

THE SEMICLASSICAL APPROXIMATION
AND
STRUTINSKY SMOOTHING

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STRUTINSKY SMOOTHING

By

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Abstract:

An expression for the semiclassical density of states for a particle in a smooth potential well is obtained from the Kirkwood expansion of the partition function. This expression for the semiclassical density of states is then shown to be essentially equivalent to the expression obtained from the Green's function method of Balian and Bloch.

The Strutinsky shell correction to the nuclear binding energy is then analytically shown to be equivalent to the shell correction obtained from a consideration of the semiclassical partition function if certain restrictions on the Strutinsky smoothing parameter can be met.

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CHAPTER I

INTRODUCTION

Although the nuclear binding displays a smooth dependence on mass number and proton number that is well reproduced by the liquid-drop mass formulae (von Weizsäcker, 1935, and Bethe, 1936) there is a small systematic structure superimposed on this smooth trend due to the grouping of single-particle levels. These deviations are called shell corrections to the liquid-drop model and greatly affect the stability of heavy and superheavy nuclei.

The shell corrections are usually calculated by means of the Strutinsky prescription (Strutinsky, 1967, 1968). In this method one first considers the single-particle quantum mechanical density of states. One then finds a smoothed density of states by replacing each delta function in the single particle quantum mechanical density of states by a Gaussian multiplied by a curvature function. The shell correction is found by taking the difference between the energy calculated from the single particle quantum mechanical density of states and the energy calculated from the smoothed single particle density of states.

Other methods have been proposed for finding the shell corrections. These methods include an extended W.K.B. method (Balian et al. 1970, 1971), an extended Thomas-Fermi

method (Tyapin, 1970, 1972, Gross, 1972) and the entropy method (Ramamurthy). Another method, the partition function method (Bhaduri et al. 1971) is somewhat similar to the Strutinsky method in that they both deal with the single-particle density of states. In the partition function method one finds the smoothed density of states from the corresponding semiclassical single-particle partition function.

In chapter two of this thesis we find an expression for the semiclassical single-particle partition function for the case where we have an infinite potential that is a smooth function of the position. The single-particle semiclassical density of states is then calculated from this partition function. This expression for the semiclassical density of states is then shown to be valid for the case of a finite well if the energy being considered is below the top of the well. The equivalence between this semiclassical density of states and the one obtained by Balian et al. (1971) is demonstrated.

In chapter three we first describe the Strutinsky method of finding shell corrections and then show analytically that the shell correction obtained by the partition function approach is the same as the shell correction obtained by the Strutinsky method. This was demonstrated numerically by Bhaduri et al. (1971) for a few model cases where the semiclassical partition function is analytically known; chapter three is a general proof of this equivalence and

lends some insight into the Strutinsky smoothing procedure.

CHAPTER II

THE SEMICLASSICAL SINGLE-PARTICLE DENSITY OF STATES

2.1 The Semiclassical Single-particle Partition Function.

The single-particle partition function, $Z_{\text{qm}}(\beta)$, is given by, $Z_{\text{qm}}(\beta) = \sum_n e^{-\beta \epsilon_n}$ where ϵ_n are the single particle energy levels and β is the reciprocal of kT where k is the Boltzmann constant and T the temperature. The sum runs over all energy levels including degeneracies. The single-particle partition function is thus just the Laplace transform of single-particle density of states as can be seen by writing the partition function as follows:

$$Z_{\text{qm}}(\beta) = \int_0^{\infty} e^{-\beta \epsilon} \left[\sum_n \delta(\epsilon - \epsilon_n) \right] d\epsilon = \int_0^{\infty} e^{-\beta \epsilon} g_{\text{qm}}(\epsilon) d\epsilon ,$$

This equation also defines the quantum mechanical density of states, $g_{\text{qm}}(\epsilon)$.

Now we want an expression for the semiclassical single particle partition function. It is convenient for this purpose to express $Z_{\text{qm}}(\beta)$ in the following form (Grossman, p. 302):

$$Z_{\text{qm}}(\beta) = \frac{1}{h^3} \iint e^{-\frac{i}{\hbar} \vec{p} \cdot \vec{r}} v(\beta) d^3 p d^3 r , \quad (2.1)$$

where \vec{p} and \vec{r} are the momentum and the position respectively and $v(\beta)$ is given by the Bloch equation (Bloch, 1932):

$$Hv + \frac{\partial v}{\partial \beta} = 0 \quad ,$$

subject to the boundary conditions $\lim_{\beta \rightarrow 0} v(\beta) = e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}}$ and v goes to zero in the limit as the absolute value of \vec{r} goes to infinity. In the above equation H denotes the Hamiltonian operator for the system. The Hamiltonian must have a discrete spectrum for this discussion to be valid. If the potential is finite the spectrum will not be discrete and thus this case must be discussed separately.

To see that eq. (2.1) is valid consider the solution of the Bloch equation given by:

$$v = \sum_n a_n f_n(\vec{r}) e^{-\beta \epsilon_n} \quad ,$$

where $f_n(\vec{r})$ is the normalized eigenfunction, with eigenvalue ϵ_n , of the corresponding time independent Schrödinger equation:

$$Hf_n(\vec{r}) = \epsilon_n f_n(\vec{r}) \quad ,$$

The coefficients, a_n , defined by the condition at $\beta=0$, are given by:

$$a_n = \int f_n(\vec{r}') e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}'} d^3 r' \quad .$$

Substituting this expression for a_n into the expression for

v we obtain:

$$v = \int (\sum_n f_n(\vec{r}) f_n(\vec{r}') e^{-\beta \epsilon_n}) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}'} d^3 r'$$

Now we multiply v by $e^{-\frac{i}{\hbar} \vec{p} \cdot \vec{r}}$, integrate with respect to p and r and thereby obtain:

$$\iint e^{-\frac{i}{\hbar} \vec{p} \cdot \vec{r}} v d^3 p d^3 r = \iiint e^{\frac{i}{\hbar} \vec{p} \cdot (\vec{r}' - \vec{r})} (\sum_n f_n(\vec{r}) f_n(\vec{r}') e^{-\beta \epsilon_n}) d^3 p d^3 r d^3 r',$$

The integrations can now be done by realizing that the p integration gives a delta function and that the f_n 's are normalized. The result is:

$$\iint e^{-\frac{i}{\hbar} \vec{p} \cdot \vec{r}} v d^3 p d^3 r = h^3 \sum e^{-\beta \epsilon_n} = h^3 Z_{qm}(\beta).$$

Dividing by h^3 we obtain eq. (2.1) and thus have shown that it is valid. This proof of eq. (2.1) shows clearly the role of the condition at $\beta=0$. It also shows that the spatial boundary conditions must be the same for both the Bloch equation and the Schrödinger equation.

A semiclassical approximation for Z can now be found by obtaining an approximate solution of the Bloch equation valid for small \hbar . This was done by Kirkwood (1933) for the case where the potential, $\phi(r)$, is a smooth function

of \vec{r} . The following solution for v was obtained:

$$v \approx e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} e^{-\beta(p^2 + \phi)} \left(1 - \frac{i\beta^2}{2m} \vec{p} \cdot \nabla \phi - \frac{1}{2m} \left\{ \frac{\beta^2}{2} \nabla^2 \phi - \frac{\beta^3}{3} [(\nabla \phi)^2] \right. \right. \\ \left. \left. + \frac{1}{m} (\vec{p} \cdot \nabla)^2 \phi \right\} + \frac{\beta^4}{4} (\vec{p} \cdot \nabla \phi)^2 \right) + \dots ,$$

where m is the mass of a particle. When this expression is substituted in eq. 2.1 the following result is obtained (Kirkwood, 1933):

$$Z_{qm}(\beta) \approx Z_{sc}(\beta) = \left(\frac{2\pi m}{h^3 \beta^{3/2}} \right)^{3/2} \int d^3r e^{-\beta \phi} \left[1 - \frac{\hbar^2 \beta^2}{12m} [\nabla^2 \phi - \frac{\beta}{2} (\nabla \phi)^2] \right. \\ \left. + \dots \right] .$$

The first term is just the classical partition function while the next terms are semiclassical corrections.

2.2 The Classical Density of states

The semiclassical single particle density of states can now be obtained by taking the Laplace inverse of the semiclassical partition function. This will be done term by term starting with the classical term.

The classical term is the first term in the semiclassical expansion (Bhaduri et al. 1971) even when the Kirkwood expansion is not valid. As such it holds

considerable interest and therefore we will work out what the contribution from this term looks like in two specific situations (where the Kirkwood expansion is not valid) as well as its general form.

To illustrate the way the density of states is obtained for the second two terms we will obtain the classical density of states from the first term in Kirkwood expansion. It is given by:

$$g_{\text{cl}}(\epsilon) = \mathcal{L}^{-1} \left[\frac{(2\pi m)^{3/2}}{h^3} \int \frac{e^{-\beta\phi}}{\beta^{3/2}} d^3r \right],$$

where \mathcal{L}^{-1} denotes the Laplace inverse. It should be noted that the energy scale must be such that the minimum value of ϕ is zero. If the potential goes to infinity as the absolute value of r goes to infinity the Laplace inverse can be taken inside the integral sign. The Laplace inverse can now be taken and the following results obtained:

$$g_{\text{cl}}(\epsilon) = \frac{(2m)^{3/2}}{4\pi^2 \hbar^3} \int d^3r \sqrt{\epsilon - \phi(\vec{r})} u(\epsilon - \phi(\vec{r})), \quad (2.2)$$

where $u(\epsilon - \phi(\vec{r}))$ is the Heaviside unit step function.

We will now consider two examples. The first is a spherical well with sloping walls:

$$\phi(\vec{r}) = \begin{cases} 0 & |\vec{r}| < r_0 \\ a(|\vec{r}| - r_0) & |\vec{r}| \geq r_0 \end{cases}.$$

Substituting this expression for the potential into eq. (2.2) and doing the integral we obtain:

$$g_{cl}(\epsilon) = \frac{(2m)^{3/2}}{3\pi\hbar^3} \sqrt{\epsilon} r_0^3 + \frac{2}{3} \frac{(2m)^{3/2}}{\pi\hbar^3} \epsilon^{3/2} \frac{r_0^2}{a} \\ + \frac{8}{15} \frac{(2m)^{3/2}}{\pi\hbar^3} \epsilon^{5/2} \frac{r_0}{a^2} + \frac{16}{105} \frac{(2m)^{3/2}}{\pi\hbar^3} \frac{\epsilon^{7/2}}{a^3}$$

The first term is the classical result for an infinite spherical well. The rest of the terms are corrections resulting from the sloping walls. The factor r_0^3 in the first term shows that it is a volume term. The case of the rest of the terms is not so clear. The powers of r_0 in the next two terms cause them to look like surface and curvature terms. The factor of $1/a$, which has units of length over energy, in the second term indicates that this term can be thought of as a volume term due to an effective thickness of the surface. Similarly the third term can be thought of as a volume term. The final term is just the volume term that would arise if r_0 were zero. Thus in this case the classical term can be thought of either as a volume term or as a combination of volume, surface, curvature and constant term.

A similar situation exists for the case of a spherical

well with parabolic sides:

$$\phi(\vec{r}) = \begin{cases} 0 & |\vec{r}| < r_0 \\ \frac{1}{2} w^2 m (|\vec{r}| - r_0)^2 & |\vec{r}| \geq r_0 \end{cases} .$$

The classical density of states in this case is given by:

$$g_{cl}(\epsilon) = \frac{(2m)^{3/2}}{3\pi\hbar^3} \sqrt{\epsilon} r_0^3 + \frac{m \epsilon r_0^2}{\hbar^3 w} - \frac{(2m)^{3/2} \epsilon^{3/2} r_0}{3 w^2 m \pi \hbar^3} + \frac{\epsilon^2}{2w^3 \hbar^3} .$$

A similar analysis to that given for the last example holds.

2.3 Semiclassical Corrections to the Classical Density of States.

The contribution to the density of states from the second and third terms in the Kirkwood expansion will now be calculated. The second term in semiclassical density of states is:

$$g_2(\epsilon) = - \frac{(2\pi m)^{3/2}}{96\pi^3 m \hbar} \mathcal{L}^{-1} \left\{ \beta^2 \int d^3 r \frac{e^{-\beta\phi}}{\beta^{3/2}} \nabla^2 \phi \right\} . \quad (2.3)$$

The Laplace inverse in this expression is difficult to do because of the β^2 factor in the numerator. We will first consider the situation when the β^2 factor is absent. Then the Laplace inverse can be taken inside the integral and

done explicitly, giving the following result:

$$\mathcal{L}^{-1} \left[\int d^3 r \frac{e^{-\beta\phi}}{\beta^{3/2}} \nabla^2 \phi \right] = \frac{2}{\sqrt{\pi}} \int d^3 r \sqrt{\epsilon-\phi} \nabla^2 \phi u(\epsilon-\phi) \quad (2.4)$$

To obtain the Laplace inverse of the expression given in eq. (2.3) consider the second derivative with respect to ϵ of the expression on the right-hand side of eq. (2.4), take the Laplace transform (Abramowitz et al. p.1020) of it with respect to ϵ and hence obtain:

$$\begin{aligned} \mathcal{L} \left[\frac{2}{\sqrt{\pi}} \frac{\partial^2}{\partial \epsilon^2} \int d^3 r \sqrt{\epsilon-\phi} \nabla^2 \phi u(\epsilon-\phi) \right] = \\ \beta^2 \int d^3 r \frac{e^{-\beta\phi}}{\beta^{3/2}} \nabla^2 \phi - \frac{2}{\sqrt{\pi}} \beta \int d^3 r \nabla^2 \phi \sqrt{\epsilon'-\phi} u(\epsilon'-\phi) \Big|_{\epsilon'=0^+} \\ - \frac{2}{\sqrt{\pi}} \frac{\partial}{\partial \epsilon} \int d^3 r \nabla^2 \phi \sqrt{\epsilon-\phi} u(\epsilon-\phi) \Big|_{\epsilon=0^+} . \end{aligned}$$

In all cases the second term in this expression will be zero because $u(\epsilon-\phi)$ will equal zero unless $\phi=\epsilon'=0$. The first term is just the expression we want the Laplace inverse of. Therefore we solve for the first term, take the Laplace inverse of both sides and substitute into eq. (2.3) thereby obtaining:

$$\begin{aligned} g_2(\epsilon) = - \frac{(2m)^{1/2}}{24\pi^2 \hbar} \left[\frac{\partial^2}{\partial \epsilon^2} \int d^3 r \sqrt{\epsilon-\phi} \nabla^2 \phi u(\epsilon-\phi) \right. \\ \left. + \delta(\epsilon) \frac{\partial}{\partial \epsilon'} \int d^3 r \sqrt{\epsilon'-\phi} \nabla^2 \phi u(\epsilon'-\phi) \Big|_{\epsilon'=0^+} \right] . \end{aligned}$$

The third term in the semiclassical density of states is given by:

$$g_3(\epsilon) = \frac{(2\pi m)^{3/2}}{192\pi^3 m \hbar} \mathcal{L}^{-1} \left[\beta^3 \int d^3 r \frac{e^{-\beta\phi}}{\beta^{3/2}} (\nabla\phi)^2 \right]$$

The Laplace inverse can be taken by the same method as the Laplace inverse in the second term, and the following result obtained:

$$g_3(\epsilon) = \frac{(2m)^{1/2}}{48\pi^2 \hbar} \left[\frac{\partial^3}{\partial \epsilon^3} \int d^3 r (\nabla\phi)^2 \sqrt{\epsilon - \phi} u(\epsilon - \phi) \right. \\ \left. + \delta'(\epsilon) \frac{\partial}{\partial \epsilon} \int d^3 r (\nabla\phi)^2 \sqrt{\epsilon' - \phi} u(\epsilon' - \phi) \Big|_{\epsilon' = 0^+} \right. \\ \left. + \delta(\epsilon) \frac{\partial^2}{\partial \epsilon'^2} \int d^3 r (\nabla\phi)^2 \sqrt{\epsilon' - \phi} u(\epsilon' - \phi) \Big|_{\epsilon' = 0^+} \right] \quad (2.5)$$

The contribution to the density of states from the second and third terms can be combined by the use of Green's first identity. To do this we will apply Green's first identity to the integral in eq. (2.3) and get the following result (Landau et al. p.97):

$$\int d^3 r \frac{e^{-\beta\phi}}{\beta^{3/2}} \nabla^2 \phi = - \int d^3 r \frac{(\nabla\phi)(\nabla e^{-\beta\phi})}{\beta^{3/2}} \\ = \beta \int d^3 r \frac{(\nabla\phi)^2}{\beta^{3/2}} e^{-\beta\phi}$$

This is valid when $\nabla^2\phi$ is continuous and $\nabla\phi e^{-\beta\phi}$ goes to zero faster than $1/r^2$ as the absolute value of \vec{r} goes to infinity. If we now take the Laplace inverse of both sides we have the following result:

$$\begin{aligned} & \int d^3r \sqrt{\epsilon-\phi} \nabla^2\phi u(\epsilon-\phi) \\ &= \frac{\partial}{\partial\epsilon} \int d^3r \sqrt{\epsilon-\phi} (\nabla\phi)^2 u(\epsilon-\phi) \end{aligned} \quad (2.6)$$

The second term in eq. (2.3) contains the right-hand side of eq. (2.5) evaluated at $\epsilon=0$, but this must be zero because as we have seen the left-hand side of eq. (2.6) evaluated at $\epsilon=0$ is zero. The use of eq. (2.6) allows the sum of the first three terms in semiclassical density of states to be written in any of the three following forms:

$$\begin{aligned} g_{sc}(\epsilon) &= \frac{(2m)^{3/2}}{4\pi^2\hbar^3} \int d^3r \sqrt{\epsilon-\phi} u(\epsilon-\phi) + \frac{(2m)^{1/2}}{24\pi^2\hbar} \left[\frac{1}{2} \frac{\partial^3}{\partial\epsilon^3} \right. \\ & \int d^3r (\nabla\phi)^2 \sqrt{\epsilon-\phi} u(\epsilon-\phi) - \frac{\partial^2}{\partial\epsilon^2} \int d^3r \nabla^2\phi \sqrt{\epsilon-\phi} u(\epsilon-\phi) \\ & + \delta(\epsilon) \left(\frac{1}{2} \frac{\partial^2}{\partial\epsilon'^2} \int d^3r \sqrt{\epsilon'-\phi} (\nabla\phi)^2 u(\epsilon'-\phi) - \frac{\partial}{\partial\epsilon'} \right. \\ & \left. \left. \int d^3r \sqrt{\epsilon'-\phi} \nabla^2\phi u(\epsilon'-\phi) \right) \Big|_{\epsilon'=0^+} \right] \\ &= \frac{(2m)^{3/2}}{4\pi^2\hbar^3} \int d^3r \sqrt{\epsilon-\phi} u(\epsilon-\phi) - \frac{(2m)^{1/2}}{48\pi^2\hbar} \left[\frac{\partial^2}{\partial\epsilon^2} \int d^3r \nabla^2\phi \sqrt{\epsilon-\phi} \right. \end{aligned}$$

$$\begin{aligned}
& u(\epsilon - \phi) + \delta(\epsilon) \left. \frac{\partial}{\partial \epsilon'} \int d^3 r \nabla^2 \phi \sqrt{\epsilon' - \phi} u(\epsilon' - \phi) \right|_{\epsilon' = 0} \\
&= \frac{(2m)^{3/2}}{4\pi^2 \hbar^3} \int d^3 r \sqrt{\epsilon - \phi} u(\epsilon - \phi) - \frac{(2m)^{1/2}}{48\pi^2 \hbar} \left[\frac{\partial^3}{\partial \epsilon^3} \int d^3 r (\nabla \phi)^2 \sqrt{\epsilon - \phi} \right. \\
& \quad \left. u(\epsilon - \phi) + \delta(\epsilon) \frac{\partial^2}{\partial \epsilon'^2} \int d^3 r (\nabla \phi)^2 \sqrt{\epsilon' - \phi} u(\epsilon' - \phi) \right]_{\epsilon' = 0^+}.
\end{aligned} \tag{2.7}$$

2.4 The Case of a Finite Potential

We now have the first few terms in the semiclassical expansion of the density of states for a particle in a smooth infinite well. Next we will extend the results to the case of a finite well. In this case the integrals in the expression for the partition function do not converge. To avoid this difficulty we replace the finite potential, ϕ , with the infinite potential $\phi_a = \phi - (1 - e^{ar})$. If we are dealing with energies below the top of the well the Heaviside unit step functions limits the r integration to a finite region of space. If a is small enough ϕ_a and ϕ will be approximately equal in this region.

Consider for example the first integral in the first part eq. (2.7). Upon substitution of ϕ_a for ϕ in the original

Hamiltonian, this integral becomes:

$$\int d^3r \sqrt{\epsilon - \phi_a} u(\epsilon - \phi_a) = \int d^3r \sqrt{\epsilon - \phi + (1 - e^{-ar})} u(\epsilon - \phi + (1 - e^{-ar})).$$

If ϵ is an energy below the top of the well we can take limit of this expression as a goes to zero and obtain the original expression. If ϵ is above the top of the well, ϕ , the integral diverges as a goes to zero. A similar analysis holds for the other terms. Thus we have unambiguously defined a semiclassical density of states for energies below the top of the well. This is of some interest in obtaining a smoothed density of states for shell corrections to nuclear binding energy as other methods of finding the smoothed density of states run into difficulties (Ross et al. 1972). The semiclassical result however is difficult to use if there is a spin orbit interaction.

2.5 Comparison of Results of Kirkwood Expansion and W.K.B Approximation.

The Kirkwood expansion used to obtain the semiclassical partition function is similar (Kirkwood, 1933) to the W.K.B. solution of the Schrödinger equation. It will now be shown that the density of states obtained here is the same as that obtained by the extended W.K.B. solution

of Balian et al. (1970, 1971). We now consider part one of eq. (2.7) and take only the smooth part (i.e. we neglect the terms containing delta functions). Instead of having the Heaviside unit step functions limit the range of integration we can take the real part of the square root before integrating. The result is:

$$g_{sc}(\epsilon) = \frac{(2m)^{3/2}}{4\pi^2 \hbar^3} \int d^3r \operatorname{Re}(\sqrt{\epsilon - \phi}) + \frac{(2m)^{1/2}}{24\pi^2 \hbar} \left[- \frac{\partial^2}{\partial \epsilon^2} \int d^3r \operatorname{Re}(\sqrt{\epsilon - \phi}) \nabla^2 \phi + \frac{1}{2} \frac{\partial^3}{\partial \epsilon^3} \int d^3r \operatorname{Re}(\sqrt{\epsilon - \phi}) (\nabla \phi)^2 \right],$$

where Re denotes the real part of the quantity in brackets. Next we replace ϵ inside the square roots by $\epsilon + i\gamma$ where γ is a real number and take the limit as γ goes to zero. The limit can be taken outside integral and done after the derivative because both the limit and the integral are uniformly convergent. The following result is obtained:

$$g_{sc}(\epsilon) = \lim_{\gamma \rightarrow 0} \left(\frac{(2m)^{3/2}}{4\pi^2 \hbar^3} \int d^3r \operatorname{Re}(\sqrt{\epsilon + i\gamma - \phi}) + \frac{(2m)^{1/2}}{24\pi^2 \hbar} \left[- \frac{\partial^2}{\partial \epsilon^2} \int d^3r \operatorname{Re}(\sqrt{\epsilon + i\gamma - \phi}) \nabla^2 \phi + \frac{1}{2} \frac{\partial^3}{\partial \epsilon^3} \int d^3r (\nabla \phi)^2 \operatorname{Re}(\sqrt{\epsilon + i\gamma - \phi}) \right] \right).$$

For non-zero γ the derivatives can be taken inside the integrals and done explicitly. Replacing $\epsilon + i\gamma$ by z and combining the second two integrals we have:

$$g_{sc}(\epsilon) = \lim_{\gamma \rightarrow 0} \left(\frac{(2m)^{3/2}}{4\pi^2 \hbar^3} \int d^3r \operatorname{Re}(\sqrt{z-\phi}) \right. \\ \left. + \frac{(2m)^{1/2}}{384\pi^2 \hbar} \int d^3r \operatorname{Re} \left[\frac{4 \nabla^2 \phi}{(z-\phi)^{3/2}} + \frac{3(\nabla\phi)^2}{(z-\phi)^{5/2}} \right] \right) .$$

This result is now the same as that obtained Balian et al. (1971). The two methods are thus equivalent at least to this order.

CHAPTER III
 STRUTINSKY SMOOTHING AND THE PARTITION
 FUNCTION APPROACH

3.1 The Strutinsky Method.

In this section the Strutinsky and Partition function methods of obtaining the shell correction are described. The Strutinsky smoothed single-particle density of states, denoted by $\bar{g}(\epsilon)$, is obtained from a density of states, $g(\epsilon)$, by Gaussian smoothing modulated with a curvature function:

$$\bar{g}(\epsilon) = \int_0^{\infty} d\epsilon' g(\epsilon') \frac{e^{-(\epsilon-\epsilon')^2/\gamma^2}}{\gamma\sqrt{\pi}} L_n^{1/2} [(\epsilon-\epsilon')^2/\gamma^2] . \quad (3.1)$$

In this expression $g(\epsilon)$ can be either the single-particle density of states, denoted $g_{qm}(\epsilon)$, or the single-particle semiclassical density of states, $g_{sc}(\epsilon)$. It should be noted that in this chapter $g_{sc}(\epsilon)$ and the corresponding partition function, $Z_{sc}(\beta)$, are considered to have more terms than those discussed in chapter 2. The exact number of terms will be discussed later. The $L_n^{1/2}$ is an associated Laguerre polynomial (Abramowitz et al. p.775); γ is the smoothing parameter. The Strutinsky smoothed quantum mechanical density of states is denoted by $\bar{g}_{qm}(\epsilon)$, and the Strutinsky smoothed semiclassical density of states is denoted by $\bar{g}_{sc}(\epsilon)$.

If the lower limit in the integral in eq. (3.1) is replaced by $-\infty$ and $g(\epsilon')$ is a polynomial of order less than or equal to $2n+1$ then $\bar{g}(\epsilon')$ will equal $g(\epsilon')$ (Strutinsky 1967, 1968 and Tsang 1969). This is called the self-consistency condition for the Strutinsky method.

Two energies E and \bar{E} are now defined by the following equations:

$$E = \int_0^{\mu} \epsilon g(\epsilon) d\epsilon \quad \bar{E} = \int_{-\infty}^{\bar{\mu}} \epsilon \bar{g}(\epsilon) d\epsilon \quad . \quad (3.2)$$

The lower limit in the second integral must be minus infinity because $\bar{g}(\epsilon)$ is non-zero for negative ϵ . Energies calculated from $g_{qm}(\epsilon)$ and $\bar{g}_{qm}(\epsilon)$ will be denoted E_{qm} and \bar{E}_{qm} respectively while those calculated from $g_{sc}(\epsilon)$ and $\bar{g}_{sc}(\epsilon)$ will be denoted E_{sc} and \bar{E}_{sc} . The chemical potentials μ and $\bar{\mu}$ are defined by the two following equations:

$$N = \int_0^{\mu} g(\epsilon) d\epsilon \quad , \quad N = \int_{-\infty}^{\bar{\mu}} \bar{g}(\epsilon) d\epsilon \quad , \quad (3.3)$$

where N is the number of particles.

In the Strutinsky method the shell correction is found by subtracting \bar{E}_{qm} from E_{qm} . This difference must be independent of γ over a considerable range of γ if the Strutinsky method is to be valid. In the partition function method the shell correction found by subtracting E_{sc} from E_{qm} . The name "partition function method" comes from the fact $g_{sc}(\epsilon)$,

which is used to calculate E_{sc} , can be found by taking the Laplace inverse of the semiclassical expansion of the partition function.

To show that the two methods are equivalent we must show that E_{sc} equals \bar{E}_{qm} . This is done in two steps. In section 3.2 we show that $\bar{g}(\epsilon)$ and $\bar{g}_{sc}(\epsilon)$ are equal if γ is large enough and hence \bar{E}_{qm} equals \bar{E}_{sc} . The proof is then completed in section 3.3 where it is shown that \bar{E}_{sc} and E_{sc} are equal if γ is not too large.

3.2 Smoothing and the Partition Function.

In this section we show that \bar{E}_{sc} and \bar{E}_{qm} are equal by a consideration involving the quantum mechanical and semiclassical partition functions. We start by taking the two-sided Laplace transform of $\bar{g}(\epsilon)$ (see appendix), obtaining:

$$\begin{aligned} \mathcal{L}[\bar{g}(\epsilon)] &= \int_{-\infty}^{\infty} e^{-\beta\epsilon} \bar{g}(\epsilon) d\epsilon \\ &= Z(\beta) \int_{-\infty}^{\infty} e^{-\beta\gamma y} \frac{e^{-y^2}}{\sqrt{\pi}} L_n^{1/2}[y^2] dy, \end{aligned} \quad (3.4)$$

where β is the transform variable and $Z(\beta)$ is the Laplace transform of $g(\epsilon)$, thus it is just the partition function corresponding to $g(\epsilon)$. The partition function corresponding to $g_{qm}(\epsilon)$ will be denoted $Z_{qm}(\beta)$.

The integral in eq. (3.4) is done in the appendix and the following expression obtained:

$$\mathcal{L}[\bar{g}(\epsilon)] = z(\beta) e^{\beta^2 \gamma^2 / 4} p_n(\beta \gamma) ,$$

Here $p_n(\beta \gamma)$ is the polynomial of order $2n$ in the variable $\beta \gamma$.

We now consider the identity:

$$\mathcal{L}^{-1}[\mathcal{L}[\bar{g}(\epsilon)]] = \bar{g}(\epsilon) .$$

The inverse Laplace transform can be written as (Van der Pol et al. p.16):

$$\mathcal{L}^{-1}[z(\beta)] = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} z(\beta) e^{\beta \epsilon} d\beta ,$$

where c is a constant chosen such that the line of integration lies in the strip of convergence of the Laplace transform. In this case c can be any positive number.

Writing out the above identity explicitly we have:

$$\bar{g}(\epsilon) = \mathcal{L}^{-1}[\mathcal{L}[\bar{g}(\epsilon)]] = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} z(\beta) e^{\beta^2 \gamma^2 / 4} p_n(\beta \gamma) e^{\beta \epsilon} d\beta .$$

(3.5)

In eq. (3.5) we make the substitution $\beta = c+ix$ and obtain:

$$\bar{g}(\epsilon) = \frac{e^{c^2 \gamma^2 / 4 + c\epsilon}}{2\pi} \int_{-\infty}^{\infty} z(c+ix) e^{-x^2 \gamma^2 / 4} e^{ixc\gamma^2 / 2} e^{ix\epsilon} \times p_n[(c+ix)\gamma] dx .$$

(3.6)

Due to the presence of the factor $e^{-x^2 \gamma^2 / 4}$ the only significant contribution to the integral comes from x near zero. (Gross, 1972). Also since the positive parameter c can be chosen as small as we like as long as it is not zero, we see that the integral depends only on $Z(\beta)$ near $\beta=0$.

We now consider an expansion of the quantum mechanical partition function valid for small β . One such expansion that has been used (Bhaduri et al. 1971) is the semiclassical expansion given by:

$$Z_{sc}(\beta) = Z_c(\beta) (1 + \hbar \chi_1(\beta) + \hbar^2 \chi_2(\beta) + \dots), \quad (3.7)$$

where $Z_c(\beta)$ is the classical partition function and the χ 's are defined in terms of the one body potential. Other expansions valid for small β , such as a Laurent expansion, could also be used, but we will use the semiclassical expansion in this thesis for the sake of definiteness. If γ is large enough, the integral in eq. (3.6) has almost the same value whether $Z_{qm}(\beta)$ or $Z_{sc}(\beta)$ is used in it. If $Z_{qm}(\beta)$ is used the smooth density of states obtained is $\bar{g}_{qm}(\epsilon)$ while $\bar{g}_{sc}(\epsilon)$ is obtained if $Z_{sc}(\beta)$ is used. Thus it follows that $\bar{g}_{qm}(\epsilon)$ and $\bar{g}_{sc}(\epsilon)$ are approximately equal, and hence the energy, \bar{E}_{qm} , calculated from $\bar{g}_{qm}(\epsilon)$ is the same as the energy, \bar{E}_{sc} , calculated from $\bar{g}_{sc}(\epsilon)$. From eq. (3.7) we see that $Z_{sc}(\beta)$ and hence $\bar{g}_{sc}(\epsilon)$ consists of an infinite number of terms. Only those terms that do not make a significant contribution

to the energy calculated from $g_{sc}(\epsilon)$ can be neglected.

For example, the first three terms must be kept for a harmonic oscillator although the third term is a derivative of a delta function.

It should be noted that we have not implied that the two partition functions are approximately equal for all β , in fact they differ considerably for large β .

The equivalence of \bar{E}_{qm} and \bar{E}_{sc} was checked numerically for the case of an axial symmetric deformed harmonic oscillator well. The solid line in fig. 1 shows $\bar{E}_{qm} - \bar{E}_{sc}$ as a function of γ for three different particle numbers. The lower bound on γ in case is seen to be about $lh\omega$.

3.3 Strutinsky Smoothed Semiclassical Density of States.

In this section we will show that the energies \bar{E}_{sc} and E_{sc} are the same. This is done in two steps; first it is shown that the chemical potentials are the same in both cases and then this fact is used to show that the energies are the same.

From eq. (3.3) we see that the condition for the chemical potentials to be equal is:

$$\int_0^{\mu} g_{sc}(\epsilon) d\epsilon - \int_{-\infty}^{\mu} g_{sc}(\epsilon) d\epsilon = 0 . \quad (3.8)$$

The second integral in this expression will now be considered. Let us denote it by I_N . Substituting for $\bar{g}_{SC}(\epsilon)$ in I_N from eq. (3.1) we obtain:

$$I_N = \int_{-\infty}^{\mu} d\epsilon \int_0^{\infty} g_{SC}(\epsilon') \frac{e^{-(\epsilon - \epsilon')^2/\gamma^2}}{\gamma\sqrt{\pi}} L_n^{1/2}[(\epsilon - \epsilon')^2/\gamma^2] d\epsilon'$$

We now change the order of integration and substitute $y = (\epsilon - \epsilon')/\gamma$ to obtain:

$$I_N = \int_0^{\infty} d\epsilon' g_{SC}(\epsilon') \int_{-\infty}^{(\mu - \epsilon')/\gamma} \frac{e^{-y^2}}{\sqrt{\pi}} L_n^{1/2}(y^2) dy .$$

The ϵ' integration is now done by parts and the following result obtained:

$$I_N = \int_0^{\epsilon'} g_{SC}(\epsilon'') d\epsilon'' \int_{-\infty}^{(\mu - \epsilon')/\gamma} \frac{e^{-y^2}}{\sqrt{\pi}} L_n^{1/2}(y^2) dy \Big|_0^{\infty} \\ + \int_0^{\infty} d\epsilon' \left[\int_0^{\epsilon'} d\epsilon'' g_{SC}(\epsilon'') \right] \frac{e^{-(\mu - \epsilon')^2/\gamma^2}}{\gamma\sqrt{\pi}} L_n^{1/2}[(\mu - \epsilon')^2/\gamma^2] .$$

The first term is zero at the lower limit because the range of integration of the first integral goes to zero when $\epsilon' = 0$.

The situation at the upper limit is not so clear. As ϵ' goes to infinity the second integral goes to zero but the first integral tends to diverge. Fortunately the second integral goes to zero fast enough to make the term equal to zero in most cases of interest.

The second term is more interesting as it makes a finite contribution to I_N . Due to the Gaussian the only significant contribution to integral comes from ϵ' near μ , the size of the region determined by γ and $g_{SC}(\epsilon'')$. If $\int_0^{\epsilon'} g_{SC}(\epsilon'') d\epsilon''$ can be approximated by a polynomial in this region then it can be replaced by that polynomial everywhere without affecting the value of the integral. Similarly the lower limit can be replaced by $-\infty$ and the polynomial approximation extended to regions of negative ϵ' . If γ is small enough for the polynomial used in the approximation to be of order $2n + 1$ or less then the self-consistency condition for Strutinsky smoothing gives us:

$$I_N \approx \int_0^{\mu} g_{SC}(\epsilon') d\epsilon', \quad (3.9)$$

thus proving eq. (3.8).

Now we consider the energies E_{SC} and \bar{E}_{SC} defined by eq. (3.2). As μ and $\bar{\mu}$ are equal the condition for E_{SC} and \bar{E}_{SC} to be equal is:

$$\int_0^{\mu} \epsilon g_{SC}(\epsilon) d\epsilon - \int_{-\infty}^{\mu} \epsilon \bar{g}_{SC}(\epsilon) d\epsilon = 0 \quad (3.10)$$

As with eq. (3.8) we substitute for $\bar{g}_{SC}(\epsilon)$ from eq. (3.1), change the order of integration and make the substitution $y = (\epsilon - \epsilon')/\gamma$ to obtain the following form for eq. (3.9):

$$\int_0^{\mu} \epsilon g_{SC}(\epsilon) d\epsilon - \int_0^{\infty} d\epsilon' g_{SC}(\epsilon') \int_{-\infty}^{(\mu - \epsilon')/\gamma} \frac{e^{-y^2}}{\sqrt{\pi}} L_n^{1/2}(y^2) dy = 0$$

This difference will now be denoted I_E . Both the ϵ and the ϵ' integrations are now done by parts and the following results obtained:

$$\begin{aligned}
 I_E &= \mu \int_0^\mu g_{sc}(\epsilon') d\epsilon' - \int_0^\mu \left[\int_0^\epsilon g_{sc}(\epsilon') d\epsilon' \right] d\epsilon \\
 &- \mu \int_0^\infty \left[\int_0^{\epsilon'} g_{sc}(\epsilon'') d\epsilon'' \right] \frac{1}{\gamma\sqrt{\pi}} e^{-(\mu-\epsilon')^2/\gamma^2} L_n^{1/2}[(\mu-\epsilon')^2/\gamma^2] d\epsilon' . \\
 &+ \int_0^\infty \left[\int_0^{\epsilon'} g_{sc}(\epsilon'') d\epsilon'' \right] \int_{-\infty}^{(\mu-\epsilon')/\gamma} \frac{1}{\sqrt{\pi}} e^{-y^2} L_n^{1/2}(y^2) dy d\epsilon'
 \end{aligned}$$

Since the third term is just μ times I_N eq. 3.9 shows that it is approximately equal to the first term. The fourth term is I_N with $g_{sc}(\epsilon')$ replaced by $\int_0^{\epsilon'} g_{sc}(\epsilon'') d\epsilon''$ and thus it is seen to be approximately equal to the second term if $\int_0^{\epsilon'} g_{sc}(\epsilon'') d\epsilon''$ can be approximated by a polynomial of order less than $2n+1$ for ϵ' near μ . Thus I_E is approximately equal to zero and \bar{E}_{sc} and E_{sc} are approximately equal. This was checked numerically for the case of an axially symmetric deformed harmonic oscillator and a plot of $\bar{E}_{sc} - E_{sc}$ against γ for three different particle numbers is shown by the dashed line in fig. 1. The upper limit on γ is seen to be less than $3\hbar\omega$ and to increase with particle number.

3.4 Conclusions.

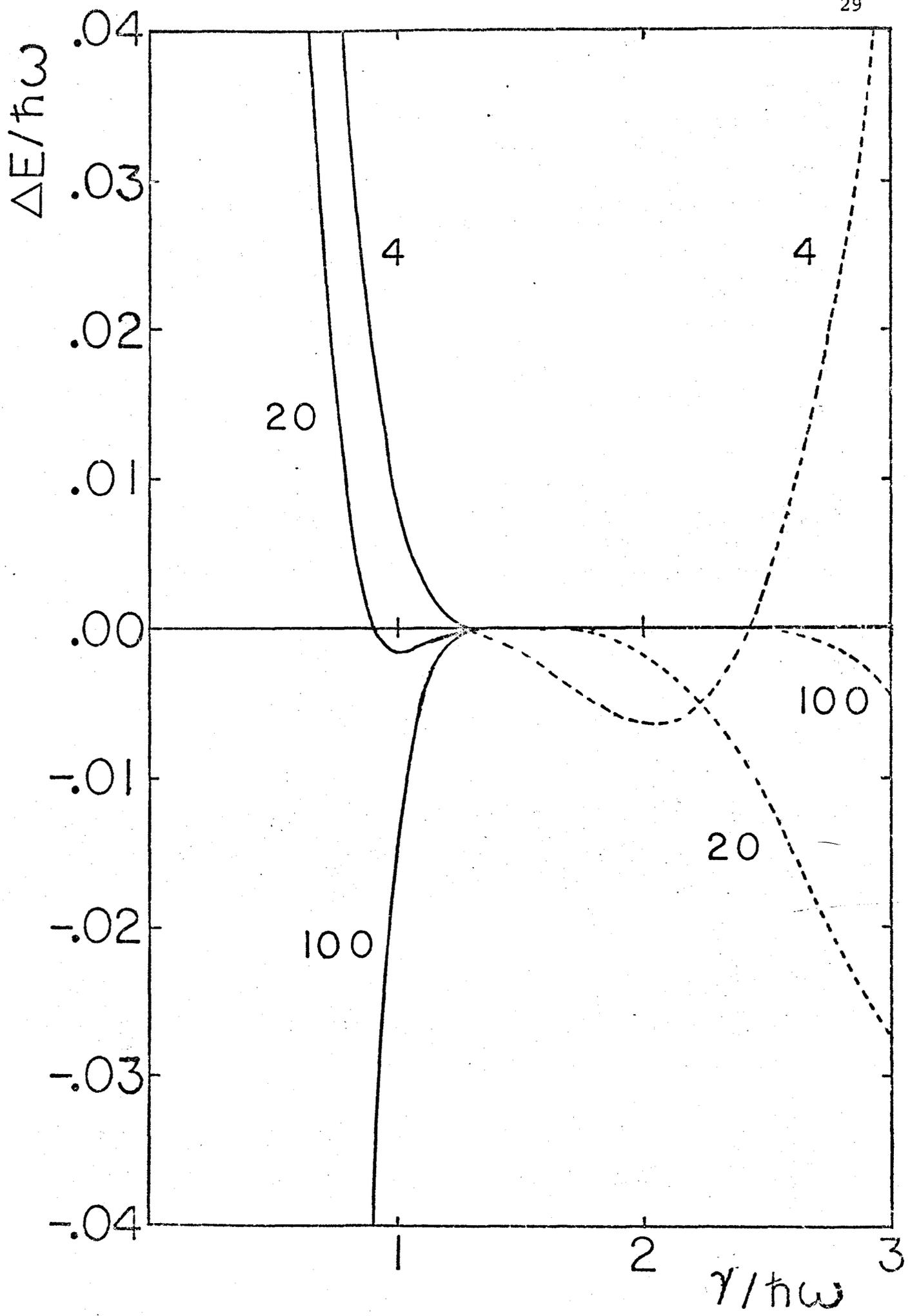
It has now been shown that if certain restrictions on γ and $g_{sc}(\epsilon)$ are met, $\bar{E}_{qm} \sim \bar{E}_{sc}$ and $\bar{E}_{sc} \sim E_{sc}$. It follows

immediately that \bar{E}_{qm} and E_{sc} are approximately equal, and hence the Strutinsky procedure yields the same shell corrections as the partition function approach.

There are two restrictions placed on γ . The first is a lower bound associated with part one of the proof. The second is an upper bound associated with the second part of the proof. If these two restrictions are met, the Strutinsky shell correction will be independent of γ and equal to the shell corrections obtained by the partition function approach.

Figure Caption

Fig. 1 A plot of ΔE , representing $\bar{E}_{qm} - \bar{E}_{sc}$ (solid line) and $\bar{E}_{sc} - E_{sc}$ (dotted line), as a function of γ for 4, 20 and 100 particles in an axially symmetric harmonic oscillator well with a deformation parameter of 0.4. Both ΔE and γ are expressed in units of $h\omega$. The range of γ for which \bar{E}_{qm} and E_{sc} are equal can be seen by comparing the solid and dotted lines.



APPENDIX

Here we consider the Laplace transform of:

$$\bar{g}(\varepsilon) = \int_{-\infty}^{\infty} d\varepsilon' g(\varepsilon') \frac{e^{-(\varepsilon-\varepsilon')^2/\gamma^2}}{\gamma\sqrt{\pi}} L_n^{1/2}[(\varepsilon-\varepsilon')^2/\gamma^2]$$

Taking the Laplace transform of both sides we have:

$$\begin{aligned} \mathcal{L}[\bar{g}(\varepsilon)] &= \int_{-\infty}^{\infty} e^{-\beta\varepsilon} \bar{g}(\varepsilon) d\varepsilon = \int_{-\infty}^{\infty} e^{-\beta\varepsilon} d\varepsilon \int_0^{\infty} d\varepsilon' g(\varepsilon') \\ &\times e^{-(\varepsilon-\varepsilon')^2/\gamma^2} L_n^{1/2}[(\varepsilon-\varepsilon')^2/\gamma^2] \end{aligned}$$

where the two-sided Laplace transform is used because $\bar{g}(\varepsilon)$ is not zero for ε less than zero. By changing the order of integration and making the change of variable $\varepsilon = \varepsilon' + \gamma y$ we obtain:

$$\begin{aligned} \mathcal{L}[\bar{g}(\varepsilon)] &= \int_0^{\infty} g(\varepsilon') d\varepsilon' \int_{-\infty}^{\infty} e^{-\beta(\gamma y + \varepsilon')} \frac{e^{-y^2}}{\sqrt{\pi}} L_n^{1/2}(y^2) dy \\ &= \int_0^{\infty} g(\varepsilon') e^{-\beta\varepsilon'} d\varepsilon' \int_{-\infty}^{\infty} e^{-\beta\gamma y} \frac{e^{-y^2}}{\sqrt{\pi}} L_n^{1/2}(y^2) dy . \end{aligned}$$

The second integration is independent of ε' . The first integral is just the one-side Laplace transform of $g(\varepsilon')$, that is the partition function $Z(\beta)$. Thus we have:

$$\mathcal{L}[\bar{g}(\varepsilon)] = Z(\beta) \int_{-\infty}^{\infty} e^{-\beta\gamma y} \frac{e^{-y^2}}{\sqrt{\pi}} L_n^{1/2}(y^2) dy .$$

Now we consider the y integral:

$$I_Y = \int_{-\infty}^{\infty} e^{-\beta\gamma Y} \frac{e^{-Y^2}}{\sqrt{\pi}} L_n^{1/2}(Y^2) dy \quad . \quad \text{A.1}$$

By using identities (Abramowitz et al. p.785) involving the associated Laguerre polynomial we obtain:

$$\sum_{m=0}^n L_m^{-1/2}(x^2) = L_n^{1/2}(x^2) \quad ,$$

$$\text{and: } L_n^{-1/2}(x^2) = \frac{(-1)^n}{n! 2^{2n}} H_{2n}(x) \quad .$$

These two equations can be combined to give:

$$L_n^{1/2}(x^2) = \sum_{m=0}^n \frac{(-1)^m}{m! 2^{2m}} H_{2m}(x) \quad .$$

Substituting this in eq. (A.1) we obtain:

$$I_Y = \sum_{m=0}^n \frac{(-1)^m}{m! 2^{2m}} \int_{-\infty}^{\infty} e^{-\beta\gamma Y} \frac{e^{-Y^2}}{\sqrt{\pi}} H_{2m}(Y) dy \quad .$$

The integral is the two-sided Laplace transform of $\frac{e^{-Y^2}}{\sqrt{\pi}} H_{2m}(Y)$, given by Van der Pol et al. (p.83) to be $(\gamma\beta)^{2m} e^{\beta^2\gamma^2/4}$. We now obtain:

$$I_Y = \sum_{m=0}^n \frac{(-1)^m}{m! 2^{2m}} (\gamma\beta)^{2m} e^{\beta^2\gamma^2/4} = e^{\beta^2\gamma^2/4} P_n(\gamma\beta) \quad ,$$

where $P_n(\gamma\beta)$ is a polynomial of order $2n$ in $\gamma\beta$.

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