n)^{1/2}}$$

where we have used

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}} .$$

In order to evaluate this integral, all the eigen-values F_i must be positive. Now, the product of all the eigen-values of a matrix is equal to the determinant of the matrix and therefore we finally obtain

$$I = \frac{\exp[f(\alpha_{10}, \ldots, \alpha_{n0})]}{(2\pi)^{n/2} [\det|(\partial^2 f / \partial\alpha_i \partial\alpha_j)_0|]^{1/2}} \qquad \text{(AI.3)}$$

APPENDIX II

DENSITY OF STATES IN THE HARTREE-FOCK THEORY

Let us consider the case when pairing correlation is either absent or unimportant. Thus at any temperature, the nucleus is a system of independent particles. However the system now is not necessarily spherical. Therefore, the wave functions of orbitals can change as a function of temperature. The Hamiltonian $(H - \lambda\hat{N})$ is given by

$$H - \lambda\hat{N} = \Sigma(T_{ab} - \lambda\delta_{ab})\ c_a^\dagger c_b + \frac{1}{4}\Sigma\ V_{acbd}\ c_a^\dagger c_c^\dagger c_d c_b \qquad \text{(AII.1)}$$

where T_{ab} is a one body part and V_{acbd} is an antisymmetrized two-body matrix element, and for convenience, taken to be real. If in some orthonormal single particle basis $|a>$, we can reduce the Hamiltonian to the form

$$H - \lambda\hat{N} \approx K + \Sigma(\epsilon_a - \lambda)\ c_a^\dagger c_a\ ,$$

then the grand partition function will be given as

$$Z = \mathrm{Tr}\ e^{-\beta(H-\lambda\hat{N})}$$

$$= e^{-\beta K}\ \Pi(1+e^{-\beta(\epsilon_a-\lambda)}) \qquad \text{(AII.2)}$$

The probability of occupation in the state $|a>$ is

$$<c_a^\dagger c_a> = 1/(1+e^{\beta(\epsilon_a-\lambda)}) = f_a \qquad \text{(AII.3)}$$

and

$$\langle c_a^\dagger c_b \rangle = \delta_{ab} f_a \qquad \text{(AII.4)}$$

The basis $|a\rangle$ is not a priori known; it can be expanded in terms of some known fixed basis.

Let us define a normal product

$$: c_a^\dagger c_b : = c_a^\dagger c_b - \langle c_a^\dagger c_b \rangle .$$

Using Wick's theorem for the grand canonical ensemble, we write

$$H - \lambda \hat{N} = A_0 + A_2 + A_4$$

with

$$A_0 = \Sigma (T_{ab} - \lambda \delta_{ab}) \langle c_a^\dagger c_b \rangle + \frac{1}{2} \Sigma V_{acbd} \langle c_c^\dagger c_d \rangle \langle c_a^\dagger c_b \rangle$$

$$= \Sigma (T_{aa} - \lambda) f_a + \frac{1}{2} \Sigma V_{acac} f_a f_c$$

$$A_2 = \Sigma (T_{ab} - \lambda \delta_{ab}) : c_a^\dagger c_b : + \Sigma V_{acbd} \langle c_c^\dagger c_d \rangle : c_a^\dagger c_b :$$

$$= \Sigma (T_{ab} - \lambda \delta_{ab})(c_a^\dagger c_b - \delta_{ab} f_a) + \Sigma V_{acbc} f_c (c_a^\dagger c_b - \delta_{ab} f_b)$$

$$A_4 = \frac{1}{4} \Sigma V_{acbd} : c_a^\dagger c_c^\dagger c_d c_b :$$

Neglecting A_4 we obtain

$$H - \lambda \hat{N} = A_0 + A_2$$

$$= - \frac{1}{2} \Sigma V_{acac} f_a f_c + \Sigma [T_{ab} + \Sigma V_{acac} f_c - \lambda \delta_{ab}] \times c_a^\dagger c_b \qquad \text{(AII.5)}$$

The above equation shows that the basis $|a\rangle$ is to be chosen

such that

$$T_{ab} + \Sigma\, V_{acac}\, f_c = \varepsilon_a\, \delta_{ab} \qquad \text{(AII.6)}$$

Then the grand partition function will be given by

$$Z = \exp\left[\frac{1}{2}\,\beta\, \Sigma\, V_{abab}\, f_a\, f_b\right] \prod_a \left(1+e^{-\beta(\varepsilon_a-\lambda)}\right)$$

and therefore

$$\ell n\, Z = \frac{1}{2}\,\beta\, \Sigma\, V_{abab}\, f_a\, f_b + \Sigma\, \ell n\, \left[1+e^{-\beta(\varepsilon_a-\lambda)}\right]$$

It is convenient to introduce a "fixed" basis $|A\rangle$ in terms of which the H.F. orbitals can be expanded

$$|a\rangle = \sum_A d_{aA}\, |A\rangle \qquad \text{(AII.7)}$$

where we take the transformation coefficients d_{aA} to be real. We have, for example,

$$\langle c_A^\dagger\, c_B\rangle \doteq \rho_{BA} = \sum_a d_{aA}\, d_{aB}\, f_a = \rho_{AB}$$

The logarithm of the grand partition function can now be written as

$$\ell n\, Z = \frac{1}{2}\,\beta\, \Sigma\, V_{ACBD}\, \rho_{DC}\, \rho_{BA} + \Sigma\, \ell n\, \left[1+e^{-\beta(\varepsilon_a-\lambda)}\right] \qquad \text{(AII.8)}$$

where

$$\sum_B \left[T_{AB} + \sum_{CD} V_{ACBD}\, \rho_{DC}\right] d_{aB} = \varepsilon_a\, d_{aA}$$

$$\sum_A d_{aA}\left(T_{AB} + \sum_{CD} V_{ACBD}\, \rho_{DC}\right) = d_{aB}\, \varepsilon_a$$

$$\sum_A d_{aA}^2 = 1$$

We now need the derivatives of $\ln Z$ and an expression for entropy.

$$N = \frac{\partial \ln Z}{\partial \alpha}$$

$$= \frac{1}{\beta} \frac{\partial \ln Z}{\partial \lambda}$$

$$= \frac{1}{2} \frac{\partial}{\partial \lambda} \sum V_{ACBD}\, \rho_{DC}\, \rho_{BA} - \sum \frac{e^{-\beta(\varepsilon_a - \lambda)}}{1+e^{-\beta(\varepsilon_a - \lambda)}} \frac{\partial}{\partial \lambda} (\varepsilon_a - \lambda)$$

$$= \sum f_a - \sum f_a \frac{\partial \varepsilon_a}{\partial \lambda} + \frac{1}{2} \frac{\partial}{\partial \lambda} \sum V_{ACBD}\, \rho_{DC}\, \rho_{BA}$$

Physically, the answer must be simply $\sum f_a$ and hence the two terms of Eq. (AII.8) must cancel each other. We have

$$\frac{1}{2} \frac{\partial}{\partial \lambda} \sum V_{ACBD}\, \rho_{DC}\, \rho_{BA} = \frac{1}{2} \sum \left[V_{ACBD} \left(\frac{\partial \rho_{DC}}{\partial \lambda}\right) \rho_{BA} + V_{ACBD} \times \rho_{DC} \left(\frac{\partial \rho_{BA}}{\partial \lambda}\right)\right]$$

$$= \sum \rho_{BA}\, V_{ACBD} \frac{\partial \rho_{DC}}{\partial \lambda}$$

Let us now consider

$$\sum_a f_a \frac{\partial \varepsilon_a}{\partial \lambda} = \sum_a f_a \frac{\partial}{\partial \lambda} \sum_{AB} [d_{aA} (T_{AB} + \sum_{CD} V_{ACBD} \rho_{DC}) d_{aB}]$$

$$= \sum f_a d_{aA} \sum V_{ACBD} (\frac{\partial \rho_{DC}}{\partial \lambda}) d_{aB}$$

$$+ \sum f_a (\frac{\partial d_{aA}}{\partial \lambda}) [T_{AB} + \sum V_{ACBD} \rho_{DC}] d_{aB}$$

$$+ \sum f_a d_{aA} [T_{AB} + \sum V_{ACBD} \rho_{DC}] (\frac{\partial d_{aB}}{\partial \lambda})$$

$$= \sum \rho_{BA} V_{ACBD} \frac{\partial \rho_{DC}}{\partial \lambda} + \sum f_a (\frac{\partial d_{aA}}{\partial \lambda}) \varepsilon_a d_{aA}$$

$$+ \sum f_a \varepsilon_a d_{aB} (\frac{\partial d_{aB}}{\partial \lambda})$$

$$= \sum \rho_{BA} V_{ACBD} \frac{\partial \rho_{DC}}{\partial \lambda} + \sum f_a \varepsilon_a \frac{\partial}{\partial \lambda} \sum_A d_{aA}^2 .$$

Since in any variation, the norm of the vector must be conserved, we get

$$\sum f_a \frac{\partial \varepsilon_a}{\partial \lambda} = \sum \rho_{BA} V_{ACBD} \frac{\partial \rho_{DC}}{\partial \lambda}$$

and therefore

$$N = \sum f_a . \qquad \text{(AII.9)}$$

Consider now

$$-E = \frac{\partial \ln Z}{\partial \beta}$$

$$= \frac{1}{2} \sum V_{ACBD} \rho_{DC} \rho_{BA} + \frac{1}{2} \beta \sum V_{ACBD} \frac{\partial}{\partial \beta} (\rho_{DC} \rho_{BA})$$

$$- \sum \varepsilon_a f_a - \beta \sum f_a \frac{\partial \varepsilon_a}{\partial \beta} .$$

Using techniques as before,

$$\frac{\partial \ln Z}{\partial \beta} = \frac{1}{2} \Sigma V_{ACBQ} \rho_{DC} \rho_{BA} - \Sigma \varepsilon_a f_a$$

$$= \frac{1}{2} \Sigma V_{abab} f_a f_b - \Sigma \varepsilon_a f_a \qquad \text{(AII.10)}$$

The expression for entropy will be

$$S = \ln Z - \alpha N + \beta E$$

$$= \frac{1}{2} \beta \Sigma V_{abab} f_a f_b + \ln [1 + e^{-\beta(\varepsilon_a - \lambda)}]$$

$$- \beta \lambda \Sigma f_a - \frac{1}{2} \beta \Sigma V_{abab} f_a f_b + \beta \Sigma \varepsilon_a f_a$$

$$= \beta \Sigma (\varepsilon_a - \lambda) f_a - \Sigma \ln \left[\frac{1}{1 + e^{-\beta(\varepsilon_a - \lambda)}}\right]$$

$$= \Sigma f_a \ln \left[\frac{1-f_a}{f_a}\right] - \Sigma \ln [1 - f_a]$$

$$= - \Sigma [f_a \ln f_a + (1-f_a) \ln (1-f_a)] \qquad \text{(AII.11)}$$

which is the same as obtained for non-interacting fermions.

We also need the second derivatives of $\ln Z$. They are given as

$$\frac{\partial^2 \ln Z}{\partial \alpha^2} = \Sigma \frac{\partial f_a}{\partial \alpha}$$

$$= \Sigma f_a (1-f_a) \left(1 - \beta \frac{\partial \varepsilon_a}{\partial \alpha}\right)$$

$$\frac{\partial^2 \ln Z}{\partial \beta^2} = - \Sigma \varepsilon_a \frac{\partial f_a}{\partial \beta}$$

$$= \Sigma\ \varepsilon_a\ f_a(1-f_a)\left(\varepsilon_a+\beta\ \frac{\partial \varepsilon_a}{\partial \beta}\right) ,$$

$$\frac{\partial^2\ \ell n\ Z}{\partial \alpha \partial \beta} = \frac{\partial^2\ \ell n\ Z}{\partial \beta \partial \alpha} = \Sigma\ \frac{\partial f_a}{\partial \beta} = -\ \Sigma\ \varepsilon_a\ \frac{\partial f_a}{\partial \alpha} .$$

Thus in order to evaluate the second derivatives of $\ell n\ Z$, we need the values of $\partial f_a/\partial \alpha$ and $\partial f_a/\partial \beta$. The evaluation of quantities like $\Sigma\ f_a(1-f_a)\ \frac{\partial \varepsilon_a}{\partial \alpha}$ are difficult, although these can always be evaluated numerically.

APPENDIX III

DERIVATIONS OF EQUATIONS (II.33), (II.34) AND (II.35)

The expression for the logarithm of the grand partition function [Eq. (II.32)] is

$$\ell n\ Z = -\frac{1}{2}\beta \sum [\eta_a - E_a + \mu_a \rho_a + \Delta_a k_a] + \sum \ell n [1 + e^{-\beta E_a}] \tag{AIII.1}$$

We have two independent variables α, and β and $\alpha = \beta\lambda$. Therefore,

$$\frac{\partial \lambda}{\partial \alpha} = \frac{1}{\beta} \quad \frac{\partial \lambda}{\partial \lambda} = \frac{1}{\beta} \quad ;$$

and

$$\frac{\partial \alpha}{\partial \beta} = \frac{\partial}{\partial \beta}(\beta\lambda) = \beta \frac{\partial \lambda}{\partial \beta} + \lambda = 0$$

which gives

$$\frac{\partial \lambda}{\partial \beta} = -\frac{\lambda}{\beta}$$

Now,

$$\frac{\partial\ \ell n\ Z}{\partial \alpha} = -\frac{1}{2}\beta \frac{\partial}{\partial \alpha} \sum [\varepsilon_a - \mu_a - \lambda - E_a + \mu_a \rho_a + \Delta_a k_a]$$

$$+ \frac{\partial}{\partial \alpha} \sum \ell n [1 + e^{-\beta E_a}]$$

$$= \frac{1}{2}\beta \sum_a \left[\frac{\partial \mu_a}{\partial \alpha} + \frac{1}{\beta} + \frac{\partial E_a}{\partial \alpha}\right] - \frac{1}{2}\beta \frac{\partial}{\partial \alpha} \sum_a \mu_a \rho_a$$

$$- \frac{1}{2}\beta \frac{\partial}{\partial \alpha} \sum_a \Delta_a k_a + \beta \sum_a f_a \frac{\partial E_a}{\partial \alpha} .$$

Using

$$\frac{\partial E_a}{\partial \alpha} = \frac{1}{E_a}\left[\Delta_a \frac{\partial \Delta_a}{\partial \alpha} - \eta_a \left(\frac{\partial \mu_a}{\partial \alpha} + \frac{1}{\beta}\right)\right] , \qquad \text{(AIII.2)}$$

$$\frac{\partial \ln Z}{\partial \alpha} = \frac{1}{2} \sum_a \left[1 - \frac{\eta_a}{E_a}(1-2f_a)\right]$$

$$+ \frac{1}{2}\beta \sum_a \left[1 - \frac{\eta_a}{E_a}(1-2f_a)\right] \frac{\partial \mu_a}{\partial \alpha}$$

$$- \frac{1}{2}\beta \frac{\partial}{\partial \alpha} \sum_a \mu_a \rho_a + \frac{1}{2}\beta \sum_a \frac{\Delta_a}{E_a}(1-2f_a) \frac{\partial \Delta_a}{\partial \alpha}$$

$$- \frac{1}{2}\beta \frac{\partial}{\partial \alpha} \sum_a \Delta_a k_a$$

$$= \sum_a \rho_a + \beta \sum_a \rho_a \frac{\partial \mu_a}{\partial \alpha} - \frac{1}{2}\beta \frac{\partial}{\partial \alpha} \sum_a \mu_a \rho_a$$

$$+ \beta \sum_a k_a \frac{\partial \Delta_a}{\partial \alpha} - \frac{1}{2}\beta \frac{\partial}{\partial \alpha} \sum_a \Delta_a k_a .$$

Let us now consider

$$\frac{1}{2} \frac{\partial}{\partial \alpha} \sum_a \mu_a \rho_a = \frac{1}{2} \sum_a \rho_a \frac{\partial \mu_a}{\partial \alpha} + \frac{1}{2} \sum_a \mu_a \frac{\partial \rho_a}{\partial \alpha}$$

$$= \frac{1}{2} \sum_a \rho_a \frac{\partial \mu_a}{\partial \alpha} - \frac{1}{2} \sum_{a\,b} V_{abab}\, \rho_b \frac{\partial \rho_a}{\partial \alpha}$$

$$= \frac{1}{2} \sum_a \rho_a \frac{\partial \mu_a}{\partial \alpha} - \frac{1}{2} \sum_{ba} \rho_b \frac{\partial}{\partial \alpha}(V_{abab}\, \rho_a)$$

$$= \frac{1}{2} \Sigma \rho_a \frac{\partial \mu_a}{\partial \alpha} + \frac{1}{2} \Sigma \rho_b \frac{\partial \mu_b}{\partial \alpha}$$

$$= \Sigma \rho_a \frac{\partial \mu_a}{\partial \alpha} \qquad \text{(AIII.3)}$$

Similarly

$$\frac{1}{2} \frac{\partial}{\partial \alpha} \Sigma \Delta_a k_a = \Sigma k_a \frac{\partial \Delta_a}{\partial \alpha} \qquad \text{(AIII.4)}$$

and therefore we obtain

$$\frac{\partial \ln Z}{\partial \alpha} = \Sigma \rho_a \,. \qquad \text{(II.33)}$$

Consider now

$$\frac{\partial \ln Z}{\partial \beta} = -\frac{1}{2} \Sigma [\varepsilon_a - \mu_a - \lambda - E_a + \mu_a \rho_a + \Delta_a k_a]$$

$$+ \frac{1}{2} \beta \Sigma [\frac{\partial \mu_a}{\partial \beta} - \frac{\lambda}{\beta} + \frac{\partial E_a}{\partial \beta}] - \frac{1}{2} \beta \frac{\partial}{\partial \beta} \Sigma \mu_a \rho_a$$

$$- \frac{1}{2} \beta \frac{\partial}{\partial \beta} \Sigma \Delta_a k_a - \beta \Sigma f_a \frac{\partial E_a}{\partial \beta} - \Sigma f_a E_a$$

Using

$$\frac{\partial E_a}{\partial \beta} = \frac{1}{E_a} [\frac{\lambda}{\beta} (\varepsilon_a - \mu_a - \lambda) - (\varepsilon_a - \mu_a - \lambda) \frac{\partial \mu_a}{\partial \beta} + \Delta_a \frac{\partial \Delta_a}{\partial \beta}], \qquad \text{(AIII.5)}$$

$$\frac{1}{2} \frac{\partial}{\partial \beta} \Sigma \mu_a \rho_a = \Sigma \rho_a \frac{\partial \mu_a}{\partial \beta} \,, \qquad \text{(AIII.6)}$$

$$\frac{1}{2} \frac{\partial}{\partial \beta} \Sigma \Delta_a k_a = \Sigma k_a \frac{\partial \Delta_a}{\partial \beta} \,, \qquad \text{(AIII.7)}$$

we get

$$\frac{\partial \ell n\, Z}{\partial \beta} = -\frac{1}{2}\Sigma\ (\varepsilon_a-\mu_a-E_a)$$

$$+\frac{1}{2}\Sigma\ \frac{\lambda}{E_a}\ (\varepsilon_a-\mu_a-\lambda)(1-2f_a)$$

$$-\Sigma\ f_a\ E_a - \frac{1}{2}\Sigma\ \Delta_a k_a - \frac{1}{2}\Sigma\ \mu_a\rho_a$$

$$+\frac{1}{2}\beta\ \Sigma\ \left[1 - \frac{1-2f_a}{E_a}\ (\varepsilon_a-\mu_a-\lambda) - 2\rho_a\right]\ \frac{\partial \mu_a}{\partial \beta}$$

$$+\beta\ \Sigma\ \left[\frac{\Delta_a}{2E_a}(1-2f_a) - k_a\right]\ \frac{\partial \Delta_a}{\partial \beta}\ .$$

The coefficients of $\partial\mu_a/\partial\beta$ and $\partial\Delta_a/\partial\beta$ obviously vanish. Rearranging the surviving terms, we get

$$\frac{\partial \ell n\, Z}{\partial \beta} = -\frac{1}{2}\Sigma\ (\varepsilon_a-\mu_a) + \frac{1}{2}\Sigma\ E_a(1-2f_a)$$

$$+\frac{1}{2}\Sigma\ \frac{\lambda}{E_a}\ (\varepsilon_a-\mu_a-\lambda)(1-2f_a) - \frac{1}{2}\Sigma\ \Delta_a k_a - \frac{1}{2}\Sigma\ \mu_a\rho_a$$

$$= -\frac{1}{2}\Sigma\ (\varepsilon_a-\mu_a) + \frac{1}{2}\Sigma\ \frac{1-2f_a}{E_a}\ (\varepsilon_a-\mu_a-\lambda)(\varepsilon_a-\mu_a)$$

$$+\Delta_a^2] - \frac{1}{2}\Sigma\ \Delta_a k_a - \frac{1}{2}\Sigma\ \mu_a\rho_a$$

$$= -\frac{1}{2}\Sigma\ (\varepsilon_a-\mu_a)\ \left[1 - \frac{\eta_a}{E_a}\ (1-2f_a)\right]$$

$$+\Sigma\ \Delta_a k_a - \frac{1}{2}\Sigma\ \Delta_a k_a - \frac{1}{2}\Sigma\ \mu_a\rho_a$$

$$= -\Sigma\ \varepsilon_a\rho_a + \frac{1}{2}\Sigma\ \Delta_a k_a + \frac{1}{2}\Sigma\ \mu_a\rho_a \qquad \text{(II.34)}$$

Lastly from Eqs. (AIII.1), (II.33) and (II.34), the expression for entropy is

$$S = \ell n\ Z - \alpha N + \beta E$$

$$= -\frac{1}{2}\beta\Sigma[\eta_a - E_a + \mu_a\rho_a + \Delta_a k_a] + \Sigma\,\ell n[1 + e^{-\beta E_a}]$$

$$- \beta\lambda\Sigma\rho_a + \beta\Sigma\varepsilon_a\rho_a - \frac{1}{2}\beta\Sigma\mu_a\rho_a - \frac{1}{2}\beta\Sigma\Delta_a k_a$$

$$= \frac{1}{2}\beta\Sigma(\eta_a - E_a) + \beta\Sigma(\varepsilon_a - \mu_a - \lambda)\rho_a - \beta\Sigma\Delta_a k_a$$

$$+ \Sigma\,\ell n[1 + e^{-\beta E_a}]$$

$$= -\frac{1}{2}\beta\Sigma(\eta_a - E_a) + \beta\Sigma\eta_a\frac{1}{2}\left[1 - \frac{\eta_a}{E_a}(1-2f_a)\right]$$

$$- \beta\Sigma\frac{\Delta_a^2}{2E_a}(1-2f_a) + \Sigma\,\ell n[1 + e^{-\beta E_a}]$$

$$= \beta\Sigma f_a E_a + \Sigma\,\ell n[1 + e^{-\beta E_a}] \qquad \text{(II.35)}$$

APPENDIX IV

DERIVATIVES OF ρ_a AND k_a

From Eq. (II.29) we have

$$\frac{\partial \rho_a}{\partial \alpha} = -\frac{1}{2}\frac{\partial}{\partial \alpha}\left[\frac{\epsilon_a - \mu_a - \lambda}{E_a}(1-2f_a)\right]$$

$$= \frac{1}{2E_a}\left[\frac{\partial \mu_a}{\partial \alpha} + \frac{1}{\beta}\right](1-2f_a) + \frac{\eta_a}{2E_a^2}(1-2f_a)\frac{\partial E_a}{\partial \alpha}$$

$$- \frac{\eta_a}{E_a}\beta\, f_a(1-f_a)\frac{\partial E_a}{\partial \alpha} .$$

Using (AIII.2) we obtain

$$\frac{\partial \rho_a}{\partial \alpha} = \left[\left(\frac{1}{2E_a} - \frac{\eta_a^2}{2E_a^3}\right)(1-2f_a)\right.$$

$$\left. + \frac{\eta_a^2}{E_a^2}\beta\, f_a(1-f_a)\right]\left(\frac{\partial \mu_a}{\partial \alpha} + \frac{1}{\beta}\right)$$

$$+ \left[\frac{\eta_a}{2E_a^3}(1-2f_a) - \frac{\eta_a}{E_a^2}\beta\, f_a(1-f_a)\right]\Delta_a .$$

Let us define

$$X_a = f_a(1-f_a)/E_a^2 \qquad \text{(AIV.1)}$$

$$Y_a = (1-2f_a)/(2\beta E_a^3) \qquad \text{(AIV.2)}$$

Then

$$\frac{\partial \rho_a}{\partial \alpha} = (\Delta_a^2 Y_a + \eta_a^2 X_a)(\beta \frac{\partial \mu_a}{\partial \alpha} + 1)$$

$$+ \beta \eta_a (Y_a - X_a) \Delta_a \frac{\partial \Delta_a}{\partial \alpha} .$$

Similarly

$$\frac{\partial \rho_a}{\partial \beta} = -\frac{1}{2} \frac{\partial}{\partial \beta} [\frac{\varepsilon_a - \mu_a - \lambda}{E_a} (1-2f_a)]$$

$$= \frac{1}{2E_a} (\frac{\partial \mu_a}{\partial \beta} - \frac{\lambda}{\beta})(1-2f_a) - \frac{\eta_a}{2E_a^2} (1-2f_a) \frac{\partial E_a}{\partial \beta}$$

$$- \frac{\eta_a}{E_a} f_a(1-f_a)(E_a + \beta \frac{\partial E_a}{\partial \beta})$$

Using (AIII.5) we get

$$\frac{\partial \rho_a}{\partial \beta} = [(\frac{1}{2E_a} - \frac{\eta_a}{2E_a^3})(1-2f_a)$$

$$+ \frac{\eta_a^2}{E_a^2} \beta f_a(1-f_a)] (\frac{\partial \mu_a}{\partial \beta} - \frac{\lambda}{\beta})$$

$$+ [\frac{\eta_a}{2E_a^3} (1-2f_a) - \frac{\eta_a}{E_a^2} \beta f_a(1-f_a)] \Delta_a \frac{\partial \Delta_a}{\partial \beta}$$

$$- \eta_a f_a(1-f_a)$$

$$= (\Delta_a^2 Y_a + \eta_a^2 X_a)(\beta \frac{\partial \mu_a}{\partial \beta} - \lambda) - \eta_a E_a^2 X_a$$

$$+ \beta \eta_a (Y_a - X_a) \Delta_a \frac{\partial \Delta_a}{\partial \beta} .$$

From Eq. (II.30) we have

$$\frac{\partial k_a}{\partial \alpha} = \frac{1}{2} \frac{\partial}{\partial \alpha} \left[\frac{\Delta_a}{E_a} (1-2f_a) \right]$$

$$= \frac{1}{2E_a} (1-2f_a) \frac{\partial \Delta_a}{\partial \alpha} - \frac{\Delta_a}{2E_a^2} (1-2f_a) \frac{\partial E_a}{\partial \alpha}$$

$$+ \frac{\Delta_a}{E_a} \beta f_a(1-f_a) \frac{\partial E_a}{\partial \alpha}$$

$$= \left[\left(\frac{1}{2E_a} - \frac{\Delta_a^2}{2E_a^3} \right) (1-2f_a) \right.$$

$$\left. + \frac{\Delta_a^2}{E_a^2} \beta f_a(1-f_a) \right] \frac{\partial \Delta_a}{\partial \alpha} + \left[\frac{\Delta_a}{2E_a^3} (1-2f_a) \right.$$

$$\left. - \frac{\Delta_a}{E_a^2} \beta f_a(1-f_a) \right] \eta_a \left(\frac{\partial \mu_a}{\partial \alpha} + \frac{1}{\beta} \right)$$

$$= \beta (\eta_a^2 Y_a + \Delta_a^2 X_a) \frac{\partial \Delta_a}{\partial \alpha}$$

$$+ \eta_a (Y_a - X_a) \Delta_a \left(\beta \frac{\partial \eta_a}{\partial \alpha} + 1 \right) .$$

Similarly

$$\frac{\partial k_a}{\partial \beta} = \frac{1}{2} \frac{\partial}{\partial \beta} \left[\frac{\Delta_a}{E_a} (1-2f_a) \right]$$

$$= \frac{1}{2E_a} (1-2f_a) \frac{\partial \Delta_a}{\partial \alpha} - \frac{\Delta_a}{2E_a^2} (1-2f_a) \frac{\partial E_a}{\partial \beta}$$

$$+ \frac{\Delta_a}{E_\alpha} f_a(1-f_a) \left(E_a + \beta \frac{\partial E_a}{\partial \beta} \right)$$

$$= \left[\left(\frac{1}{2E_a} - \frac{\Delta_a^2}{2E_a^3}\right)\ (1-2f_a)\right.$$

$$\left. + \frac{\Delta_a^2}{E_a^2}\ \beta\ f_a(1-f_a)\right]\ \frac{\partial \Delta_a}{\partial \beta} + \left[\frac{\Delta_a}{2E_a^3}\ (1-2f_a)\right.$$

$$\left. - \frac{\Delta_a}{E_a^2}\ \beta\ f_a(1-f_a)\right]\ \eta_a\left(\frac{\partial \mu_a}{\partial \beta} - \frac{\lambda}{\beta}\right) + \Delta_a\ f_a(1-f_a)$$

$$= \beta(\eta_a^2\ Y_a + \Delta_a^2\ X_a)\ \frac{\partial \Delta_a}{\partial \beta}$$

$$+ \eta_a(Y_a - X_a)\ \Delta_a\left(\beta\ \frac{\partial \mu_a}{\partial \beta} - \lambda\right) + \Delta_a\ E_a^2\ X_a\ .$$

APPENDIX V

THE COUPLED MATRIX ELEMENTS OF THE POTENTIAL

The two-body interaction term of the Hamiltonian is

$$\frac{1}{4} \Sigma V_{acbd} c_a^\dagger c_c^\dagger c_d c_b .$$

It is appropriate to write the interaction Hamiltonian in a way which exhibits its invariance under rotations and reflections. This can be done, for example, by coupling two of the particles, say a and c, to angular momentum JM, coupling the other two also to JM, and writing an invariant tensor product. We may therefore write V_{acbd} in the form

$$V_{acbd} = - 2 \sum_{JM} G(ACBDJ) C^J_{ac} C^J_{bd} \qquad (AV.1)$$

where C's are the Clebsch-Gordon coefficients

$$C^J_{ac} = (j_a m_a j_c m_c | J m_a + m_c)$$

The parity of $\ell_a + \ell_c$ must be the same as that of $\ell_b + \ell_d$, otherwise G vanishes. We must also have $q_a + q_c = q_b + q_d$. From the Hermiticity of the Hamiltonian and time-reversal invariance, it follows that G is real and satisfies

$$G(acbdJ) = G(bdacJ)$$
$$= - (-)^{j_a+j_c+J} G(cabdJ)$$

$$= - (-)^{j_b+j_d+J} G(acdbJ)$$

Now we may also couple two of the particles, say a and b to angular momentum $J' M'$ and similarly c and d; or alternatively a and d to $J''M''$, as well as c and b. We can therefore define another matrix element F as

$$V_{acbd} = - 2 \sum_{J'} F(ABDCJ') \; s_b \; C^{J'}_{a-b} \; s_c \; C^{J'}_{d-c}$$

$$= 2 \sum_{J''} F(ADBCJ'') \; s_d \; C^{J''}_{a-d} \; s_c \; C^{J''}_{b-c} \qquad \text{(AV.2)}$$

where -c is obtained from c by changing the sign of the magnetic quantum number m_c. The function F is related to the two-body matrix element for a particle and a hole. It is real and satisfies

$$F(abdcJ) = F(dcabJ) = (-)^{j_a+j_c+j_b+j_d} F(bacdJ)$$

but it is not simple to interchange a and b. F and G are related by

$$F(abdcJ') = - \sum_{J} (2J+1) \; W(j_a \; j_c \; j_b \; j_d ; \; J \; J') \; G \; (cabdJ)$$

Now we defined [Eqs. (II.20) and (II.21)]

$$\mu_a = - \sum_b V_{abab} \; \rho_b \; ,$$

$$\Delta_a = - \frac{1}{2} s_a \sum_b V_{a-ab-b} \; s_b \; k_b \; .$$

From (AV.2), we can write

$$\sum_{m_b} V_{abab} = -2 \sum_{m_b J} F(AABBJ)\,(-)^{j_a-m_a}\,(j_a\ m_a\ j_a\ -\ m_a\,|JO)$$

$$\times\ (-)^{j_b-m_b}\,(j_b\ m_b\ j_b\ -\ m_b\,|JO)$$

But,

$$\sum_{m_b} (-)^{j_b-m_b}\,(j_b\ m_b\ j_b\ -\ m_b\,|JO) = (2j_b+1)^{\frac{1}{2}}\,\delta_{JO}$$

and

$$(-)^{j_a-m_a}\,(j_a\ m_a\ j_a\ -\ m_a\,|0\ 0) = (2j_a+1)^{-\frac{1}{2}}$$

Therefore, summing over m_b and then over J, we obtain

$$\sum_{m_b} V_{abab} = -\,2\,[(j_b+\tfrac{1}{2})/(j_a+\tfrac{1}{2})]^{\frac{1}{2}}\ F(AABBO)\ , \qquad (AV.3)$$

and

$$\mu_a = \mu_A = 2 \sum_B [(j_B+\tfrac{1}{2})/(j_A+\tfrac{1}{2})]^{\frac{1}{2}}\ F(AABBO)\ \rho_B\ . \qquad (AV.4)$$

Similarly from (AV.1), we obtain,

$$s_a \sum_{m_b} s_b\, V_{a-ab-b} = -\,2\,[(j_b+\tfrac{1}{2})/(j_a+\tfrac{1}{2})]^{\frac{1}{2}}\ G(AABBO)\ , \qquad (AV.5)$$

and

$$\Delta_a = \Delta_A = \sum_B [(j_B+\tfrac{1}{2})/(j_A+\tfrac{1}{2})]^{\frac{1}{2}}\ G(AABBO)\ k_B\ . \qquad (AV.6)$$

APPENDIX VI

ALTERNATIVE MATRIX EQUATIONS

Simpler matrix equations than those in Eqs. (II.44) and (II.45) can be obtained. Eqs. (II.40) and (II.41) can be solved for $\frac{\partial \mu_a}{\partial \alpha}$ and $\frac{\partial \Delta_a}{\partial \alpha}$ to give

$$\frac{\partial \mu_a}{\partial \alpha} = -\frac{1}{\beta} + \frac{1}{\beta X_a Y_a E_a^4} [\eta_a (X_a - Y_a) \Delta_a \frac{\partial k_a}{\partial \alpha} + (\eta_a^2 Y_a + \Delta_a^2 X_a) \frac{\partial \rho_a}{\partial \alpha}]$$

$$\frac{\partial \Delta_a}{\partial \alpha} = \frac{1}{\beta X_a Y_a E_a^4} [(\Delta_a^2 Y_a + \eta_a^2 X_a) \frac{\partial k_a}{\partial \alpha} + \eta_a (X_a - Y_a) \Delta_a \frac{\partial \rho_a}{\partial \alpha}]$$

Using these equations in conjunction with Eqs. (II.42) and (II.43) we get

$$\begin{pmatrix} p & r \\ r & q \end{pmatrix} \begin{pmatrix} \frac{\partial \rho}{\partial \alpha} \\ \frac{\partial k}{\partial \alpha} \end{pmatrix} = \frac{1}{\beta} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

where

$$p_{AB} = \delta_{AB} \frac{\eta_A^2 Y_A + \Delta_A^2 X_A}{\beta X_A Y_A E_A^4} - 2[(j_B + \tfrac{1}{2})/(j_A + \tfrac{1}{2})]^{\frac{1}{2}} \cdot F(AABBO)$$

$$r_{AB} = \delta_{AB} \frac{\eta_A (X_A - Y_A)\ \Delta_A}{\beta\ X_A\ Y_A\ E_A^4}$$

$$q_{AB} = \delta_{AB} \frac{\Delta_A^2\ Y_A + \eta_A^2\ X_A}{\beta\ X_A\ Y_A\ E_A^4} - [(j_B+\tfrac{1}{2})/(j_A+\tfrac{1}{2})]^{\frac{1}{2}}$$

$$\times\ G(AABBO)$$

A similar technique can be used for $\partial\rho/\partial\beta$ and $\partial k/\partial\beta$. After considerable algebra, one gets

$$\begin{pmatrix} p & r \\ r & q \end{pmatrix} \begin{pmatrix} \frac{\partial\rho}{\partial\beta} \\ \frac{\partial k}{\partial\beta} \end{pmatrix} = \frac{1}{\beta} \begin{pmatrix} -\varepsilon + \mu \\ \Delta \end{pmatrix}$$

APPENDIX VII

THE F AND G MATRICES OF THE AUXILIARY HAMILTONIAN

The extra term introduced to the actual Hamiltonian is

$$-\frac{1}{4} M(\delta_{ab}\,\delta_{cd} - \delta_{ad}\,\delta_{bc})\; c_a^\dagger\, c_c^\dagger\, c_d\, c_b \,.$$

If we write the new two-body interaction term as V'_{acbd}, then

$$V'_{acbd} = V_{acbd} - M(\delta_{ab}\,\delta_{cd} - \delta_{ad}\,\delta_{bc})$$

Therefore,

$$V'_{abab} = V_{abab} - M(1-\delta_{ab}) \qquad \text{(AVII.1)}$$

$$V'_{a-a\;b-b} = V_{a-a\;b-b} - M(\delta_{ab} - \delta_{a-b}) \qquad \text{(AVII.2)}$$

From Eqs. (AV.3) and (AV.5), we have

$$F(AABBO) = -\frac{1}{2}\left[(j_A+\tfrac{1}{2})/(j_B+\tfrac{1}{2})\right]^{\frac{1}{2}} \sum_{m_b} V_{abab} \qquad \text{(AVII.3)}$$

$$G(AABBO) = -\frac{1}{2}\left[(j_A+\tfrac{1}{2})/(j_B+\tfrac{1}{2})\right]^{\frac{1}{2}} \Sigma\; s_a\, s_b\, V_{a-a\;b-b} \qquad \text{(AVII.4)}$$

The new F-matrix will then be

$$F'(AABBO) = -\frac{1}{2}\left[(j_A+\tfrac{1}{2})/(j_B+\tfrac{1}{2})\right]^{\frac{1}{2}} \sum_{m_b} \left[V_{abab} - M(1-\delta_{ab})\right]$$

$$= F(AABBO) + M[(j_A+\tfrac{1}{2})(j_B+\tfrac{1}{2})]^{\frac{1}{2}} - \delta_{AB}\frac{M}{2} .$$

Similary, G-matrix will become

$$G'(AABBO) = -\frac{1}{2}[(j_A+\tfrac{1}{2})/(j_B+\tfrac{1}{2})]^{\frac{1}{2}} \sum_{m_b} s_a s_b [V_{a-a\ b-b} - M(\delta_{ab}-\delta_{a-b})]$$

$$= G(AABBO) + \frac{1}{2} M[(j_A+\tfrac{1}{2})/(j_B+\tfrac{1}{2})]^{\frac{1}{2}} \times (s_a s_a - s_a s_{-a})\ \delta_{AB}$$

$$= G(AABBO) + \delta_{AB}\ M .$$

APPENDIX VIII

GENERALIZATIONS OF EQS. (II.33), (II.34) AND (II.35) FOR TWO KINDS OF PARTICLES

For two kinds of particles, the logarithm of the grand partition function will be given as

$$\ell n\ Z = -\frac{1}{2}\beta \sum_{a,i} [\eta_a(i) - E_a(i) + \mu_a(i)\ \rho_a(i) + \Delta_a(i)\ k_a(i)] + \sum_{a,i} \ell n[1 + e^{-\beta E_a(i)}] .$$

Hence,

$$N_j = \frac{\partial}{\partial \alpha_j} \ell n\ Z$$

$$= -\frac{1}{2}\beta \sum_{a,i} [\frac{\partial \mu_a}{\partial \alpha_j} - \frac{1}{\beta}\delta_{ij} - \frac{\partial}{\partial \alpha_j} E_a(i)]$$

$$- \frac{1}{2}\beta \frac{\partial}{\partial \alpha_j} \Sigma\ \mu_a(i)\ \rho_a(i) - \frac{1}{2}\beta \frac{\partial}{\partial \alpha_j} \Sigma\ \Delta_a(i)\ k_a(i)$$

$$- \beta \Sigma\ f_a(i) \frac{\partial E_a(i)}{\partial \alpha_j} .$$

As before,

$$\frac{1}{2} \frac{\partial}{\partial \alpha_j} \Sigma\ \mu_a(i)\ \rho_a(i) = \frac{1}{2} \Sigma\ \rho_a(i) \frac{\partial \mu_a(i)}{\partial \alpha_j} + \frac{1}{2} \Sigma\ \mu_a(i) \frac{\partial \rho_a(i)}{\partial \alpha_j}$$

$$= \frac{1}{2} \Sigma \rho_a(i) \frac{\partial \mu_a(i)}{\partial \alpha_j} + \frac{1}{2} \sum_{a,i} [- \sum_{c,k} V^{ik}_{acac} \rho_c(k)] \frac{\partial \rho_a(i)}{\partial \alpha_j}$$

$$= \frac{1}{2} \Sigma \rho_a(i) \frac{\partial \mu_a(i)}{\partial \alpha_j} + \frac{1}{2} \sum_{c,k} \rho_c(k) [- \sum_{a,i} V^{ik}_{acac} \frac{\partial \rho_a(i)}{\partial \alpha_j}]$$

$$= \frac{1}{2} \Sigma \rho_a(i) \frac{\partial \mu_a(i)}{\partial \alpha_j} + \frac{1}{2} \Sigma \rho_c(k) \frac{\partial \mu_c(k)}{\partial \alpha_j} = \Sigma \rho_a(i) \frac{\partial \mu_a(i)}{\partial \alpha_j}$$

Similarly,

$$\frac{1}{2} \frac{\partial}{\partial \alpha_j} \Sigma \Delta_a(i) k_a(i) = \Sigma k_a(i) \frac{\partial \Delta_a(i)}{\partial \alpha_j} ,$$

and using

$$\frac{\partial E_a(i)}{\partial \alpha_j} = \frac{1}{E_a(i)} [\eta_a(i) [\frac{\partial \mu_a(i)}{\partial \alpha_j} - \frac{1}{\beta} \delta_{ij}] + \Delta_a(i) \frac{\partial \Delta_a(i)}{\partial \alpha_j}],$$

we obtain

$$N_j = \frac{1}{2} \sum_{a,i} [1 - \frac{\eta_a(i)}{E_a(i)} (1 - 2f_a(i))] \delta_{ij}$$

$$+ \frac{1}{2} \beta \sum_{a,i} [1 - \frac{\eta_a(i)}{E_a(i)} (1 - 2f_a(i))] \frac{\partial \mu_a(i)}{\partial \alpha_j}$$

$$+ \frac{1}{2} \beta \Sigma \frac{\Delta_a(i)}{E_a(i)} [1 - 2f_a(i))] \frac{\partial \Delta_a(i)}{\partial \alpha_j}$$

$$- \beta \Sigma \rho_a(i) \frac{\partial \mu_a(i)}{\partial \alpha_j} - \beta \Sigma k_a(i) \frac{\partial \Delta_a(i)}{\partial \alpha_j}$$

$$= \Sigma_a \rho_a(j) .$$

The energy of the system will be

$$E = -\frac{\partial}{\partial\beta}\,\ell n\, Z$$

$$= \frac{1}{2}\,\Sigma\,[\eta_a(i) - E_a(i) + \mu_a(i)\,\rho_a(i) + \Delta_a(i)\,k_a(i)]$$

$$- \frac{1}{2}\,\beta\,\Sigma\,[-\frac{\partial\mu_a(i)}{\partial\beta} - \frac{\lambda_i}{\beta} + \frac{\partial E_a(i)}{\partial\beta}] + \frac{1}{2}\,\beta\,\frac{\partial}{\partial\beta}\,\Sigma\,\mu_a(i)\,\rho_a(i)$$

$$+ \frac{1}{2}\,\beta\,\frac{\partial}{\partial\beta}\,\Sigma\,\Delta_a(i)\,k_a(i) + \beta\,\Sigma\,f_a(i)\,\frac{\partial E_a(i)}{\partial\beta}\,.$$

Using

$$\frac{\partial E_a(i)}{\partial\beta} = \frac{1}{E_a(i)}\,[(\epsilon_a(i) - \mu_a(i) - \lambda_i)(-\frac{\partial\mu_a(i)}{\partial\beta} + \frac{\lambda_i}{\beta})$$

$$+ \Delta_a(i)\,\frac{\partial\Delta_a(i)}{\partial\beta}]\,,$$

$$\frac{1}{2}\,\frac{\partial}{\partial\beta}\,\Sigma\,\mu_a(i)\,\rho_a(i) = \Sigma\,\rho_a(i)\,\frac{\partial\mu_a(i)}{\partial\beta}\,,$$

$$\frac{1}{2}\,\frac{\partial}{\partial\beta}\,\Sigma\,\Delta_a(i)\,k_a(i) = \Sigma\,k_a(i)\,\frac{\partial\Delta_a(i)}{\partial\beta}\,,$$

we get

$$E = \frac{1}{2}\,\Sigma\,[\epsilon_a(i) - \mu_a(i) - E_a(i)] + \frac{1}{2}\,\Sigma\,\Delta_a(i)\,k_a(i)$$

$$+ \frac{1}{2}\,\Sigma\,\mu_a(i)\,\rho_a(i) + \Sigma\,f_a(i)\,E_a(i)$$

$$- \frac{1}{2}\,\Sigma\,\frac{\lambda_i}{E_a(i)}\,[\epsilon_a(i) - \mu_a(i) - \lambda_i]\,[1 - 2f_a(i)]$$

$$- \beta\,\Sigma\,[\frac{1}{2}(1 - \frac{\epsilon_a(i) - \mu_a(i) - \lambda_i}{E_a(i)}\,[1 - 2f_a(i)])$$

$$- \rho_a(i)]\,\frac{\partial\mu_a(i)}{\partial\beta} - \beta\,\Sigma\,[\frac{\Delta_a(i)}{2E_a(i)}\,(1 - 2f_a(i)) - k_a(i)]$$

$$\times\,\frac{\partial\Delta_a(i)}{\partial\beta}$$

Simplifying, we finally obtain

$$E = \Sigma\ \varepsilon_a(i)\ \rho_a(i) - \frac{1}{2}\ \Sigma\ \Delta_a(i)\ k_a(i) - \frac{1}{2}\ \Sigma\ \mu_a(i)\ \rho_a(i)\ .$$

The entropy will be given as

$$\begin{aligned} S &= \ln Z - \alpha_n N_n - \alpha_p N_p + \beta E \\ &= -\frac{1}{2}\beta \sum_{a,i} [n_a(i) - E_a(i) + \mu_a(i)\ \rho_a(i) + \Delta_a(i)\ k_a(i)] \\ &\quad + \sum_{a,i} \ln[1 + e^{-\beta E_a(i)}] - \beta \sum_{a,i} \lambda_i\ \rho_a(i) + \beta \sum_{a,i} \varepsilon_a(i)\ \rho_a(i) \\ &\quad - \frac{1}{2}\beta \sum_{a,i} \mu_a(i)\ \rho_a(i) - \frac{1}{2}\beta \sum_{a,i} \Delta_a(i)\ k_a(i) \\ &= \beta \sum_{a,i} E_a(i)/(1 + e^{\beta E_a(i)}) + \sum_{a,i} \ln[1 + e^{-\beta E_a(i)}] \end{aligned}$$

APPENDIX IX

GENERALIZATION OF THE MATRIX EQUATIONS (EQS. (II.44) AND (II.45)) FOR TWO KINDS OF PARTICLES

By straightforward algebra, the matrix equation of Eq. (II.44) generalizes, in the case of two kinds of particles, to

$$\begin{pmatrix} P11 & P12 & Q11 & 0 \\ P12 & P22 & 0 & Q22 \\ R11 & R12 & S11 & 0 \\ R21 & R22 & 0 & S22 \end{pmatrix} \begin{pmatrix} \frac{\partial \rho(1)}{\partial \alpha_1} \\ \frac{\partial \rho(2)}{\partial \alpha_1} \\ \frac{\partial k(1)}{\partial \alpha_1} \\ \frac{\partial k(2)}{\partial \alpha_1} \end{pmatrix} = \begin{pmatrix} Y(1)\Delta^2(1)+X(1)\eta^2(1) \\ 0 \\ -\eta(1)(X(1)-Y(1))\Delta(1) \\ 0 \end{pmatrix},$$

where the index 1 stands for proton orbitals and 2 for neutron orbitals or vice versa and we have

$$(Pij)_{AB} = \delta_{ij}\,\delta_{AB} - \beta\,[Y_A(i)\Delta_A^2(i) + X_A(i)\eta_A^2(i)] \times 2\,[(j_B+\tfrac{1}{2})/(j_A+\tfrac{1}{2})]^{\frac{1}{2}}\,F^{ij}(AABBO)\,,$$

$$(Qii)_{AB} = \beta\eta_A(i)\,[X_A(i) - Y_A(i)]\,\Delta_A(i)\,[(j_B+\tfrac{1}{2})/(j_A+\tfrac{1}{2})]^{\frac{1}{2}} \times G^{ii}(AABBO)\,,$$

$$(Rij)_{AB} = \beta\eta_A(i)\,[X_A(i)-Y_A(i)]\,\Delta_A(i)\;2\,[(j_B+\tfrac{1}{2})/(j_A+\tfrac{1}{2})]^{\frac{1}{2}}\;F^{ij}(AABBO),$$

$$(Sii)_{AB} = \delta_{AB} - \beta\,[Y_A(i)\eta_A^2(i) + X_A(i)\Delta_A^2(i)]$$

$$\times\,[(j_B+\tfrac{1}{2})/j_A+\tfrac{1}{2})]^{\frac{1}{2}}\;G^{ii}(AABBO)\;.$$

The corresponding generalization for Eq. (II.45) is

$$\begin{pmatrix} P11 & P12 & Q11 & 0 \\ P21 & P22 & 0 & Q22 \\ R11 & R12 & S11 & 0 \\ R21 & R22 & 0 & S22 \end{pmatrix} \begin{pmatrix} \frac{\partial\rho_a(1)}{\partial\beta} \\ \frac{\partial\rho_a(2)}{\partial\beta} \\ \frac{\partial k_a(1)}{\partial\beta} \\ \frac{\partial k_a(2)}{\partial\beta} \end{pmatrix}$$

$$= \begin{pmatrix} -\lambda(1)Y(1)\Delta^2(1) - \eta(1)X(1)[E^2(1)+\eta(1)\lambda(1)] \\ -\lambda(2)Y(2)\Delta^2(2) - \eta(2)X(2)[E^2(2)+\eta(2)\lambda(2)] \\ \Delta(1)E^2(1)X(1) + \Delta(1)[X(1)-Y(1)]\,\eta(1)\lambda(1) \\ \Delta(2)E^2(2)X(2) + \Delta(2)[X(2)-Y(2)]\,\eta(2)\lambda(2) \end{pmatrix}$$

APPENDIX X

LEVEL DENSITY FOR THE ODD-PARTICLE SYSTEM

The expressions for state and level densities obtained in Chapter II refer only to doubly even nuclei, since the formalism of the superconductivity theory describes the behavior of pairs of particles. If one or both of the nucleon numbers are odd, the presence of the last odd particle (or particles) must be taken into account in the calculation of level densities. In the ground state, the odd nucleus (with A+1 nucleons) has already one quasi particle compared to the doubly even nucleus (with A nucleons) and the odd nucleon occupies the first level over the Fermi one. The ground state of a nucleus with an odd number of neutrons or protons corresponds, therefore, to the state of doubly even nucleus with an excitation energy $E_a = [(\epsilon_a - \mu_a - \lambda)^2 + \Delta_a^2]^{\frac{1}{2}}$ (or $E_a + E_{a'}$, if both the number of neutrons or protons are odd), where a(a') is the level nearest to the Fermi level for the given kind of particles. Also, the odd particle has the effect of reducing the pairing gap through blocking. For these reasons, the odd A nucleus reaches the same level density as the adjacent doubly even nucleus at a lower excitation energy. The level density of an odd-mass (or doubly odd) nucleus with an excitation energy E^* corresponds to the level density of an even nucleus with an excitation energy $E^* + E_a$ (or $E^* + E_a + E_{a'}$).

When calculating the level densities of odd-mass nuclei, the statistical quantities are evaluated for the adjacent doubly even nucleus and then the energy scale is shifted by an energy equivalent to that required to produce one quasi-particle.

$$\rho_{ee}(E^*,I) = \rho_{oe}[E^* - E_a(p), I]$$
$$= \rho_{eo}[E^* - E_a(n), I]$$
$$= \rho_{oo}[E^* - E_a(p) - E_a(n), I] .$$

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