Finite Temperature Cranked Nilsson-Strutinsky Method

The Nilsson-Strutinsky method is one among the most feasible way to do systematic calculations of the nuclear energy as a function of deformation and/or excitation. These calculations are based on the developments of Bohr and Mottelson in the early 1950s and the subsequent calculation of the nuclear single-particle orbitals as functions of deformation. However, it was the methods of calculating shell correction energy developed by Strutinsky \cite{37,38} that made it possible to do large-scale calculations with some realism that describe, for example, the fission process.

The Strutinsky's method of shell corrections \cite{37-39} has been successfully used in calculations of the nuclear deformation energy, with the concept of dividing the total nuclear binding energy into a smooth liquid-drop energy $E_{LDM}$ and an oscillating shell correction energy $\delta E$. In this macroscopic-microscopic method, shell corrections can be attributed to the fluctuations in the actual distribution of single-particle levels relative to a smooth distribution of levels. The macroscopic part is represented by a Rotating Liquid Drop Model (RLDM) discussed in §2.1 and the microscopic part is represented by an appropriate single-
2.1. The Rotating Liquid Drop Model

The liquid drop model of the nucleus draws an analogy between the nucleus and a charged liquid drop. It emphasizes the strong coupling between the motion of the individual nucleons in the nucleus. The first systematic study of a nucleus with very high spin, represented by a structureless, charged liquid drop subject to Coulomb and surface forces, was undertaken by Cohen, Plasil and Swiatecki [64]. Considering the nucleus to be spherical, the surface energy and Coulomb energy are given by

\[ E_s^0 = a_s A^{2/3} , \]
\[ E_c^0 = a_c \frac{Z^2}{A^{1/3}} , \]

where \( a_s \) and \( a_c \) are surface and Coulomb constants, \( Z \) and \( A \) the atomic number and the mass number of the nucleus.

For a deformed nucleus represented by the deformation parameters \( \beta \) and \( \gamma \), the surface and Coulomb energies are given by

\[ E_s(\beta, \gamma) = E_s^0 B_s(\beta, \gamma) , \]
\[ E_c(\beta, \gamma) = E_c^0 B_c(\beta, \gamma) . \]

The function \( B_s(\beta, \gamma) \) gives the dependence of the surface energy on shape and
is equal to the dimensionless ratio of the surface area of the shape in question to the area of the original sphere. The functions \( B_c(\beta, \gamma) \) is the dimensionless ratio of the electrostatic energy of a distorted shape distribution to that of the sphere. Both \( B_s(\beta, \gamma) \) and \( B_c(\beta, \gamma) \) are elliptic integrals which depend on the semi-axes lengths. Here the liquid drop energy \( E_{LDM} \) is given by the sum of Coulomb and surface energies as

\[
E_{LDM}(\beta, \gamma) = [(B_s(\beta, \gamma) - 1) + 2\chi(B_c(\beta, \gamma) - 1)a_s] A^{2/3}.
\]  

The values used for the parameters \( a_s \) and \( \chi \) are as follows: \( a_s = 19.7 \text{ MeV} \) and the fissility parameter \( \chi = \frac{2^2}{45A} \). It has to be noted that \( E_{LDM}(\beta, \gamma) \) is the binding energy relative to the binding energy of a sphere and hence is termed as deformation energy. Such a quantity is enough for us as we study only the variation of energy over the deformation space rather than its absolute value.

For rotating nuclei the simple rigid rotor formula can be applied and hence the total energy of the rotating nucleus is

\[
E_{RLDM}(\beta, \gamma) = E_{LDM} + \frac{\hbar^2 I^2}{2\mathcal{I}_{\text{rig}}(\beta, \gamma)},
\]

where \( \mathcal{I}_{\text{rig}}(\beta, \gamma) \) is the rigid body moment of inertia defined by \( \beta \) and \( \gamma \) including the surface diffuseness correction. In the case of an ellipsoidal shape described by the deformation parameter \( \beta \) and the triaxiality parameter \( \gamma \) the semi-axes \( R_x, R_y, R_z \) are given by

\[
R_x = R_0 \exp \left[ \sqrt{\frac{5}{4\pi}} \beta \cos \left( \gamma - \frac{2\pi}{3} \right) \right],
\]

\[
R_y = R_0 \exp \left[ \sqrt{\frac{5}{4\pi}} \beta \cos \left( \gamma - \frac{4\pi}{3} \right) \right],
\]

\[
R_z = R_0 \exp \left[ \sqrt{\frac{5}{4\pi}} \beta \cos \gamma \right].
\]
By volume conservation we have

\[ R_x R_y R_z = R_o^3, \tag{2.8} \]

where \( R_o = r_o A^{1/3} \) with \( r_o = 1.16 \text{ fm} \) is the radius of the spherical nucleus.

The moment of inertia about the z-axis is given by

\[ \frac{\Omega_{ng}(\beta, \gamma) + 2M b^2}{h^2} = \frac{1}{5} \frac{AM(R_x^2 + R_y^2)}{h^2} + \frac{2M b^2}{h^2}, \tag{2.9} \]

where the diffuseness correction to the moment of inertia is \( 2M b^2 \) and the diffuseness parameter \( b = 0.87 \text{ fm} \).

### 2.2. The Single-Particle Potential

The shell energy calculations for non-rotating case \((I = 0)\) assumes a single particle field

\[ H_0 = \sum h_0, \tag{2.10} \]

where \( h_0 \) is the triaxial Nilsson Hamiltonian given by

\[ h_0 = \frac{p^2}{2m} + \frac{1}{2} m \sum_{i=1}^{3} \omega_i^2 x_i^2 + C \ell \cdot s + D \left( \ell^2 - 2 \langle \ell^2 \rangle \right). \tag{2.11} \]

The three oscillator frequencies \( \omega_i \) are given by the Hill Wheeler parameterization as

\[
\begin{align*}
\omega_x &= \omega_0 \exp \left[ -\sqrt{\frac{5}{4\pi}} \beta \cos \left( \gamma - \frac{2}{3} \pi \right) \right], \tag{2.12a} \\
\omega_y &= \omega_0 \exp \left[ -\sqrt{\frac{5}{4\pi}} \beta \cos \left( \gamma - \frac{4}{3} \pi \right) \right], \tag{2.12b} \\
\omega_z &= \omega_0 \exp \left[ -\sqrt{\frac{5}{4\pi}} \beta \cos \gamma \right]. \tag{2.12c}
\end{align*}
\]
with the constraint of constant volume for equipotentials

\[ \omega_x \omega_y \omega_z = \dot{\omega}_0^3 = \text{constant}, \quad (2.13) \]

where the oscillator frequency is chosen as

\[ h\dot{\omega}_0 = \frac{45.3}{(A^{1/3} + 0.77)} \text{MeV}. \quad (2.14) \]

In the expression for \( h_0 \) (Eq. 2.11), the term \( \langle \ell^2 \rangle \) has been doubled to obtain better agreement between the Strutinsky-smoothed moment of inertia and the rigid rotor value. Accordingly, the parameter \( D \) corresponding to a mass region has to be redetermined with the help of single-particle levels in the given mass region. The Hamiltonian (2.11) is diagonalized in cylindrical representation [65] upto \( N = 11 \) shells using the matrix elements given in [6]. Here \( N_{osc} \) is the harmonic oscillator principal quantum number.

For the rotating case \((I \neq 0)\), the Hamiltonian becomes

\[ H_\omega = H_0 - \omega J_z = \sum h_\omega, \quad (2.15) \]

where

\[ h_\omega = h_0 - \omega j_z, \quad (2.16) \]

if it is assumed that the rotation takes place around the \( z \)-axis. The single particle energy \( e_\omega \) and the wave function \( \phi_\omega \) are given by

\[ h_\omega \phi_\omega = e_\omega \phi_\omega. \quad (2.17) \]

The spin projections are obtained as

\[ \langle m_i \rangle = \langle \phi_\omega | j_z | \phi_\omega \rangle. \quad (2.18) \]
The total shell energy is given by

\[ E_{sp} = \sum \langle \phi_i^\omega | h_0 | \phi_i^\omega \rangle = \sum \langle e_i \rangle , \quad (2.19) \]

where

\[ e_i^\omega = \langle e_i \rangle - \hbar \omega \langle m_i \rangle . \quad (2.20) \]

Thus

\[ E_{sp} = \sum e_i^\omega + \hbar \omega I . \quad (2.21) \]

The total spin \( I \) from the shell model is given by

\[ I = \sum \langle m_i \rangle . \quad (2.22) \]

The sums should be carried out over the occupied states where the occupation is determined from the order of the quantities \( e_i^\omega \).

2.3. Finite Temperature Effects

The natural way to study the hot nuclear systems is to apply our knowledge about Fermi-Dirac statistics to nuclei. For an ideal Fermi-Dirac gas of \( N \) particles, the most probable number of particles with energy \( e_i \) is

\[ n_i = \frac{g_i}{1 + \exp (\alpha + \beta e_i)} . \quad (2.23) \]

where \( \beta = 1/kt \) and \( \alpha = -e_F/kt \) and \( g_i \) is the degeneracy of the \( i^{th} \) level. Here \( k \) is the Boltzmann's constant, \( t \) is the Temperature and \( e_F \) is the energy of the
Fermi level. Since due to Pauli’s exclusion principle no energy state can accommodate more than one particle, the maximum number of particles that can be accommodated in an energy level, \( g_i = 1 \) for our problem. Also for our practical calculation purposes, we represent the temperature in units of the Boltzmann’s constant \( (T = kT) \), which makes the temperature to have the units of energy. With these choices, the quantity \( n_i \) gives the probability for the level \( i \) with energy \( e_i \) being occupied and hence we define \( n_i \) as the occupation probability given by

\[
n_i(e_i, \lambda) = \frac{1}{1 + \exp \left( \frac{e_i - \lambda}{T} \right)}.
\]

The chemical potential \( \lambda \) is obtained using the constraint \( \sum_{i=1}^{\infty} n_i = N \), where \( N \) is the total number of particles. The internal energy is given by

\[
E = \sum_{i=1}^{\infty} e_i n_i. \tag{2.25}
\]

The entropy is given by

\[
S = \sum_{i=1}^{\infty} s_i = - \sum_{i=1}^{\infty} \left[ n_i \ln n_i - (1 - n_i) \ln(1 - n_i) \right]. \tag{2.26}
\]

The nuclear spin is obtained as

\[
I = \sum_{i=1}^{\infty} m_i n_i. \tag{2.27}
\]

The quantities \( E, S \) and \( I \) have to be calculated separately for protons and neutrons. The total summed energy \( E = E_p + E_N \), the total entropy \( S = S_P + S_N \) and the total spin \( I = I_P + I_N \). To study equilibrium properties of statistically distributed particles, it is meaningful to use the free energy instead of the summed energy. The free energy is given by

\[
F = E - TS. \tag{2.28}
\]
Fig. 2.1. Dependence of single-proton energies upon single-particle number for the \(^{90}\text{Zr}\) nucleus. The discrete energies are shown by a “staircase” function \(e_{\text{stair}}(\mathcal{N})\). The smooth curve \(e_{\text{smooth}}(\mathcal{N})\) removes the local fluctuations of \(e_{\text{stair}}(\mathcal{N})\) but retains its long-range behaviour.

2.4. Shell Correction Methods

2.4.1. The Strutinsky Energy Theorem

According to Strutinsky [37] the total energy is written as the sum of the LDM energy and the shell correction

\[
E_{TOT} = E_{LDM} + \sum_{p,n} \delta E .
\]  

(2.29)

Following Refs. [36,41] we illustrate the method with the aid of Fig. 2.1. For a deformed \(^{90}\text{Zr}\) nucleus, the step curve \((e_{\text{stair}}(\mathcal{N}))\) gives the dependence of the calculated single-proton energies \(e_{\mathcal{N}}\) upon the single-particle number \(\mathcal{N}\). This
pattern is however universal and is independent of the choice of the nucleus. For a macroscopic system without single-particle effects all the energies would lie on a smooth curve, but the discreteness of the single-particles causes some fluctuations about a monotonic increasing function of $N$. The discrete energies $e_i$ can be regarded as a "staircase" function $e_{\text{stair}}(N)$ formed by horizontal and vertical lines through the points.

The deformation energy within any single-particle model is given by the sum of single-particle energies of all occupied states, i.e,

$$E = \sum_{i=1}^{N} e_i = \int_0^{N} e_{\text{stair}}(N)$$ \hspace{1cm} (2.30)

We next remove the local fluctuations of $e_{\text{stair}}(N)$ while retaining its long-range behaviour by passing a smooth curve $e_{\text{smooth}}(N)$ through the staircase function. Then the shell correction for a specified particle number $N$ is given simply by the difference between the area under staircase curve and the area under smooth curve up to $N$, that is,

$$\delta E = \int_0^{N} [e_{\text{stair}}(N) - e_{\text{smooth}}(N)]dN.$$ \hspace{1cm} (2.31)

Hence the shell correction is the difference between the deformation energies evaluated with a discrete single-particle spectrum and with a smooth (averaged) spectrum corresponding to the discrete single-particle spectrum. We require a consistent method to get a smooth spectrum corresponding to a given single-particle energy spectrum. As the difference in energies between deformations is of the order of few MeVs, any uncertainty in our method should be well below that level. Also the results of the method we adopt should not vary with the choice of free parameters, if any.
Let us rewrite Eq. (2.31) as

$$\delta E = E - \bar{E} = \int_0^N e(N)dN - \int_0^N \bar{e}(N)dN .$$

(2.32)

Now our problem is to evaluate the integrals $E$ and $\bar{E}$. Practically $E$ can be evaluated by summing up the single particle energies. But $E$ is defined by an integral in our discussion for the sake of generality. As the single-particle number $N$ may not serve well as a continuous independent variable, and for later convenience we choose $e$ as the independent variable. In other words we choose the single-particle energy $e$ as a function of the single-particle number $N$. Changing the variable and corresponding limits, we have
\[ \delta E = \int_{-\infty}^{\lambda} e \frac{dN(e)}{de} \, de - \int_{-\infty}^{\lambda} e \frac{d\tilde{N}(e)}{de} \, de. \quad (2.33) \]

One can easily identify the term \( \frac{dN(e)}{de} \) as the level density \( g(e) \) and writing the above relation in terms of level densities, we have

\[ \delta E = \int_{-\infty}^{\lambda} e \, g(e) \, de - \int_{-\infty}^{\lambda} e \, \tilde{g}(e) \, de. \quad (2.34) \]

Recollecting that \( N(e) \) is the total number of nucleons that can be accommodated by the levels with energies \( \leq e \), we can write

\[ N(e) = \int_{-\infty}^{e} \frac{dN(e)}{de'} \, de' = \int_{-\infty}^{e} g(e') \, de'. \quad (2.35) \]

Since \( \lambda \) and \( \tilde{\lambda} \) can be found using the constraints \( N(\lambda) = N \) and \( \tilde{N}(\tilde{\lambda}) = N \), the only thing that remains is the evaluation of level density. The evaluation of the level density and its smooth counterpart can be well understood using the occupation number representation which follows. If we have \( e_i \) set of energy levels, we can write the total number of nucleons in terms of the occupation numbers \( n_i \) as

\[ N = \sum_{i=1}^{\infty} n_i(e_i, \lambda) = N(\lambda). \quad (2.36) \]

From the above relation we can write the level density as

\[ g(e) = \frac{dN(e)}{de} = \frac{dN(\lambda)}{d\lambda} \bigg|_{\lambda=e} = \sum_{i=1}^{\infty} \frac{dn_i(e_i, \lambda)}{d\lambda} \bigg|_{\lambda=e}. \quad (2.37) \]

### 2.4.2. Shell corrections at ground state

At the ground state the occupation probability can be defined as
\[ n_i = \begin{cases} 1 & -\infty \leq e_i \leq \lambda \\ 0 & \text{otherwise} \end{cases} \quad (2.38) \]

\[ = \sum_{k=1}^{N} \delta(e_k, e_i) . \quad (2.39) \]

Assuming \( e_k \) to be continuous, we can replace the summation with an integration and the Kronocker delta function with a Dirac delta function. Now we have

\[ n_i = \int_{-\infty}^{\lambda} \delta(e - e_i) \, de . \quad (2.40) \]

Substituting the above relation in Eq. (2.37), we can write directly

\[ g(e) = \sum_{i=1}^{\infty} \delta(e - e_i) . \quad (2.41) \]

From Eqs. (2.34) and (2.41) we have

\[ E = \int_{-\infty}^{\lambda} e \sum_{i=1}^{\infty} \delta(e - e_i) \, de = \sum_{i=1}^{N} e_i . \quad (2.42) \]

If we have to write an expression for \( \tilde{g}(e) \) similar to Eq. (2.41), the only possible difference will be the width of the delta function. Such a smooth level density will have the form

\[ \tilde{g}(e) = \sum_{i=1}^{\infty} \tilde{f} \left( \frac{e - e_i}{\gamma_s} \right) . \quad (2.43) \]

The function \( \tilde{f} \) should be smooth similar to a Gaussian

\[ \tilde{f}(u_i) = \frac{1}{\sqrt{\pi}} \exp(-u_i^2) , \quad (2.44) \]

with an integral normalized to unity. Here \( u_i = \frac{e - e_i}{\gamma_s} \) and the parameter \( \gamma_s \) should be chosen suitably such that the smoothed level distribution shows fluctuations only near major shell structures, and this suggests a value near \( \hbar \omega \) for the oscillator model. Using these expressions we can plot the Strutinsky smeared energy.
spectrum corresponding to a given single particle energy spectrum (See Fig. 2.2).

For simplicity we have derived the expression for smooth level density (2.43) using a direct comparison with the expression for its exact counterpart (2.41). A more precise definition is that the smooth level density is obtained by averaging out the exact single-particle level density with a weighting function. The weighting function here is \( f \). Hence the natural way of applying Strutinsky averaging to the level density is to convolute \( g(e) \) with the function \( \tilde{f}(u) \) [46]:

\[
\tilde{g}(e) = \frac{1}{\gamma_s} \int_{-\infty}^{\infty} \tilde{f} \left( \frac{e - e'}{\gamma_s} \right) g(e') \, de'.
\]  

(2.45)

2.4.2.1. Curvature correction

In practical calculations taking a Gaussian is not quite sufficient. The reason is that a smoothing procedure should not change the result appreciably when applied a second time. In principle we should require

\[
\tilde{g}(e) = \frac{1}{\gamma_s} \int_{-\infty}^{\infty} \tilde{f} \left( \frac{e - e'}{\gamma_s} \right) \tilde{g}(e') \, de'.
\]  

(2.46)

which is clearly not true for \( \tilde{f} \) of Gaussian form, but can be fulfilled exactly only with a delta function, which of course is unacceptable because it corresponds to no smoothing at all. The solution is that the formula need not be valid for an arbitrary function \( \tilde{g}(e) \), but only for those which are already sufficiently smooth on the scale of \( \gamma_s \) [3].

The customary way to construct \( \tilde{f} \) is to use a product of a Gaussian and a polynomial. The polynomial must be even in order not to change the averages over a level. The result of the calculations is
\[ \tilde{f}(u_i) = \frac{1}{\sqrt{\pi}} \exp\left(-u_i^2\right) \sum_{m=0}^{p} C_m H_m(u_i), \quad (2.47) \]

where \( C_m = \begin{cases} \frac{(-1)^{m/2}}{2^m(m/2)!} & \text{if } m \text{ is even} \\ 0 & \text{if } m \text{ is odd} \end{cases} \), and \( u_i = \frac{\varepsilon_{\xi_i}}{\gamma_s} \) with \( \gamma_s \) a new parameter determining the degree of the polynomial or the order of smearing and \( H_m \) are the Hermite polynomials. The lower order polynomials give smooth distribution and higher order polynomials are sharp functions. We call the new function as Gaussian with curvature correction. The illustration of getting the level densities with higher order curvature corrections (sharp functions) and lower order curvature corrections (smooth functions) is depicted in Fig. 2.3.

From Fig. 2.3(b), it is clear that the smooth level density and hence the shell corrections get contributions from levels far from the Fermi energy also. Hence while calculating shell corrections, one essentially has to work with a large configuration space (more energy levels). The choice of the configuration space depends on how far the smoothing function \( \tilde{f} \) spreads over, or in other words it depends on the width of the smoothing function. Obviously this width can be related to the smearing parameter \( \gamma_s \). Hence as an optimum choice [66], levels which are placed within the energy range \( 2\gamma_s \) from the Fermi energy should be included in the calculations.

2.4.2.2. Plateau condition

It remains to determine the parameters \( p \) and \( \gamma_s \). Ideally, the results should not depend on the precise values in a "broad" range of reasonable values. In practice one finds that \( p = 6 \) usually is sufficient, and for oscillator potentials there is indeed a broad range of \( \gamma_s \) values near \( \gamma_s = \hbar \omega \) with approximately
Fig. 2.3. (a) Illustration of getting level density carrying local fluctuations using a sharp Gaussian with curvature corrections. The sharp lines in the middle represents the actual energy levels used. (b) Illustration of getting level density without local fluctuations using a smooth Gaussian with curvature corrections.
constant $\delta E$. In compact notations we can write the plateau conditions as [40]

$$\frac{d\bar{E}}{d\gamma_s} = 0$$ \hspace{1cm} (2.48)

and

$$\bar{E}^p(\gamma_s^p) = \bar{E}^{p+2}(\gamma_s^{p+2})$$ \hspace{1cm} (2.49)

2.4.2.3. Exact solutions

Now we write the smooth level density as

$$\tilde{g}(e) = \sum_{i=1}^{\infty} \tilde{g}_i(e) = \frac{1}{\gamma_s} \sum_{i=1}^{\infty} f \left( \frac{e - e_i}{\gamma_s} \right) ,$$ \hspace{1cm} (2.50)

where $\tilde{f}$ is given by Eq. (2.47). Given the smooth level density, the first quantity to be determined is the Fermi energy $\lambda$. To evaluate $\lambda$ we use the particle number constraint $\bar{N}(\lambda) = N$. Writing $\bar{N}(e)$ in terms of $\tilde{g}(e)$ we get a relation similar to Eq.(2.35),

$$\bar{N}(e) = \frac{1}{\gamma_s} \sum_{i=1}^{\infty} \int_{-\infty}^{e} \tilde{f}(u_i) \, du' .$$ \hspace{1cm} (2.51)

This integral can be solved analytically [41] to give

$$\bar{N}(e) = \sum_{i=1}^{\infty} \left\{ \frac{1}{2} [1 + \text{erf}(u_i)] - \frac{1}{\sqrt{\pi}} \exp(-u_i^2) \sum_{m=1}^{p} C_m H_{m-1}(u_i) \right\} .$$ \hspace{1cm} (2.52)

From the above relations we can write

$$N = \bar{N}(\bar{\lambda}) = \sum_{i=1}^{\infty} \bar{n}_i ,$$ \hspace{1cm} (2.53)

where $\bar{n}_i$ are the smoothed occupation numbers given by
\[ \bar{n}_i = \frac{1}{2} \left[ 1 + \text{erf}(u_i) \right] - \frac{1}{\sqrt{\pi}} \exp(-u_i^2) \sum_{m=1}^{p} C_m H_{m-1}(u_i) . \] (2.54)

From Eqs. (2.34) and (2.50) we have

\[ \tilde{E} = \frac{1}{\gamma_s} \sum_{i=1}^{\infty} \int_{-\infty}^{\lambda} e^{-\frac{1}{\gamma_s} \left( \frac{e - e_i}{e} \right)} \, de . \] (2.55)

This integral also can be solved analytically [41] to give

\[ \tilde{E} = \sum_{i=1}^{\infty} \left\{ \frac{1}{2} e_i \left[ 1 + \text{erf}(\tilde{u}_i) \right] - \frac{1}{2\sqrt{\pi}} \gamma_s \exp(-\tilde{u}_i^2) - \frac{1}{\sqrt{\pi}} \exp(-\tilde{u}_i^2) \right\} , \] (2.56)

where \( \tilde{u}_i = \frac{\lambda - e_i}{\gamma_s} \). The above relation can also be written as [47]

\[ \tilde{E} = \sum_{i=1}^{\infty} e_i \tilde{n}_i - \gamma_s \tilde{M}_c , \] (2.57)

with

\[ \tilde{M}_c = \frac{1}{2\sqrt{\pi}} \sum_{i=1}^{\infty} C_p H_p(\tilde{u}_i) \exp(-\tilde{u}_i^2) . \] (2.58)

The term \( \tilde{M}_c \) can be shown equivalent to \( \frac{d\tilde{E}}{d\gamma_s} \) and can be neglected utilizing the plateau condition (2.48). However inclusion of this term makes \( \tilde{E} \) to be less sensitive to \( \gamma_s \) and hence gives us a broader plateau. Finally the expression for shell corrections at ground state reads

\[ \delta E = \sum_{i=1}^{N} e_i - \left( \sum_{i=1}^{\infty} e_i \tilde{n}_i - \gamma_s \tilde{M}_c \right) . \] (2.59)

Similarly for the spin distribution, the Strutinsky smoothed spin is given by

\[ \tilde{I} = \sum_{i=1}^{\infty} m_i \tilde{n}_i . \] (2.60)
2.4.3. Shell corrections at finite temperature

As we have already defined the level density in terms of occupation probability, the extraction of shell corrections can be done straight away by evaluating the level density using the definition of temperature dependent occupation probability. At finite temperature the occupation probability follows a Fermi-Dirac distribution defined by

\[
    n_i = \frac{1}{1 + \exp \left( \frac{e_i - \lambda}{T} \right)} .
\]

(2.61)

The temperature dependent level density can be easily derived using Eq. (2.37) as \[46,67\],

\[
    g_T(e) = \sum_{i=1}^{\infty} \frac{dn_i(e_i, \lambda)}{d\lambda} \bigg|_{\lambda=e} = \sum_{i=1}^{\infty} f_T(e - e_i) ,
\]

(2.62)

where

\[
    f_T(e - e_i) = \frac{1}{4T \cosh^2[(e - e_i)/2T]} .
\]

(2.63)

From the definition (2.62) it is clear that our energy spectrum is no longer discrete as we allow the level density to vary smoothly with its peaks at our old discrete levels. Increasing the temperature will result in the increase of the width of the function (2.63) and subsequently will make the level density to vary smoothly with respect to the single particle energy. This situation is well explained by Fig. 2.4, in which the temperature dependent single-particle level density (2.62) is plotted as a function of single-particle energy. It is clearly seen in the figure that around \( T = 3 \) MeV the level density ceases to fluctuate. This
Fig. 2.4. Temperature dependent single-particle level densities at different temperatures. The energy levels are the same used in Figs. 2 and 4. One component corresponding to a single energy level has been shown in the inset for sample. It is evident that the rise in temperature leads to an increase in the width of the components and hence leads to a smooth energy spectrum.

behavior of $g_T(e)$ is very similar to the Strutinsky smoothing function $\tilde{g}(e)$ and hence there is no difference between the Strutinsky smoothed spectrum and the exact single-particle spectrum at high temperatures. This implies that the shell correction will become zero at such instances.

A simulation of such temperature induced smoothing of energy levels has been carried out and and the resulting spectrum is shown in Fig. 2.5. As ex-
Fig. 2.5. (a) A typical single-particle energy spectrum. (b) Simulation of thermal effect on smoothing of the single-particle spectrum (a) at a temperature 0.5 MeV. (c) Simulation of Strutinsky smoothing of the single-particle spectrum (a). Now the shell correction comes from the difference between (b) and (c) which will always be less than that between (a) and (c). At higher temperatures, (b) and (c) will be similar leading to the disappearance of shell correction.

Expected, at higher temperatures the exact single-particle spectrum coincides with the Strutinsky smoothed spectrum. Examination of the width of the function (2.63) will reveal the enlargement to be made to the configuration space comprising single-particle levels.

The function (2.63) is very close to a Gaussian and we have our Strutinsky smeared single-particle level density as a Gaussian with curvature correction given by Eq.(2.50). The relation between the two smoothing quantities is given by [67]
Fig. 2.6. Upper limits for critical temperatures (in MeV) as a function of mass number and smearing width.

\[ T \approx 0.472 \gamma_s . \] (2.64)

If we have \( \gamma_s \) in the order of the inter-shell spacing (\( \hbar \omega \)), the above relation suggests that temperatures above half of the inter-shell spacing will wash out shell corrections.

Now we proceed to look for a consistent method to calculate shell corrections at finite temperatures. We have to get a Strutinsky smoothed level density (or energy spectrum) which is already smoothed to some extent due to the thermal effect (See Figs. 2.4 and 2.5). From Eq.(2.45), the natural way of applying Strutinsky averaging to the level density is to convolute \( g_T(\epsilon) \) with the function \( \tilde{f}(u_i) \) [46]:

\[
\bar{g}_T(\epsilon) = \frac{1}{\gamma_s} \int_{-\infty}^{\infty} \tilde{f} \left( \frac{\epsilon - \epsilon'}{\gamma_s} \right) g_T(\epsilon') \, d\epsilon'. \] (2.65)
The shell correction at finite temperature is given by

$$\delta F = F - \bar{F} = \int_{-\infty}^{\lambda} e \ g_T(e) \ de - \int_{-\infty}^{\tilde{\lambda}} e \ \tilde{g}_T(e) \ de , \tag{2.66}$$

where $F = E - TS$ is the free energy. Let us first evaluate the integral $F$. Using Eq. (2.62) we can write

$$F = \sum_{i=1}^{\infty} \int_{-\infty}^{\lambda} e \ f_T(e - e_i) \ de . \tag{2.67}$$

Utilizing the constraint for the number of particles,

$$N = \int_{-\infty}^{\lambda} g_T(e) \ de = \sum_{i=1}^{\infty} \int_{-\infty}^{\lambda} f_T(e - e_i) \ de = \sum_{i=1}^{\infty} n_i , \tag{2.68}$$

and after some calculations we can evaluate the integral for $F$ to yield the usual expression

$$F = \sum_{i=1}^{\infty} e_i n_i - T \sum_{i=1}^{\infty} s_i = E - TS . \tag{2.69}$$

The above relation and the expression for $\bar{F}$ has been derived in ref. [46]. Here we attempt a compact derivation involving minimum mathematical details. Inserting Eq. (2.65) in the expression for $\bar{F}$, we have

$$\bar{F} = \int_{-\infty}^{\lambda} e \ \frac{1}{\gamma_s} \int_{-\infty}^{\infty} \tilde{f} \left( \frac{e - e'}{\gamma_s} \right) g_T(e') \ de' \ de , \tag{2.70}$$

$$\bar{F} = \sum_{i=1}^{\infty} 1 \ \gamma_s \int_{-\infty}^{\lambda} e \ \int_{-\infty}^{\infty} \tilde{f} \left( \frac{e - e'}{\gamma_s} \right) f_T(e' - e_i) \ de' \ de . \tag{2.71}$$

After substituting $e' = e - \gamma_s x$ and using the fact that $\tilde{f}(x)$ is an even function, we get

$$\bar{F} = \sum_{i=1}^{\infty} \int_{-\infty}^{\infty} \tilde{f}(x) \int_{-\infty}^{\lambda} e \ f_T(e - \gamma_s x - e_i) \ de \ dx = \int_{-\infty}^{\infty} \tilde{f}(x) F(x) \ dx , \tag{2.72}$$

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where $F(x)$ is defined exactly as $F$, Eq. (2.67), if we replace there $e_i \rightarrow e_i + \gamma_s x$ and $\lambda \rightarrow \tilde{\lambda}$. We can therefore immediately use the form of $F$, Eq. (2.69), to write with the same replacements

$$
\tilde{F} = \int_{-\infty}^{\infty} \tilde{f}(x) \sum_i \left[ (e_i + \gamma_s x)n_i(x) - Ts_i(x) \right] dx ,
$$

(2.73)

where

$$
n_i(x) = \frac{1}{1 + \exp\left( \frac{e_i + \gamma_s x - \lambda}{\tilde{\lambda}} \right)} ,
$$

(2.74)

$$
s_i = - \left[ n_i(x) \ln n_i(x) + (1 - n_i(x)) \ln (1 - n_i(x)) \right] .
$$

(2.75)

Again we can split the integral (2.73) as

$$
\tilde{F} = \sum_i \left[ e_i \int_{-\infty}^{\infty} \tilde{f}(x)n_i(x)dx + \gamma_s \int_{-\infty}^{\infty} \tilde{f}(x)xn_i(x)dx - T \int_{-\infty}^{\infty} \tilde{f}(x)s_i(x)dx \right] ,
$$

(2.76)

$$
= \sum_i \left[ e_i \tilde{n}_i - Ts_i \right] + \gamma_s \int_{-\infty}^{\infty} \tilde{f}(x)x \sum_i n_i(x)dx ,
$$

(2.77)

where

$$
\tilde{n}_i = \int_{-\infty}^{\infty} \tilde{f}(x) n_i(x) \ dx ,
$$

(2.78)

$$
\tilde{s}_i = \int_{-\infty}^{\infty} \tilde{f}(x) s_i(x) \ dx .
$$

(2.79)

After substituting $x = \frac{e - e_i}{\gamma_s}$ in Eqs. (2.78) and (2.79) we get

$$
\tilde{n}_i = \frac{1}{\gamma_s} \int_{-\infty}^{\infty} \tilde{f} \left( \frac{e - e_i}{\gamma_s} \right) n_i(e, \tilde{\lambda}) \ de ,
$$

(2.80)

$$
\tilde{s}_i = \frac{1}{\gamma_s} \int_{-\infty}^{\infty} \tilde{f} \left( \frac{e - e_i}{\gamma_s} \right) s_i(e, \tilde{\lambda}) \ de ,
$$

(2.81)
which are consistent with our previous argument [Eq. (2.65)]. However, now we have to get rid of the last term in Eq. (2.77). To recognize the relevance of that term, we calculate the total derivative of \( \bar{F} \) with respect to \( \gamma_s \) from the following equations.

\[
\bar{F} = \int_{-\infty}^{\lambda} \epsilon \, \bar{g}_T(\epsilon) \, d\epsilon ,
\]

(2.82)

and

\[
N = \int_{-\infty}^{\lambda} \bar{g}_T(\epsilon) \, d\epsilon = \sum_{i=1}^{\infty} \bar{n}_i^T ;
\]

(2.83)

\[
\frac{d\bar{F}}{d\gamma_s} = \frac{d}{d\gamma_s} \left( \bar{F} - \lambda N \right) = \int_{-\infty}^{\lambda} (e - \lambda) \frac{d}{d\gamma_s} \bar{g}_T(\epsilon) \, d\epsilon .
\]

(2.84)

From Eqs. (2.65) and (2.62), we find, substituting again \( e' = e - \gamma_s x \),

\[
\frac{d}{d\gamma_s} \bar{g}_T(\epsilon) = \int_{-\infty}^{\infty} f(x) dx \sum_i (-x) \frac{d}{de} f_T(e - \gamma_s x - e_i) .
\]

(2.85)

Inserting Eq. (2.85) into Eq. (2.84), we get after partial integration over \( e \) and using Eq. (2.62),

\[
\frac{d\bar{F}}{d\gamma_s} = \sum_i \int_{-\infty}^{\infty} f(x) x n_i(x) dx.
\]

(2.86)

This give for \( \bar{F} \), with Eq. (2.77),

\[
\bar{F} = \sum_i \left[ e_i \bar{n}_i - T \bar{s}_i \right] + \gamma_s \frac{d\bar{F}}{d\gamma_s} .
\]

(2.87)

Now, when Strutinsky averaging one wants to obtain results that are (at least locally) independent of the averaging parameter \( \gamma_s \). Thus, we use here, the plateau condition

\[
\frac{d\bar{F}}{d\gamma_s} = 0,
\]

(2.88)
which then leads to the result for $\bar{F}$,

$$\bar{F} = \sum_i [e_i \bar{n}_i - T \bar{s}_i] = \bar{E} - T \bar{S}.$$  \hfill (2.89)

2.4.3.1. Numerical evaluation

We can evaluate $\bar{n}_i$ and $\bar{s}_i$ given by the relations (2.80) and (2.81) respectively, using a 32 point Gauss-Hermite quadrature. We call this method as the Numerically Exact Method (NEM). However, we can obtain an alternative form of $\bar{F}$ starting from Eq. (2.71) again. Adding and subtracting the same quantity [46], we can rewrite $\bar{F}$ as

$$\bar{F} = \sum_i \frac{1}{\gamma_s} \int_{-\infty}^{e_i} \int_{-\infty}^{\tilde{\lambda}} (e - e') f\left(\frac{e - e'}{\gamma_s}\right) f_T(e' - e_i) \, de \, de'$$

$$+ \sum_i \frac{1}{\gamma_s} \int_{-\infty}^{e_i} e' f_T(e' - e_i) \, de' \int_{-\infty}^{\tilde{\lambda}} f\left(\frac{e - e'}{\gamma_s}\right) \, de. \hfill (2.90)$$

The first term in Eq. (2.90), after substituting $e - e' = \gamma_s x$, is recognized as $\gamma_s d\bar{F}/d\gamma_s$ with Eq. (2.86), and thus is vanishing. The second term, with Eq. (2.62) gives the result for $\bar{F}$ as

$$\bar{F} = \int_{-\infty}^{\tilde{\lambda}} e g_T(e) \bar{n}(e - \tilde{\lambda}) \, de,$$  \hfill (2.91)

where $\bar{n}(e - \tilde{\lambda})$ is the usual Strutinsky occupation number function:

$$\bar{n}(e - \tilde{\lambda}) = \frac{1}{\gamma_s} \int_{-\infty}^{\tilde{\lambda}} f\left(\frac{e - e'}{\gamma_s}\right) \, de'.$$  \hfill (2.92)

which has analytical solution given by Eq. (2.52). Hence while using this alternate form we need have to perform only one numerical integration. However the function $g_T(e)$ is too sharp to perform 32 point Gauss-Hermite quadrature at
low temperatures and in all our calculations we evaluate the integrals given by Eqs. (2.80) and (2.81). The Strutinsky smoothed spin is given by

$$\bar{I} = \sum_{i=1}^{\infty} m_i \bar{n}_i ,$$

(2.93)

where $\bar{n}_i$ is defined by Eq. (2.80)

2.4.3.2. Evaluation by Maximum Term Approximation Method (MTAM)

The maximum term approximation method proposed by Civitarese et al. [47] provides an approximate solution for the integrals given in Eqs. (2.80) and (2.81) using the "maximum term approximation" of quantum statistical mechanics. The final result of the application of this approximation reads

$$\delta F = E(T) - TS - E(T = 0) + \bar{a}(\lambda_0)T^2 ,$$

(2.94)

where

$$\bar{a} = \frac{\pi^2}{6} \bar{g}(\lambda_0) .$$

(2.95)

The term $\bar{g}$ is given by

$$\bar{g}(e) = \frac{1}{\gamma_s} \int_{-\infty}^{\infty} f \left( \frac{e - e'}{\gamma_s} \right) g(e') \, de' ,$$

(2.96)

which has analytical solution.

Thus in this method we have contributions which can be considered of completely different nature, namely,

1. The $T$-independent shell correction $\bar{E}(\lambda_0, \gamma_s)$ (Eq.2.56), which is evaluated at $T = 0$;
2. The $T$-dependent discrete single-particle contribution $F(T)$ (Eq.2.69);

3. The smooth $T$-dependent term $(\pi^2/6)\bar{g}(\lambda_0)T^2$ in which $\bar{g}(\lambda_0)$ is evaluated at $T = 0$.

It has to be noted that in this method there is no need to perform any smoothing at finite temperatures. The above facts depict the advantages of this method over the numerically exact method described earlier. The final result of this rigorous mathematical derivation can be well understood with the aid of the following derivation based on few elementary relations. Let us start with the expression for the smoothed excitation energy

$$\tilde{E}^* = \tilde{E}(T) - \tilde{E}(T = 0).$$ \hfill (2.97)

Substituting $\tilde{E}^* = \tilde{a}T^2$ and rearranging, we get

$$\tilde{E}(T) = \tilde{E}(T = 0) + \tilde{a}T^2.$$ \hfill (2.98)

Subtracting $T\tilde{S}$ from both the sides give

$$\tilde{F}(T) = \tilde{E}(T = 0) + \tilde{a}T^2 - T\tilde{S}.$$ \hfill (2.99)

Substituting $\tilde{S} = 2\sqrt{\tilde{a}\tilde{E}^*} = 2\tilde{a}T$ on the right hand side, we get

$$\tilde{F}(T) = \tilde{E}(T = 0) - \tilde{a}T^2.$$ \hfill (2.100)

Hence the shell correction at finite temperature obtained by assuming $\tilde{E}^* = \tilde{a}T^2$ and $\tilde{S} = 2\sqrt{\tilde{a}\tilde{E}^*}$ is

$$\delta F = F(T) - \tilde{F}(T) = E(T) - TS - \tilde{E}(T = 0) + \tilde{a}T^2,$$ \hfill (2.101)
which is exactly the same result obtained using the maximum term approximation. It is interesting to note that in this expression for shell correction if we neglect the final term in the right hand side, this method reduces to the cold-nucleus approximation method (CNAM). Also the smooth level density $\bar{g}(\lambda_0)$ in the final term is a smeared or averaged quantity which is not much sensitive to the deformation of the nucleus. Hence while calculating the relative deformation energies at fixed temperature, the contribution from the final term is very low. If we assume $\bar{g}(\lambda_0)$ to be totally deformation independent, MTAM and CNAM give same results in deformation energy calculations. Otherwise we can say that within CNAM, the topography of the smoothed free energy surface with respect to deformation does not vary with temperature except by a constant factor due to the excitation energy. This is not a crude approximation and hence explains the success of the CNAM.

2.4.3.3. Statistical Method (SM)

The influence of shell effects in hot nuclei was first studied within the statistical theory [67,53]. In fact it was found that the statistical theory can explain the ground state shell corrections as well and it was first identified by Ramamurthy et al. [53]. This approach starts with the identification of the nuclear level density parameter 'a' as the key to extract information about the distribution of levels. The Fermi gas expression or the equidistant model gives the expression $S = 2\sqrt{aE^*}$. This expression, however, which is valid only for a system having a uniform spacing of single-particle levels, should be modified to include the nuclear shell effects. Hence a liquid drop behavior or an averaged energy spectrum will lead to a constant level density parameter and the variation of $S^2$ with
$E^*$ will be linear. On the other hand for a discrete single-particle spectrum exhibiting fluctuations in the distribution of levels, the variation of $S^2$ with $E^*$ will not be linear. The difference between these two trends contains the information about the shell effect. Further more asymptotically (at higher excitation energies) the single-particle spectrum also is expected to diffuse into a continuum having smooth variation in level density. Hence the study of variation of $S^2$ as a function of $E^*$ at asymptotic limits give information about the smooth (liquid drop) behavior and at lower excitation energies give the information about the shell structure.

This method is best explained with the aid of Fig. 2.7, following the original material [53], in which the calculations were done with a modified spherical harmonic-oscillator potential. It is seen that the curve deviates considerably from a straight line of the form $S^2 = 4aE^*$, expected from the Fermi gas model. However at excitation energies $E^2 > 30 - 40$ MeV an asymptotic behavior of the form

$$S^2 = 4a(E^* \pm \Delta E)$$

(2.102)

where $\Delta E$ represents the magnitude of the intercepts on the energy axis of the asymptotic straight lines, and $\pm$ signs refer to the two cases of positive and negative shell corrections, respectively. From the calculations for $^{208}Pb$ and $^{242}Pu$, it is seen that the shell corrections calculated using the Strutinsky's method are numerically equal to the energy intercepts $\Delta E$ of the asymptotic straight lines in both the cases within 0.2 MeV.

Moretto [67] later on claimed that the entropy square never becomes linear with excitation energy and $\Delta E$ never becomes a constant. The arguments be-
Fig. 2.7. Plot of $S^2$ vs $E^*$, for the cases of the doubly magic nucleus $^{208}\text{Pb}$ and the nucleus $^{242}\text{Pu}$ (spherical shape). The dashed curves in each case represent the asymptotic behavior at high excitation energies. (After [53])

hind such conclusion follow. Expanding the single-particle level density $g_T(e)$ about the chemical potential (similar to the maximum term approximation described in §2.4.3.2) and retaining terms up to second order, one obtains

$$S = \frac{2\pi^2}{6} T g_T(\lambda) \left( 1 + \frac{7\pi^2}{30} T^2 \frac{g''_T(\lambda)}{g'_T(\lambda)} \right)$$

(2.103)

It can be seen immediately that only if $g''_T(\lambda) = g'_T(\lambda) = 0$ then $\lambda = \text{constant}$
and \( S = (\pi^2/3)Tg_T = 2aT = 2\sqrt{aE^*} \). Only in such case a linear dependence of \( S^2 \) versus \( E^* \) is obtained. The condition \( g''_T(\lambda) = g'_T(\lambda) = 0 \) corresponds to a rather unrealistic case. Even the simple Fermi gas model deviates substantially from such conditions. However Moretto admits that if the excitation energy is suitably chosen, a correlation between the local value of \( \Delta E \) and the shell effect determined from the Strutinsky procedure is to be expected. Such a difficulty is always there while calculating shell corrections i.e. a crucial parameter has to be chosen such that the results doesn’t vary with the choice at least locally. In Strutinsky’s method it is the choice of smearing parameter \( \gamma_s \), and here it is the choice of optimum excitation energy (or temperature) range in which the asymptotic straight line fit has to be done.

Evaluation of shell corrections in this framework is quite easy that after choosing the optimum temperature we just have to fit a straight line for the asymptotical part of the \( S^2 \) versus \( E^* \) curve and deduct shell corrections at fixed temperature (and hence fixed entropy) by simply calculating the difference between the excitation energies given by the actual curve and the fitted line.

2.5. Pairing correlations

The analogy between the excitation spectra of nuclei and those of the superconducting metallic state was proposed by Bohr, Mottelson and Pines [68] soon after the work of Bardeen, Cooper and Schrieffer [69] on the theory of superconductivity. The inclusion of pairing correlations in the BCS approach provides accurate description of the ground state of medium and heavy nuclei. However the above mentioned analogy can be extended to describe excited nuclei as well.
The extension of BCS theory to describe hot nuclei is rather simple and straightforward thanks to the original work of Bardeen et al., [69] which itself comprises the BCS theory for excited states (hot metallic states). Sano and Yamasaki [70] demonstrated that hot nuclei can be treated with an approach very similar to that of BCS. In fact the BCS equations as well as the estimate for critical temperature at which pairing vanishes were found to be the same for both the hot metallic states and the hot nuclei.

2.5.1. The BCS Theory

2.5.1.1. The Ground State

We start by considering a reduced problem in which we include configurations in which the states are occupied in pairs such that if $k^+(k \uparrow)$ is occupied so is $k^-(k \downarrow)$ [69]. A pair is designated by the wave vector $k$, independent of spin. The Hamiltonian describing the pairing interaction may be written in the following form [71]:

$$H = \sum_k e_k (c^+_k c^+_k + c^+_k c^-_k) - G \sum_{kk'} c^+_k c^+_k c^-_k c^-_{k'},$$

(2.104)

where symbols $c^+_k$ and $c^-_k$ are creation and annihilation operators of the particles with opposite spin projections and the quantity $e_k$ the energy state of non-interacting fermions.

The most general wave function satisfying the pairing condition $(k^+, k^-)$ is of the form [69]:

$$\sum_{k_1 \cdots k_n} \left[ v^2(k_1 \cdots k_n) \right]^\frac{1}{2} f(\cdots 1(k_1) \cdots 1(k_n) \cdots),$$

(2.105)
where the sum extends over all distinct pair configurations. To construct our
ground state function we make a Hartree-like approximation in which the prob-
ability that a specific configuration of pairs occurs in the wave function is given
by a product of occupancy probabilities for the individual pair states. If for the
moment we relax the requirement that the wave function describes a system
with a fixed number of particles then a function having this Hartree-like prop-
erty is

$$\Psi = \prod_k [u_k + v_k c_{k+}^+ c_{k-}^+] \Phi_0,$$

(2.106)

where $\Phi_0$ is the vacuum. It follows from (2.106) that the probability of the $n$
states $k_1 \ldots k_n$ being occupied is $v^2(k_1) \ldots v^2(k_n)$, and since $n$ is unrestricted we
see that $\Psi$ is closely related to the intermediate coupling approximation.

Decomposing the wave function (2.106) and evaluating the matrix elements,
we get an expression for the ground-state energy. Minimizing the ground-state
energy with respect to $v_k^2$ yields the ground state BCS equations

$$\Delta = G \sum_k u_k v_k$$

(2.107)

and

$$N = 2 \sum_k v_k^2,$$

(2.108)

where

$$v_k^2 = \frac{1}{2} \left[ 1 - \frac{(e_k - \lambda)}{E_k} \right],$$

(2.109)

$$E_k = \sqrt{(e_k - \lambda)^2 + \Delta^2}$$

and $v_k^2 + u_k^2 = 1$. The parameter $\lambda$ is approximate to the
Fermi energy of the non-interacting fermion system. The quantity $\Delta$ is referred
to as the energy gap.

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2.5.1.2. Excited States

An excited state of the system will be formed by specifying the set of states, \( S \), which are occupied by single particles and the set of states, \( P \), occupied by excited pairs. The rest of the states, \( G \), will be available for occupation by ground pairs. The term "single-particle" occupation means that either \( k^+ \) or \( k^- \) is occupied by one particle, but not both.

According to Sano and Yamasaki [70], the sum of a fermion system taking account the pairing interaction may be represented by the formula

\[
Z = \text{Tr} \exp(-H_0/T),
\]

where

\[
H_0 = \sum_k (e_k - \lambda - E_k) + \frac{\Delta^2}{G} + \sum_{ks} E_k \alpha_{ks}^+ \alpha_{ks}.
\]

Summation over \( s \) means that summation is both over negative and positive values of spin projection, and \( T \) is the temperature of the system. The symbols \( \alpha_{ks}^+ \) and \( \alpha_{ks} \) are creation and annihilation operators of the quasi-particle in the \( ks \) state, respectively and are defined by the canonical Bogoliubov transformation.

A typical excited state wave function can be written as the projection of

\[
\Psi_{exc} = \prod_{k(G)} [u_k + v_k c_{k+} c_{k-}] \prod_{k'(P)} [u_{k'} c_{k'+} c_{k'-} - v_{k'}] \prod_{k''(S)} c_{(k'')}^+ \Phi_0,
\]

onto the space with \( N \) pairs, where \( G, P \) and \( S \) specify the states occupied by ground pairs, excited pairs, and single particles respectively and \( c_{(k'')}^+ \) denotes either \( k''+ \) or \( k''- \) is included in the product.

To determine the distribution functions, we need the free energy
\[ F = E - TS \] 

where \( E \) is the energy calculated by an ensemble average over the wave functions of the form (2.112) and \( S \) is the entropy. Decomposing the wave function and evaluating the matrix elements, we get an expression for the free energy. Minimization of the free energy with respect to \( v_k^2 \) gives the BCS equations for hot nuclei:

\[ \Delta = G \sum_k u_k v_k (1 - 2n_k^T) \]  
\[ \text{and } N = 2 \sum_k n_k^T + (1 - 2n_k^T)v_k^2 \]

where \( v_k^2 \) and \( u_k^2 \) are as same as defined earlier and \( n_k^T \) is the probability for a state \( k \) to be occupied by a thermally excited single particle. Minimizing the free energy with respect to \( n_k^T \) we get

\[ n_k^T = \frac{1}{1 + \exp(E_k/T)} . \]

Substituting the expressions for \( v_k^2 \), \( u_k^2 \) and \( n_k^T \) in (2.114 and 2.115) we get the explicit form of the BCS equations as

\[ \frac{2}{G} = \sum_k \left[ \frac{\tanh(E_k/2T)}{E_k} \right] \]  
\[ \text{and } N = \sum_k \left[ 1 - \frac{e_k - \lambda}{E_k} \tanh(E_k/2T) \right] . \]

The free energy including the pairing correlations is given by

\[ E_P = \sum_k e_k \left[ 1 - \frac{e_k - \lambda}{E_k} \tanh(E_k/2T) \right] - \frac{\Delta^2}{G} - TS , \]

where \( S \) is the entropy which is caused purely by the thermally excited nucleons. Hence the entropy is given by

\[ S = - \sum_k \left[ n_k^T \ln n_k^T + (1 - n_k^T) \ln(1 - n_k^T) \right] . \]
2.5.1.3. Ground state energy gap and critical temperature

It is possible to establish a relation between the ground state energy gap \[\Delta(T = 0) \equiv \Delta(0)\] and the critical temperature \(T_c\) at which the pairing correlations vanish \[\Delta(T_c) = 0\] with the aid of the following simplifying assumptions [69,70]:

1. The pairing strength \(G\) is constant within an energy interval \(\omega\) around the Fermi surface

\[|e_k - \lambda| \leq \omega, \tag{2.121}\]

and is equal to zero otherwise.

2. The sums over \(k\) can be approximated by integrals with the single particle level density set equal to a constant \(g\). In every case of our interest the assumption \(gG \ll 1\) is justified.

The energy gap \(\Delta(0)\) in the ground state is determined by the relation (2.107) which can be written as

\[\frac{2}{G} = \sum_k \frac{1}{\sqrt{(e_k - \lambda)^2 + \Delta^2}}. \tag{2.122}\]

With the aid of our assumptions we see that the energy gap is zero outside the region (2.121), while it is given by the solution of the following equation inside the region (2.121)

\[\frac{2}{gG} = \int_{-\infty}^{\infty} \frac{d\xi}{\sqrt{\xi^2 + \Delta^2(0)}}, \quad \xi = e - \lambda. \tag{2.123}\]

This equation gives
\[ \Delta(0) = \frac{\omega}{\sinh 1/gG}, \]  
\text{(2.124)}

and as \( gG \ll 1 \) is valid in our case, we have the approximate equality

\[ \Delta(0) = 2\omega \exp(-1/gG). \]  
\text{(2.125)}

At the critical temperature \( (T = T_c, \Delta = 0) \) the gap equation (2.117) becomes

\[ \frac{2}{G} = \sum_k \frac{\tanh[(e_k - \lambda)/2T_c]}{(e_k - \lambda)}. \]  
\text{(2.126)}

Utilizing our assumptions the above equation can be written as

\[ \frac{2}{gG} = \int_{-\infty}^{\infty} d\xi \frac{\tanh \frac{\xi}{2T_c}}{\xi}, \]  
\text{(2.127)}

from which we obtain

\[ T_c = 1.14\omega \exp(-1/gG). \]  
\text{(2.128)}

From Eqs. (2.125) and (2.128) we have the estimate for the critical temperature as

\[ T_c = 0.57 \Delta(0). \]  
\text{(2.129)}

The above relations are the same as those obtained by Bardeen et al. [69],

\[ 2\Delta(0)/T_c = 3.50. \]  
\text{(2.130)}

This gives a fairly good estimate for the critical temperature. The approximated function for the pairing gap is given by

\[ \Delta(T) = \Delta(0)\sqrt{1 - (T/T_c)^2} \]  
\text{(2.131)}

for \( T < T_c \), and \( \Delta(T) = 0 \) for \( T \geq T_c \).
2.5.2. A probabilistic view

The pairing problem as well as the statistical theory for hot nuclei, deal with partially filled energy levels and were essentially built on the probability theory. This section briefs the interplay between various probabilities we come across in the hot superconducting nuclei. Before entering further discussions, let us define explicitly the various probabilities we have.

\[
v_k^2 = \frac{1}{2} \left\{ 1 - \frac{e_k - \Delta}{E_k} \right\} \quad \text{Probability for which a state to be occupied by a pair at the limit } T \to 0.
\]

\[
n_k^T = \frac{1}{1 + \exp((e_k - \lambda)/T)} \quad \text{Probability for which a state to be occupied by a thermally excited nucleon at the limit } \Delta \to 0.
\]

\[
n_k = n_k^T (1 - n_k^T) \quad \text{Probability for which a state to be occupied by a thermally excited nucleon or by a thermally excited pair.}
\]

\[
p_k = (n_k^T)^2 \quad \text{Probability for which a state to be occupied by a thermally excited single nucleon.}
\]

\[
n_k = v_k^2 (1 - n_k^T) + (1 - v_k^2) n_k^T \quad \text{Overall probability for which a state to be occupied.}
\]

\[
n_k - s_k - p_k = (1 - 2s_k - 2p_k)v_k^2 \quad \text{Probability for which a state to be occupied by a ground state pair.}
\]

\[
2u_kv_k \sim \Delta/2G \quad \text{Pairing field strength at the limit } T \to 0.
\]

\[
2u_kv_k(1 - 2n_k) \sim \Delta/2G \quad \text{Overall pairing field strength.}
\]

As stated in the previous section, our excited state can have ground pairs, excited pairs and excited single particles. The ground pairs follow the distribution defined by \( v_k^2 \) if we neglect the influence of excited pairs and excited single
particles. The excited pairs and excited single particles follow the distribution defined by $n_k^T$. Hence we can assume the resultant distribution is the combined effect of these two distributions. One interesting point to note is that the excited pairs and excited single particles block the ground pairs against occupying their own levels. If we define $h_k$ as an event caused by the distribution $v_k^2$ and $f_k$ as an event caused by the distribution $n_k^T$, we have a constraint that $h_k$ and $f_k$ are mutually exclusive events. The combined events can be $h_k f_k$ and $h_k f_k$ and the resultant probability is given by

$$P(h_k f_k \cup h_k f_k) = P(h_k f_k) + P(h_k f_k)$$

$$= P(h_k) \cdot P(f_k) + P(h_k) \cdot P(f_k)$$

$$\Rightarrow n_k = v_k^2(1 - n_k^T) + (1 - v_k^2)n_k^T. \quad (2.132)$$

This is exactly what we have used for the overall occupation probability in Eq. (2.115) to conserve the total number of particles. But now we did it just using few simple arguments as we know the behaviour of the probabilities involved. With this motivation, an investigation has been carried out on the variation of all the defined probabilities with respect to the temperature and pairing strength. The results are given in Figures 2.8-2.13. In all the figures the lines in the bottom axis represents the corresponding energy levels. The temperature and pair gap $\Delta$ are fixed and $\lambda$ is found by iteration using the constraint $2 \sum_k n_k = N$. The figures are only schematic as the $\Delta$ is not obtained by solving the BCS equations through which the dependence on external parameter $G$ will come. Hence the results may give a good description about the overall behaviour of various probabilities as a function of temperature and pairing strength independent of the parameter $G$. However the only fact affecting the generality is the choice of energy levels and particle number.
Fig. 2.8. Various probabilities versus single particle energy at $T = 0.1$ MeV and $\Delta = 1.0$ MeV for 40 particles.

Fig. 2.8 represents the case $T = 0.1$ MeV and $\Delta = 1.0$ MeV and is very similar to that of ground state pairing. We infer that such a low temperature has nothing to affect the ground state behaviour. The long tail of the curve representing the pairing strength gains much significance as it depicts the complexity in fixing the pairing phase space (number of levels to be included). Also the choice of the pairing force strength will be strongly influenced by the choice of phase space. Figures 2.10, 2.11 and 2.12 suggests that at moderate temperatures even with a presence of strong pairing field strength, the overall probability is close to that of the Fermi-Dirac distribution. From Fig. 2.13 it is clear that at temperatures greater than 2.0 MeV there is no sign of pairing correlations even if we assume $\Delta = 0.5$ MeV. Other overall trends we observe from the figures are, the temperature effect destroys the pairing effect very rapidly and the probability for producing excited pairs is low.
Fig. 2.9. Same as Fig. 2.8 but for $T = 1.0 \text{ MeV}$ and $\Delta = 0.1 \text{ MeV}$.

Fig. 2.10. Same as Fig. 2.8 but for $T = 0.5 \text{ MeV}$ and $\Delta = 5.0 \text{ MeV}$. 
Fig. 2.11. Same as Fig. 2.8 but for $T = 1.0 \text{ MeV}$ and $\Delta = 1.0 \text{ MeV}$.

Fig. 2.12. Same as Fig. 2.8 but for $T = 1.0 \text{ MeV}$ and $\Delta = 0.5$. 

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2.5.3. Pairing energy at finite temperature and spin

The pairing correlations in rotating nuclei was put forth by Mottelson and Valatin [72]. In the case of rotating nuclei the Coriolis field on a superconducting nucleus has been treated analogous to the magnetic field in a superconductor. But many such approaches are not very precise and were built on many approximations [73,74]. Following a systematic study of a paired nucleus with the inclusion of angular momentum and temperature using statistical theory by L.G. Moretto [67], we write the expression for the pairing gap at finite spin as

$$\Delta = \Delta(I = 0)\sqrt{(1 - I/I_c)} ,$$

(2.133)

where $I_c$ is the critical spin at which pairing vanishes and is given by $I_c = gm\Delta(I = 0)$. Here $g$ is the single-particle level density and $m$ is the constant angular momentum projection. Neglecting the contribution of temperature as-
Fig. 2.14. Dependence of the critical temperature upon angular momentum. The parameters used in the calculation are $\Delta(T = 0, I = 0) = 1 \text{ MeV, } g = 7 \text{ MeV}^{-1}$. The solid lines correspond to the results of [67] and the dashed lines correspond to the approximation given by Eq. (2.134).

sisted pairing [67] and assuming the temperature effect and spin effect on pairing correlations are non-interfering, we have

$$
\Delta(T, I) = \min \left\{ \Delta(T = 0, I) \sqrt{1 - I/I_c}, \right.
\Delta(T, I = 0) \sqrt{1 - (T/T_c)^2} \right\}
$$

(2.134)

In Figs. 2.14 and 2.15 the above approximation is compared with the results of calculations based on statistical theory [67]. From the figures it is clear that this approximation at spins near the critical spin and temperatures near the critical temperature overestimates the pairing gap.

To include the correction in the free energy due to the pairing correlations, let us define the energy $P$ of the pairing correlations as the difference of the sums of single-particle energies evaluated with and without the pairing correlations.
Fig. 2.15. Contour map of the gap parameter as a function both of temperature and angular momentum. The spacing in $\Delta$ between two successive lines is 1.0 MeV from $\Delta = 1.0$ MeV to $\Delta = 0.1$ MeV. The outer line corresponds to $\Delta = 0$ MeV.

The quantity $P$ is given by [39],

$$ P = \sum_k \left\{ (e_k - \lambda) \text{sign}(e_k - \lambda_0) - \frac{(e_k - \lambda)^2 + \frac{1}{2} \Delta^2}{\sqrt{(e_k - \lambda)^2 + \Delta^2}} \right\}, \quad (2.135) $$

where $\lambda_0$ is the Fermi energy for $\Delta = 0$, i.e. $\lambda_0 = (e_{N_p} + e_{N_p+1})/2$.

The shell correction in the pairing energy is determined as

$$ \delta P = P - \bar{P}, \quad (2.136) $$

where $\bar{P}$ is the pairing correlation energy for the uniform distribution

$$ \bar{P} = -\frac{1}{2} \bar{g}(\bar{\lambda}) \bar{\Delta}^2, \quad (2.137) $$

with the average pairing gap $\bar{\Delta}(T = 0, I = 0) = \frac{j_2}{\sqrt{A}}$ and the smooth single-particle level density $\bar{g}(\bar{\lambda})$ given by Eq. (2.50). The average pairing gap at finite temperature and spin can be evaluated using the expression (2.134). A more simpler approximation for the shell correction in pairing energy can be [46],
\[
\delta P = \frac{\tilde{\Delta}^2}{G} - \frac{\Delta^2}{G}. \tag{2.138}
\]

In all the above cases the pairing strength \(G\) which is evaluated at the ground state has the form
\[
\frac{1}{G} = \tilde{\rho} \ln \left\{ \left[ \frac{N_p}{2\tilde{\rho}\tilde{\Delta}} \right] + 1 \right\}^{1/2} \frac{N_p}{2\tilde{\rho}\tilde{\Delta}}, \tag{2.139}
\]
where
\[
\tilde{\rho} = \frac{1}{2} \tilde{g}(\tilde{\lambda}). \tag{2.140}
\]

2.5.4. Effect of pairing on moment of inertia

The moment of inertia given by the cranking model of Inglis is
\[
\Im = 2\hbar^2 \sum_{k \neq 0} |\langle k | J_1 | 0 \rangle|^2 \frac{E_k - E_0}{}, \tag{2.141}
\]
and it was observed to be close to the rigid body value.

Taking into account the pairing correlations, the formula gets a new form
\[
\Im = 2\hbar^2 \sum_{\nu, \mu > 0} |\langle \nu | J_1 | \mu \rangle|^2 \frac{(u_\nu v_\nu - u_\nu v_\nu)^2}{E_\mu - E_\nu}. \tag{2.142}
\]

For hot nuclei the moment of inertia is given by [39]
\[
\Im_i = \sum_{\nu, \mu > 0} \left\{ \frac{(u_\mu v_\nu - u_\nu v_\mu)^2}{2(E_\mu + E_\nu)} \left( \tanh \frac{E_\mu}{2T} + \tanh \frac{E_\nu}{2T} \right) + \frac{(u_\mu v_\nu + u_\nu v_\mu)^2}{2(E_\mu + E_\nu)} \left( \tanh \frac{E_\mu}{2T} - \tanh \frac{E_\nu}{2T} \right) \right\} |\langle \nu | J_1 | \mu \rangle|^2. \tag{2.143}
\]

Assuming only smaller deformations, Bohr and Mottelson obtained the relation
\begin{equation}
\mathcal{I} = \mathcal{I}_{rig} \left[ 1 - g \left( \frac{\delta \hbar \omega_0}{2\Delta} \right) \right], \tag{2.144}
\end{equation}

\begin{equation}
\text{where } g(x) = \frac{\ln[x + \sqrt{1 + x^2}]}{x\sqrt{1 + x^2}}, \tag{2.145}
\end{equation}

\(\mathcal{I}_{rig}\) is the moment of inertia corresponding to a rigid body value, \(\hbar \omega_0 = 41A^{-1/3}\) and \(\delta\) is the equilibrium deformation. The proton and neutron contributions can be added to give the total moment of inertia

\[
\mathcal{I}_{tot} = \frac{N}{A} \mathcal{I}_n(\Delta_n) + \frac{Z}{A} \mathcal{I}_p(\Delta_p). \tag{2.146}
\]

The moment of inertia thus calculated including the pairing effects reproduces the experimentally observed behavior of the moments of inertia. It is obvious that the evaluation of (2.144) is much more simpler than the evaluation of (2.142). In fact one can bring in to the moment of inertia, its temperature dependence if our pairing gap is a temperature dependent one [48].