EXTENDED THOMAS-FERMI THEORY

FOR

NONINTERACTING PARTICLES

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By

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ABSTRACT

For a system of noninteracting fermions in a one-body potential it is possible to derive an expression for the "smooth" part of the energy by finding corrections to the Thomas-Fermi energy. By the "smooth" part of the energy we mean that part which varies smoothly as a function of particle number and deformation. The smooth energy is needed, for example, to find the shell corrections used in conjunction with the Strutinsky energy theorem to obtain nuclear deformation surfaces. In this thesis we find corrections to the Thomas-Fermi energy as a power series in $\hbar^2$ using the Wigner-Kirkwood expansion of the one-body partition function. The resultant expression is valid for any potential whose gradients and higher order derivatives exist. The effects of a spin-orbit term in the Hamiltonian are also included. The convergence of the $\hbar^2$ series is checked by considering both the harmonic oscillator potential and realistic Woods-Saxon potentials. Expressions are also found for the spatial and kinetic energy densities. Using these expressions the kinetic energy is expressed in terms of the density and gradients of the density.

The formalism is extended to the case of a constrained Hamiltonian. In particular the pushing and cranking models are considered. When corrections are added to the Thomas-Fermi result for the cranking model the moment of inertia is found to depart somewhat from the rigid-body value.

The extended Thomas-Fermi result is used to derive the usual Strutinsky smoothing method and the good agreement between the two methods shown numerically. The $\hbar$-expansion is also compared to the A-expansion and is found to converge slightly faster than the A-expansion.

The formalism developed for the cranking model can be applied with only minor modifications to the problem of finding the magnetic susceptibility of a system of electrons. This fact is used to investigate surface effects on the magnetic susceptibility.

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CHAPTER I

INTRODUCTION

I.1 Review of Previous Work.

To gain an understanding of a nucleus it is necessary to employ simplified models. One such model, the liquid drop model (LDM), considers the nucleus to behave like a charged liquid drop. With this model one may calculate such properties as the nuclear binding energy as a function of mass number A, atomic number Z, and nuclear shape (von Weizsäcker 1935, Bethe and Bacher 1936, Myers and Swiatecki 1966). Although the resulting LDM expressions give reasonable fits throughout the periodic table there remain systematic deviations which cannot be explained with this model. The idea of a charged liquid drop also provides a qualitative explanation (Bohr and Wheeler 1939, Hill and Wheeler 1953) for the fissioning of a heavy nucleus into two or more lighter ones although it fails to account for many quantitative details (Clark 1971). This is particularly true in the actinide region where the LDM fails to give the correct fission barrier shapes. Before one can get the correct barrier shapes in this region one must take into account single particle effects.

At the other extreme is a model, the indépendant particle model, where the nucleus is assumed to consist of

nucleons moving in some average one-body potential. This model has had success in predicting the ground state spins of odd-A nuclei and in calculating the ground state deformations (Mottelson and Nilsson 1959). However it fails to reproduce such bulk properties as the total binding energy or nuclear deformation energy at the large deformations (Nilsson et.al. 1969) necessary to describe fission.

One way to calculate such properties as fission barriers would be to do a microscopic calculation such as Hartree-Fock (Flocard et. al. 1974). Although this yields reasonable results it requires a great deal of computer time. A simpler method for calculating these properties is to combine the LDM and the independant particle model. This was first done by Myers and Swiatecki (1966) who added shell corrections to the LDM by considering the grouping of single-particle states in a degenerate Fermi gas. Strutinsky (1967, 1968) proposed a general procedure for obtaining the shell correction from the independant particle model. The Strutinsky method has been successfully applied to the calculation of fission barriers (Nilsson et. al. 1969, Bolsterli et. al. 1972, Brack et. al. 1972) and has been able to explain, among other phenomena, the existence of short-lived fission isomers (Bjornholm and Strutinsky 1969). It has also been generalized to study the properties of rapidly rotating nuclei (Pashkevich and Frauendorf 1975, Bengtsson et. al. 1975, Neergard and Pashkevich 1975), which can be important in

heavy ion collisions (Johnson and Szymanski, 1973).

As the Strutinsky method has been widely applied it is of interest to look at it more closely. The total binding energy is written as the sum of the LDM energy and the shell correction. The shell correction is calculated in the independent particle model as the difference between the exact sum of occupied single particle energies and a corresponding sum over a smooth distribution of single particle states. The sum over the smooth distribution should yield an energy which varies smoothly as a function of particle number and deformation and will be referred to as the smooth energy. In the usual Strutinsky method the smooth distribution is essentially obtained by convoluting the exact single particle density of states with a Gaussian. Although this method works quite well there remain ambiguities (Jennings et. al. 1975a) especially for finite potential wells. Partly because of these ambituities other methods for obtaining the smooth energy have been developed (Siemens and Sobiczewski 1972, Gross 1972, Ramamurthy and Kapoor 1972, Balian and Bloch 1971, Bhaduri and Ross 1971). This thesis will be concerned with the further development of the alternate method first presented by Bhaduri and Ross (1971).

I.2 The Present Work.

In this work we have two main objectives. The first is to develop an alternate method of obtaining the smooth energy to check the Strutinsky smoothing method in realistic

cases. The second objective is to understand the nature and behavior of the smooth energy. Throughout this thesis we will only be concerned with systems of noninteracting particles. In the second chapter we develop an expansion for the smooth energy as a power series in $\hbar$. This expansion is obtained by using the Laplace transform of the single-particle density of states which in statistical applications is known as the single-particle partition function. The expansion, itself, is valid for arbitary local potentials, finite or infinite, which are not too rapidly varying. The effects of a spin-orbit term in the Hamiltonian are also included. The rapid convergence of this expansion is demonstrated using harmonic oscillator and realistic Woods-Saxon potentials. Expressions for the density and kinetic energy density are derived in chapter three. The kinetic energy density is expressed in terms of the density and derivatives of the density. We obtain not only the Thomas-Fermi term and the Weizsacker correction term (von Weizsacker, 1935) but also the next order term.

In chapter four the formalism is extended to the case of a constrained Hamiltonian. In particular the pushing and cranking models for noninteracting particles are discussed and the relevant mass parameters are investigated. In the case of the cranking model small corrections to the rigid-body moment of inertia are found.

Attempts have been made to obtain the smooth energy as an expansion in $A^{1/3}$ (Siemens and Sobiczewski 1972,

Dworzecka and Moszkowski 1975). It is therefore of interest to look at the A dependance of the smooth energy. This is done in chapter four. The $A^{1/3}$ expansion is found to converge somewhat slower than the $\hbar$ expansion used in this work.

In chapter six the usual Strutinsky smoothing method (Strutinsky 1967, 1968) is compared with the method presented in this work. Starting with this method the Strutinsky method is derived including the form of the curvature corrections. The case of finite wells is also discussed.

The formalism as developed in chapter 3 for the cranking model is also applicable with minor modifications to the problem of determining the magnetic susceptibility of a noninteracting electron gas. This is illustrated in chapter seven where surface effects on the susceptibility are calculated.

CHAPTER II

THE SEMICLASSICAL ENERGY

II.1 The Single-Particle Partition Function.

In this chapter we shall be concerned with developing an expression for the smooth energy of a system of noninteracting particles in a one-body potential. This smooth energy is useful, for example, in obtaining the shell correction required by the Strutinsky energy theorem (Strutinsky 1967, 1968). The smooth energy is obtained here by finding systematic corrections to the Thomas-Fermi (TF) results. In deriving these corrections we will make use of a semiclassical expansion of the one-body partition function (Wigner 1932, Kirkwood 1933). It must be stressed that the partition function is used only as a mathematical tool and we are in no sense doing statistical mechanics. The temperature that normally appears in the partition function becomes in our approach only a mathematical parameter that does not appear in our final expressions for quantities such as the energy or the spatial density. In spite of this, many of the usual results for the partition function may be used.

In the nucleus we are dealing with two types of fermions, neutrons and protons. In our approximation of noninteracting particles they may be considered completely independantly and the results trivially added in the final step.

We shall therefore work with just one kind of particle. As we are interested in the ground state, zero temperature Fermi-Dirac statistics will be used.

Before developing the $\hbar$ or semiclassical expansion it is useful to define some concepts. The first is the single-particle density of states, $g(\varepsilon)$, given by:

$$g(\varepsilon) = \Sigma_i \, \delta(\varepsilon - \varepsilon_i) \quad , \tag{1}$$

where the ε_i are the single particle energies. In terms of this density of states the particle number N and the energy E are given by:

$$N = \int_0^\lambda g(\varepsilon) d\varepsilon \quad , \tag{2}$$

$$E = \int_0^\lambda \varepsilon g(\varepsilon) d\varepsilon = \lambda N - \int_0^\lambda d\varepsilon \int_0^\varepsilon g(\varepsilon') d\varepsilon' \tag{3}$$

where λ is the Fermi energy. The second expression in eq. (3) is obtained by integrating by parts and using eq. (2). To determine the energy for a given particle number one must first use eq. (2) to determine λ and then use this value of λ in eq. (3) to determine E.

The single particle partition function can be defined in terms of the Laplace transform of the single particle density of states as:

$$Z(\beta) = \mathcal{L}[g(\varepsilon)] = \int_0^\infty e^{-\beta\varepsilon} g(\varepsilon) d\varepsilon = \Sigma_i \, e^{-\beta\varepsilon_i} \quad , \tag{4}$$

where $\mathcal{L}$ denotes the Laplace transform and β is the transformed variable. The partition function can also be expressed as:

$$Z(\beta) = \text{tr } e^{-\beta\hat{H}} , \tag{5}$$

where $\hat{H}$ is the Hamiltonian operator. The quantities $g(\varepsilon)$, N and E can now be expressed in terms of the partition function by the following equations:

$$g(\varepsilon) = \mathcal{L}_{\varepsilon}^{-1}[Z(\beta)] , \tag{6}$$

$$N = \mathcal{L}_{\lambda}^{-1}\left[\frac{Z(\beta)}{\beta}\right] , \tag{7}$$

$$E = \lambda N - \mathcal{L}_{\lambda}^{-1}\left[\frac{Z(\beta)}{\beta^2}\right] , \tag{8}$$

where $\mathcal{L}_{\lambda}^{-1}$ denotes the inverse Laplace transform with respect to the variable λ. To get eqs. (7) and (8) from eqs. (2) and (3) we have used elementary properties of Laplace transforms (Abramowitz and Stegun 1965, p. 1020). After doing the inverse transforms in eqs. (6)-(8) the dummy variable β is no longer present.

II. 2 The Semiclassical Expansion.

The energy , E, does not vary smoothly as a function

of the nucleon number or the deformation parameters of the potential because of the bunching of single particle levels. The simplest way to wash out these quantum shell effects is to replace the exact partition function in eqs. (6)-(8) by the classical partition function $Z_{Cl}(\beta)$. This, as we shall shortly see, yields the TF expressions. The classical partition function is defined in terms of the phase space integral as:

$$Z_{Cl}(\beta) = \frac{2}{h^3} \int e^{-\beta H_{Cl}} \, d^3p d^3r \qquad (9)$$

The factor 2 comes from spin degeneracy. The classical Hamiltonian, H_{Cl}, is given by:

$$H_{Cl} = \frac{p^2}{2m} + V(\underset{\sim}{r}) \quad . \qquad (10)$$

When the potential, $V(\underset{\sim}{r})$, is momentum independant, the p-integration may be done analytically to yield:

$$Z_{Cl} = \frac{1}{4\pi^{3/2}\beta^{3/2}} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int e^{-\beta V(\underset{\sim}{r})} \, d^3r \quad . \qquad (11)$$

The expressions for $g_{Cl}(\varepsilon)$, N and E_{Cl} may now be obtained from eqs. (6), (7) and (8):

$$g_{Cl}(\varepsilon) = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar}\right)^{3/2} \int d^3r (\varepsilon - V)^{1/2} \, \theta(\varepsilon - V) \qquad (12)$$

$$N = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int^{\underset{\sim}{r}_{Cl}} d^3r\ (\lambda_{Cl}-V)^{3/2} \qquad (13)$$

$$E_{Cl} = \lambda_{Cl}\,N - \frac{2}{15\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int^{\underset{\sim}{r}_{Cl}} d^3r\ (\lambda_{Cl}-V)^{5/2}$$

$$= \frac{1}{(3\pi^2)}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int^{\underset{\sim}{r}_{Cl}} d^3r\left[\frac{3}{5}(\lambda_{Cl}-V)^{5/2} + V(\lambda_{Cl}-V)^{3/2}\right] \qquad (14)$$

where the integrals for N and E_{Cl} are cut off at the classical turning point, $\underset{\sim}{r}_{Cl}$, such that $V(\underset{\sim}{r}_{Cl}) = \lambda_{Cl}$. In obtaining these results we have used the following identity (Abramowitz and Stegun, 1965, p. 1021 and p. 1022):

$$\mathcal{L}^{-1}_{\lambda}\left\{\frac{e^{-\beta V(\underset{\sim}{r})}}{\beta^{\nu}}\right\} = \frac{(\lambda-V(\underset{\sim}{r}))^{\nu-1}}{\Gamma(\nu)}\,\theta(\lambda-V(\underset{\sim}{r}))\ , \qquad (15)$$

where $\Gamma(\nu)$ is the usual gamma function and $\theta(\lambda-V(\underset{\sim}{r}))$ is the unit step function. The expressions (12), (13) and (14) may be easily recognized as the standard Thomas-Fermi (TF) results (see for example Kirzhnits, 1967 p. 45). Smooth corrections to the TF result may now be obtained by finding semiclassical correction terms to the classical partition function. Just such a semiclassical partition function, $Z_{sc}(\beta)$, was developed by Wigner (1932) and Kirkwood (1933), in which the correction terms appear as a power series in $\hbar$. Although this result is quite old, a derivation of it will be given here as it

forms the basis for the following chapters and it will be useful to present the derivation in this simple case before doing the more complicated cases in chapter IV. To do this we must express the trace in eq. (5) in terms of plane waves. This gives us:

$$Z(\beta) = \frac{2}{h^3} \int d^3r d^3p \; e^{-i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar} \; e^{-\beta\hat{H}} \; e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar} \; . \tag{16}$$

We now write:

$$e^{-\beta\hat{H}} \; e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar} = e^{-\beta H_{Cl}} \; e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar} \; w(\underset{\sim}{r},\underset{\sim}{p},\beta) = u(\underset{\sim}{r},\underset{\sim}{p},\beta) \; , \tag{17}$$

where this equation serves to define both w and u. It is easily seen that u satisfies the Bloch equation:

$$\frac{\partial u}{\partial \beta} + \hat{H}u = 0 \; , \tag{18}$$

with the boundary condition:

$$\lim_{\beta \to 0} u = e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar} \; .$$

Using eq. (17) we can write eq. (18) in terms of w, thus obtaining:

$$\frac{\partial w}{\partial \beta} = -i\hbar\left[\frac{\beta}{m}(\underset{\sim}{p}\cdot\nabla V)w - \frac{1}{m}(p\cdot\nabla w)\right]$$

$$+ \frac{\hbar^2}{2m}\left[\beta^2(\nabla V)^2 w - \beta(\nabla^2 V)w + \nabla^2 w\right.$$

$$\left. - 2\beta(\nabla V\cdot\nabla w)\right] \quad , \tag{19}$$

with the boundary condition $w=1$ at $\beta=0$. Although this equation cannot be solved exactly, it is, however, possible to make an expansion of w in a power series in $\hbar$ by substituting:

$$w = 1 + \hbar w_1 + \hbar^2 w_2 + - - - - \quad , \tag{20}$$

in eq. (19) and solving to each order in $\hbar$. The expressions for the w's, which contain $\underset{\sim}{r}, \underset{\sim}{p}$ and derivatives of V, are given, up to w_4, in Appendix A. The w's associated with odd powers of $\hbar$ (w_1, w_3, etc.) are imaginary and contain odd powers of $\underset{\sim}{p}$. The w's associated with even powers of $\hbar$ are real and contain even powers of $\underset{\sim}{p}$. With this expansion we may write the semiclassical partition function, $Z_{sc}(\beta)$, as:

$$Z_{sc}(\beta) = \frac{2}{h^3}\int e^{-\beta H_{Cl}}(1+\hbar w_1+\hbar^2 w_2+ ---)d^3p d^3r \quad . \tag{21}$$

The first term is just the classical partition function

as given by eq. (9). Although the p-integrations in eq. (21) can be done in a straightforward manner in cartesian coordinates, this is an extremely tedious process and techniques for doing them quicker will be given in Appendix B. Upon doing the p-integrations we obtain upto order $\hbar^4$:

$$Z_{sc}(\beta) = \frac{1}{4\pi^{3/2}\beta^{3/2}}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int d^3r\, e^{-\beta V}\left[1 - \frac{\beta^2}{12}\frac{\hbar^2}{2m}\nabla^2 V + \frac{\beta^3}{1440}\left(\frac{\hbar^2}{2m}\right)^2(-7\nabla^4 V+5\beta(\nabla^2 V)^2+\beta\nabla^2(\nabla V)^2)\right] . \tag{22}$$

In getting eq. (22) we have also used the fact that the space integral over a gradient is zero to obtain identities of the form:

$$\int d^3r\, e^{-\beta V}(\nabla V)^2 = \frac{1}{\beta}\int d^3r\, e^{-\beta V}\nabla^2 V . \tag{23}$$

The semiclassical partition function that we have derived may now be used in eq. (7) to obtain the Fermi energy λ_{sc}, and then in eq. (8) to find E_{sc}. It is shown in Appendix C, that to obtain E_{sc} correct to order $\hbar$, it is only necessary to take $Z_{sc}(\beta)$ to order $\hbar^{-1}$ in eq. (7), although terms of order $\hbar$ are needed in eq. (8). Eq. (22) can now be used in connection with eqs. (7) and (8) to obtain semiclassical results for N and E_{sc}. In doing this we need to use eq. (15)

and the identity:

$$e^{-\beta V} = -\frac{1}{\beta}\,\frac{\nabla V\cdot\nabla e^{-\beta V}}{(\nabla V)^2} \tag{24}$$

in connection with results like eq. (23). The final expressions are:

$$N = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int d^3r\,\left[(\lambda_{sc}-V)^{3/2} - \frac{\hbar^2}{32m}\nabla^2 V\,(\lambda_{sc}-V)^{-1/2}\right], \tag{25}$$

$$E_{sc} = \lambda_{sc}N - \frac{2}{15\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int d^3r\,(\lambda_{sc}-V)^{5/2}$$

$$+ \frac{1}{24\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}\int d^3r\,\nabla^2 V(\lambda_{sc}-V)^{1/2}$$

$$- \frac{1}{5760\pi^2}\left(\frac{\hbar^2}{2m}\right)^{1/2}\int d^3r\,\frac{1}{(\lambda_{sc}-V)^{1/2}(\nabla V)^2}\left[-7(\nabla^4 V)(\nabla V)^2\right.$$

$$+ 5(\nabla^2 V)^3 + 10[\nabla V\cdot\nabla(\nabla^2 V)]\nabla^2 V - 5(\nabla^2 V)^2\nabla V\cdot\nabla(\nabla V)^2/(\nabla V)^2$$

$$\left. + (\nabla^2 V)\nabla^2(\nabla V)^2 + \nabla V\cdot\nabla\nabla^2(\nabla V)^2 - \nabla^2(\nabla V)^2\nabla V\cdot\nabla(\nabla V)^2/(\nabla V)^2\right]. \tag{26}$$

In these equations all integrals are cut off at the turning points, $\underset{\sim}{r}_{sc}$, given by $V(\underset{\sim}{r}_{sc}) = \lambda_{sc}$.

Although it is not necessary for our main objective of obtaining the expressions for N and E_{sc}, we will give the

expression for $g_{sc}(\varepsilon)$ for completeness. It is :

$$g_{sc}(\varepsilon) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int d^3r(\varepsilon-V)^{1/2}\,\theta(\varepsilon-V)$$

$$-\frac{1}{48\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}\frac{\partial}{\partial\varepsilon}\int d^3r\,\frac{\theta(\varepsilon-V)\nabla^2V}{(\varepsilon-V)^{1/2}}$$

$$+\frac{1}{5760\pi^2}\left(\frac{\hbar^2}{2m}\right)^{1/2}\frac{\partial^3}{\partial\varepsilon^3}\int d^3r\;\theta(\varepsilon-V)\left[-14(\varepsilon-V)^{1/2}\nabla^4V\right.$$

$$\left.+\,5\,\frac{(\nabla^2V)^2}{(\varepsilon-V)^{1/2}}+\frac{\nabla^2(\nabla V)^2}{(\varepsilon-V)^{1/2}}\right] . \qquad (27)$$

In obtaining this result we have used the identity (van der Pol and Bremmer 1955, p. 48 compare p. 50):

$$\mathcal{L}_\lambda^{-1}\,\beta^n Z(\beta) = \frac{\partial}{\partial\lambda^n}\mathcal{L}_\lambda^{-1}\;Z(\beta) \quad , \qquad (28)$$

which is valid because the unit step functions are included explicitly.

We have thus completed the derivation for the smooth energy in this simple case of a momentum independant potential. We stress again that although we have used the partition function in this derivation the result is essentially an $\hbar$-expansion and not a high temperature result. In fact our result can be regarded as an extended TF expression where corrections have been added to the usual TF result, that are smooth functions of N and deformation. Similar results,

up to order $\hbar^{-1}$, have been obtained (Balian and Bloch 1971, Gross 1972) by quite different methods which do not introduce the partition function. The essential equivalence of the results obtained by Balian and Bloch (1971) and those obtained here has been shown by Jennings (1974).

II.3 The Finite Well Problem.

The results of the previous section are strictly only valid for potentials that go to infinity as $\underset{\sim}{r}$ goes to infinity. If the potential does not do this the space integrals in equations, such as eq. (21), for the partition function diverge although the eqs. (25) and (26) for N and E_{sc} remain well defined. There are two methods of making the derivation valid for finite wells. For the first we notice that the space integrals in eq. (25) and (26) are only over the classically allowed region. This means that the result will not change if the potential, V, is replaced by a potential that is almost equal to V inside the classically allowed region but goes to infinity at large $\underset{\sim}{r}$. This is essentially the same as confining the system in a large box. The derivation would then be valid and the result would not depend on the constraining potential. The potential could for example be replaced by V plus an harmonic oscillator potential with a very small oscillator frequency.

The second method is only valid for potentials whose volume integrals are finite. Instead of considering directly

the single-particle density of states we consider rather the difference, $g_d(\varepsilon)$, between the density of states, $g(\varepsilon)$, of a particle in the finite potential and the density of states, $g_f(\varepsilon)$, of a free particle (see for example Huang 1963, p. 309). Hence we have:

$$g_d(\varepsilon) = g(\varepsilon) - g_f(\varepsilon) \quad . \tag{29}$$

For the case of spherical symmetry this reduces to the well known result (Huang 1963, p. 309):

$$g_d(\varepsilon) = \Sigma \delta(\varepsilon-\varepsilon_i) + \frac{1}{\pi} \sum_J (2J+1) \frac{d\delta_J}{d\varepsilon} \quad , \tag{30}$$

where the ε_i are the bound states and δ_J are the scattering phase shifts. This density of states, eq. (29), may be used instead of $g(\varepsilon)$ in eqs. (2) and (3) to determine λ and N. It may also be used in eq. (4) to give the partition function. The partition function becomes (Gibson 1970):

$$Z_d(\beta) = \mathrm{tr}(e^{-\beta\hat{H}} - e^{-\beta\hat{H}_f}) \quad , \tag{31}$$

where $\hat{H}_f$ is the free particle Hamiltonian. When the trace is taken in the plane wave, the eigenfunctions of H_f, basis we get:

$$Z_d(p) = \frac{2}{h^3} \int d^3r d^3p \; e^{-i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar} (e^{-\beta\hat{H}} - e^{-\beta\frac{p^2}{2m}}) \; e^{-i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar} \quad . \tag{32}$$

This equation replaces eq. (16) for finite wells. In the semiclassical partition function, eq. (22), this affects only the classical term. The semiclassical partition function now becomes:

$$Z_{sc}(\beta) = \frac{1}{4\pi^{3/2}\beta^{3/2}}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int d^3r\, e^{-\beta V}\left[1-e^{\beta V}\right.$$

$$-\frac{\beta^2}{12}\frac{\hbar^2}{2m}\nabla^2 V+\frac{\beta^3}{1440}\left(\frac{\hbar^2}{2m}\right)^2(-7\nabla^4 V+5\beta(\nabla^2 V)^2$$

$$\left.+\beta\nabla^2(\nabla V)^2)\right]. \qquad (33)$$

This partition function remains finite if V(r) goes to zero faster than r^{-1}. This partition function can now be used in eqs. (6), (7) and (8) to determine $g_{sc}(\varepsilon)$, N, and E_{sc}. The new classical density of states is:

$$g_{Cl}(\varepsilon) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int d^3r\left[(\varepsilon-V)^{1/2}\theta(\varepsilon-V)-\varepsilon^{1/2}\theta(\varepsilon)\right]. \qquad (34)$$

The additional term, $\varepsilon^{1/2}\theta(\varepsilon)$, contributes to the density of states only when ε is above the top of the well. Similarly the new term contributes to the expressions for N and E_{sc} only when λ_{sc} is above the top of the well and hence can be ignored in most cases.

As using a finite potential causes only minor changes in the derivation and does not affect the results we shall

not explicitly consider finite wells in the derivations in the following sections.

II.4 Spin-orbit Effects.

In this section we shall consider the effects of a term:

$$\hat{V}_{LS} = -\frac{\kappa}{m}(\nabla f \times \hat{p})\cdot\hat{s}$$

$$= i\kappa\frac{\hbar^2}{2m}(\nabla f\times\nabla)\cdot\hat{\sigma} \qquad (35)$$

in the Hamiltonian on the semiclassical energy. Here κ is a dimensionless strength factor, $f(r)$ is a dimensionless form factor and we have used the relations $\hat{p} = -i\hbar\nabla$ and $\hat{s} = \frac{1}{2}\hbar\hat{\sigma}$, where $\hat{\sigma}$ is the unit Pauli matrix. The quantum partition function now becomes:

$$Z(\beta) = \mathrm{tr}\, e^{-\beta(\hat{H}_0+\hat{V}_{LS})} \qquad (36)$$

where $\hat{H}_0$ is the spin independant part of the Hamiltonian:

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + V(\underset{\sim}{r}) \quad . \qquad (37)$$

Since $\hat{V}_{LS}$ does not in general commute with $\hat{H}_0$, we cannot write $Z(\beta)$ as the trace over a product of two exponentials. We can however write:

$$e^{-\beta(\hat{H}_0+\hat{V}_{LS})} = e^{-\beta\hat{H}_0}\,\hat{S}(\beta) \quad , \qquad (38)$$

and develop a differential equation for $\hat{S}(\beta)$ by differentiating both sides of eq. (38) by β. This gives us:

$$\frac{\partial \hat{S}(\beta)}{\partial \beta} = -e^{\beta \hat{H}_0} \hat{V}_{LS} e^{-\beta \hat{H}_0} = -\hat{V}_{LS}(\beta) \quad , \tag{39}$$

where this equation serves to define $\hat{V}_{LS}(\beta)$. It is easily seen by direct substitution that:

$$\hat{S}(\beta) = 1 - \int_0^\beta \hat{V}_{LS}(\beta')d\beta' + \int_0^\beta \hat{V}_{LS}(\beta') \int_0^{\beta'} \hat{V}_{LS}(\beta'')d\beta'' \, d\beta' + \text{---} \tag{40}$$

provides a solution of eq. (39). The operator $\hat{V}_{LS}(\beta)$ may be further expanded as (Messiah 1965, p. 339)

$$\hat{V}_{LS}(\beta) = \hat{V}_{LS} + \beta[\hat{H}_0, \hat{V}_{LS}] + \frac{\beta^2}{2!}[\hat{H}_0, [\hat{H}_0, \hat{V}_{LS}]] + \text{----}, \tag{41}$$

From eqs. (36) and (38), using the plane wave basis, we get:

$$Z(\beta) = \frac{1}{h^3} \sum_\sigma \int e^{-i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar} e^{-\beta \hat{H}_0} \hat{S}(\beta) e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar} d^3p d^3r$$

$$= \frac{1}{h^3} \sum_\sigma \int (e^{-\beta \hat{H}_0} e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar})^* \hat{S}(\beta) e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar} d^3p d^3r \tag{42}$$

In obtaining the second expression we have used the fact that $e^{-\beta \hat{H}_0}$ is Hermitian. We may now use eq. (40) in connection with eq. (42) to obtain an expression for $Z(\beta)$ as a power series in the spin-orbit strength constant κ. The first

term is κ-independant and is the same as the partition function discussed in section (II.2). The term linear in κ is also linear in $\hat{\sigma}$ and hence vanishes upon taking the $\hat{\sigma}$ trace as $\hat{\sigma}$ is traceless. This leaves the κ^2 and higher order terms. We will only consider the κ^2, κ^3 and κ^4 terms as higher order terms are negligible as shown in next section where explicit examples are considered.

We will now use the semiclassical eqs. (17) and (20) and the definition:

$$I(\underset{\sim}{r},\underset{\sim}{p},\beta) = e^{-i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar}\,\hat{S}(\beta)\,e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar} - 1 \,, \tag{43}$$

to obtain:

$$Z_{sc}(\beta) = \frac{1}{h^3}\sum_{\sigma}\int e^{-\beta H_{Cl}}(1+\hbar\omega_1^{\star} + \hbar^2 w_2 + \text{---})I(\underset{\sim}{r},\underset{\sim}{p},\beta)\,d^3r\,d^3p$$

$$+ Z_{sc}^{0}(\beta) \,, \tag{44}$$

where $Z_{sc}^{0}(\beta)$ is the partition function as given by eq. (21) or (22). It now remains to evaluate $I(\underset{\sim}{r},\underset{\sim}{p},\beta)$. This may be done in a straightforward manner to any order in $\hbar$ by using eqs. (40), (41) and (43). The expression for $I(\underset{\sim}{r},\underset{\sim}{p},\beta)$, after the $\hat{\sigma}$-summation, is given in appendix D. Upon doing the p-integrations as outlined in appendix B we get:

$$Z_{sc}(\beta) = Z_{sc}^{0}(\beta) + \frac{\kappa^2}{8\pi^{3/2}\beta^{1/2}}\left(\frac{2m}{\hbar^2}\right)^{1/2}\int d^3r\; e^{-\beta V}(\nabla f)^2 ,$$

$$+ \frac{1}{96\pi^{3/2}} \beta^{1/2} \left(\frac{\hbar^2}{2m}\right)^{1/2} \int d^3r\, e^{-\beta V} \Big[\kappa^2\{-\beta(\nabla f)^2(\nabla^2 V)$$

$$+ \frac{1}{2}\nabla^2(\nabla f)^2 - (\nabla^2 f)^2 + \nabla f\cdot\nabla(\nabla^2 f)\} - 2\kappa^3\{(\nabla f)^2\nabla^2 f$$

$$- \frac{1}{2}\nabla f\cdot\nabla(\nabla f)^2\} + 2\kappa^4(\nabla f)^4\Big] \quad . \qquad (45)$$

To get the final results for N and E_{sc} it is only necessary to use these expressions in eqs. (7) and (8). We will here only write down the extra terms due to the spin-orbit as the κ-independant terms are already given in eqs. (25) and (26). The additional term to be added to the N equation, eq. (25), is:

$$\frac{\kappa^2}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}\int d^3r\,(\nabla f)^2(\lambda_{sc}-V)^{1/2}\,\theta(\lambda_{sc}-V) \quad , \qquad (46)$$

while the additional terms to be added to eq. (26) for E_{sc} are:

$$- \frac{\kappa^2}{6\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}\int d^3r(\nabla f)^2(\lambda_{sc}-V)^{3/2}\theta(\lambda_{sc}-V)$$

$$- \frac{1}{48\pi^2}\left(\frac{\hbar^2}{2m}\right)^{1/2}\int d^3r(\lambda_{sc}-V)^{1/2}\Big[\kappa^2\{\frac{1}{2}\nabla^2(\nabla f)^2-(\nabla^2 f)^2$$

$$+ \nabla f\cdot\nabla(\nabla^2 f) - \frac{(\nabla f)^2\nabla^2 V}{2(\lambda_{sc}-V)}\} - 2\kappa^3\{(\nabla f)^2\nabla^2 f - \frac{1}{2}\nabla f\cdot\nabla(\nabla f)^2\}$$

$$+ 2\kappa^4(\nabla f)^4\Big]\theta(\lambda_{sc}-V) \quad . \qquad (47)$$

The complete expression for E_{sc} in the case of spherical symmetry is given in appendix E.

II.5 The $\hbar$-Expansion for Harmonic Oscillator.

In this section, we consider a simple model where the one-body potential is an isotropic harmonic oscillator with a constant spin-orbit term. In this case Z_{sc} can be directly obtained from the eigenenergy spectrum without going through the Wigner-Kirkwood expansion. The relevant equations for Z_{sc} and E_{sc} derived in the earlier sections can therefore be checked here. Also the convergence of the series can be examined for reasonable values of the oscillator parameter, ω, and the spin-orbit strength, κ.

The one-body Hamiltonian is taken to be:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 r^2 - \kappa(\hbar\omega)\hat{\ell}\cdot\hat{\sigma} \quad , \tag{48}$$

where $\hat{\ell} = -i(\underset{\sim}{r}\times\nabla)$. Comparing $\hat{V}_{LS}$ of the above Hamiltonian with eq. (35), we find the form factor f for this case to be:

$$f(r) = (m\omega/\hbar)r^2 \quad . \tag{49}$$

The resulting single particle spectrum is given by:

$$\epsilon_{j=\ell+1/2} = (2n+\ell+3/2)\hbar\omega - \kappa\hbar\omega\ell \tag{50}$$

$$\varepsilon_{j=\ell-1/2} = (2n+\ell+3/2)\hbar\omega + \kappa\hbar\omega(\ell+1) \quad . \qquad (51)$$

The degeneracy of the states for a given j is $(2j+1)$. The quantum partition function, from eq. (4), is

$$Z(\beta)=2e^{-3/2\hbar\omega\beta}\sum_{n=0}^{\infty} e^{-2n\hbar\omega\beta}\sum_{\ell=0}^{\infty}[(\ell+1)e^{-\beta\hbar\omega(1-\kappa)}+\ell e^{-\beta\hbar\omega\ell(1+\kappa)} e^{-\beta\hbar\omega\kappa}] \quad . \qquad (52)$$

The sums over n and ℓ can be done explicitly to give:

$$Z(\beta) = \frac{e^{-\hbar\omega\beta/2}}{4\sinh(\hbar\omega\beta)}\left[\frac{1}{\sinh^2[\frac{1}{2}\hbar\omega\beta(1-\kappa)]} + \frac{e^{-\kappa\hbar\omega\beta}}{\sinh^2[\frac{1}{2}\hbar\omega\beta(1+\kappa)]} + \frac{2e^{\frac{1}{2}\hbar\omega\beta(1-\kappa)}}{\sinh[\frac{1}{2}\hbar\omega\beta(1-\kappa)]}\right] \quad . \qquad (53)$$

Note that for $\kappa=0$, the right hand side of the above equation reduces to the usual form $1/4\ \mathrm{cosech}^3(\hbar\omega\beta/2)$. The semi-classical partition function may now be obtained by expanding the hyperbolic and exponential functions with the result:

$$Z_{sc}(\beta) = \frac{1}{(1-\kappa^2)^2}\left[\frac{2}{(\hbar\omega\beta)^3}(1+\kappa)^2 - \frac{2\kappa^2}{(\hbar\omega\beta)^2} - \frac{1}{12\hbar\omega\beta}(3+9\kappa^2 -10\kappa^4) + \frac{1}{12}(5\kappa^3-2\kappa^5) + \frac{\hbar\omega\beta}{2880}(51+303\kappa^2-364\kappa^4+24\kappa^6) + \text{----}\right] \quad . \qquad (54)$$

In the above equation for $Z_{sc}(\beta)$ we have an expansion in powers of $\hbar$ whereas the Wigner-Kirkwood series, given by eqs. (22) and (45), is in power of $\hbar^2$. This is because in the present model the form factor, f(r), contains an explicit factor of $\hbar^{-1}$. This will not be so when more realistic form factors are chosen in the next section.

For the Hamiltonian (48), a reasonable value of κ is $\lesssim 0.1$, so that we may further expand the factor $(1-\kappa^2)^2$ in eq. (54). It is then convenient to split the resulting Z_{sc} as in eq. (45), writing:

$$Z_{sc} = Z^0_{sc} + Z_{LS} \quad . \tag{54}$$

We then get:

$$Z^0_{sc} = \frac{2}{(\hbar\omega\beta)^3} - \frac{1}{4(\hbar\omega\beta)} + \frac{17}{960}\hbar\omega\beta + \text{---} \tag{55}$$

with the κ dependant terms in Z_{LS}. This result is in agreement with that obtained by Bhaduri and Ross (1971). It is easy to verify that eq. (22), which makes no use of the spectrum, exactly reproduces eq. (55) when we put $V = m\omega^2 r^2/2$ and perform the relevant integrations. Note that two small expansion parameters, $\hbar$ and κ, are involved. Arranging the terms in the expansion such that all terms within a square bracket are of the same order, we may write:

$$Z_{LS}(\beta) = \left[\frac{6\kappa^2}{(\hbar\omega\beta)^3}\right] + \left[\frac{10\kappa^4}{(\hbar\omega\beta)^3} - \frac{2\kappa^3}{(\hbar\omega\beta)^2} - \frac{5}{4}\frac{\kappa^2}{\hbar\omega\beta}\right]$$

$$+ \left[\frac{14\kappa^6}{(\hbar\omega\beta)^3} - \frac{4\kappa^5}{(\hbar\omega\beta)^2} - \frac{17}{12}\frac{\kappa^4}{\hbar\omega\beta} + \frac{5}{12}\kappa^3 + \frac{9}{64}\kappa^2(\hbar\omega\beta)\right] + \text{---} \quad . \tag{56}$$

It is again easy to check that all terms in the first two brackets in the above equation are reproduced by the Wigner-Kirkwood formula (45) when $f = (m\omega/\hbar)r^2$. The last term will be shown to make a negligible contribution to E_{sc}.

For a given number of particles, λ_{sc} can now be calculated using Z_{sc} of eqs. (55) and (56). The smooth energy E_{sc} is then calculated with λ_{sc} using eq. (8). The resulting expression for E_{sc} is:

$$(E_{sc} - \lambda_{sc}N) = -\frac{\lambda_{sc}^4}{12(\hbar\omega)^3} + \frac{\lambda_{sc}^2}{8\hbar\omega} - \frac{17}{960}\hbar\omega$$

$$- \frac{\kappa^2}{4}\frac{\lambda_{sc}^4}{(\hbar\omega)^3} + \left(\frac{5}{8}\kappa^2\frac{\lambda_{sc}^2}{\hbar\omega} + \frac{\kappa^3}{3}\frac{\lambda_{sc}^3}{(\hbar\omega)^2} - \frac{5}{12}\kappa^4\frac{\lambda_{sc}^4}{(\hbar\omega)^3}\right)$$

$$+ \left(-\frac{7}{12}\kappa^6\frac{\lambda_{sc}^4}{(\hbar\omega)^3} + \frac{2}{3}\kappa^5\frac{\lambda_{sc}^3}{(\hbar\omega)^2} + \frac{17}{24}\kappa^4\frac{\lambda_{sc}^2}{\hbar\omega} - \frac{5}{12}\kappa^3\lambda_{sc}\right.$$

$$\left. - \frac{9}{64}\kappa^2\hbar\omega\right) + \text{----} \quad . \tag{57}$$

It is not difficult to check that above equation, neglecting the expression in the last bracket, is reproduced if one uses the Wigner-Kirkwood expansion, eqs. (22) and (45) or as given

in appendix E, with $V = m\omega^2 r^2/2$ and $f = (m\omega/\hbar)r^2$. To estimate the relative importance of these terms in a heavy nucleus, we assume $\hbar\omega$ = 7MeV and arbitrarily set λ_{sc} = 42 MeV. The first three terms of eq. (57) are respectively -756.00, 31.50 and -0.12 MeV. The leading κ^2 term gives -22.68 MeV while the three terms in the first bracket give respectively 1.58, 0.50 and -0.38 MeV. It is seen that the κ^3 and κ^4 terms almost cancel. This seems to be a general result for realistic values of κ. The terms in the second bracket give only -0.005 MeV. Considerations of this simple model therefore indicate that the semiclassical series (22) and (45) is accurate to 0.1 MeV and that the neglected terms are, in fact, negligible.

II.6 The $\hbar$-Expansion for Woods-Saxon Potentials.

In this section we consider the semiclassical expansion for Woods-Saxon potentials both with and without a spin-orbit potential. We first look at the case of hypothetical spherical "nuclei" with N=Z=A/2 and no Coulomb potential. The potential is given by:

$$V(r) = -V_0 f(r) \qquad (58)$$

with:

$$f(r) = [1 + \exp(r-R)/a]^{-1} \quad . \qquad (59)$$

Table 1

A	$E_{sc}^{(-3)}$	$E_{sc}^{(-1)}$	$E_{sc}^{(1)}$	E_{sc}	E_{str}
40	-717.7	36.2	0.7	-680.8	∿
72	-1368.3	52.5	0.8	-1315.0	-1315.4(1.2)
164	-3344.7	88.8	1.0	-3254.9	-3256.0(1.2)
204	-4229.8	102.3	1.0	-4126.5	-4126.6(0.8)
260	-5484.8	119.7	1.1	-5364.0	-5364.4(0.8)
292	-6208.4	129.1	1.1	-6078.2	-6078.6(0.8)
416	-9045.1	162.5	1.1	-8881.5	-8882.8(1.2)

Table 1. Smooth energy in a spherical Woods-Saxon well. All energies are in MeV. The parameters of the well are as given in the text. The first column gives the nucleon number A=2N=2Z. The second, third and fourth columns give $E_{sc}^{(-3)}$, $E_{sc}^{(-1)}$ and $E_{sc}^{(1)}$ which are the contributions to E_{sc} from respectively the TF term, the $\hbar^{-1}$ term, and the $\hbar$ term. The fifth column gives the total semiclassical energy E_{sc}, while the last column gives the Strutinsky energy.

For these calculations we choose V_0 = 44 MeV, a = 0.67 fm, and R = 1.27 $A^{1/3}$ fm, while $\hbar^2/(2m)$ = 20.748. The calculations for E_{sc} were done, using eq. (25) and (26), for about twenty "nuclei" in the range A = 40 to 500 and a few typical results are displayed in table 1. It can be seen that for such potentials the numerical convergence of our series is excellent, and we can claim to have found E_{sc} to an absolute accuracy of 0.1 MeV.

Our results are also compared, table 1, to the smooth energies, E_{st}, obtained from carefully done Strutinsky calculations (Jennings et. al. 1975). Due to ambiguities in the Strutinsky result the comparison is not made for A < 70; for the other cases the agreement is quite good.

To see the effects of spin-orbit we will consider the cases of 126 and 184 neutrons moving in a spherical Woods-Saxon well, as parametrized by Blomquist and Wahlborn (1960). The central part is as given by eqs. (58) and (59) while the spin-orbit part is, in the notation of eq. (35);

$$V_{LS} = -\kappa \frac{\hbar^2}{2m} \frac{1}{r} \frac{df}{dr} \hat{\ell}.\hat{\sigma} \quad , \tag{60}$$

with f as given by eq. (59). The numerical values of the parameters for N = 126 are V_0 = 44 MeV, R = 7.52 fm a = 0.67 fm and κ = -0.7491; and for N = 184 there are V_0 = 43 MeV, R = 8.48 fm, a = 0.67 fm and κ = -0.7321. In both cases

Table 2

N	$E_{sc}^{(-3)}$	$E_{sc}^{(-1)}$	$E_{sc}^{(1)}$	$E_{sc}^{LS(-1)}$	$E_{sc}^{LS(1)}$	E_{sc}	E_{st}
126	-2314.69	50.87	1.07	-23.92	4.24	-2282.43	-2282.5
184	-3267.29	61.24	1.47	-30.13	4.97	-3229.74	-3230.0
HO		31.50	-0.12	-22.68	1.70		

Table 2 Smooth energy in a spherical Woods-Saxon well with spin-orbit. All energies in MeV. The parameters are given in the text. With the exception of the first, fifth and sixth columns are as in table 1. The first column gives the neutron number N while the fifth and sixth give the contributions from V_{LS} of order $\hbar^{-1}$ and $\hbar$ respectively. The last row gives the harmonic oscillator results from the last section. The Strutinsky results are from Ross and Bhaduri (1972).

$\hbar^2/(2m)$ was taken to be 20.7219 MeV-fm^2. Compared to the harmonic oscillator model of sect. (II.5), κ is of the opposite sign and much larger. This is because df/dr is negative here and it is nonzero only in the surface region, so that a larger κ is needed to yield the same level splitting. For the same reason the contribution of V_{LS} to $\tilde{E}_{sc}$ is of the same order of magnitude as in the harmonic oscillator model, and the perturbation scheme remains satisfactory. The results for E_{sc} were obtained, using eqs. (25), (26), (46) and (47), and are given in table 2. Also given are the corresponding numbers for the harmonic oscillator as obtained in the previous section. Although the convergence here is not as good as for the harmonic oscillator it is still adequate. As we noted in the last section the next higher order contribution of V_{LS} to E_{sc} in the harmonic oscillator model is only 0.005 MeV. Even if it were twenty times bigger for the Woods-Saxon case, the neglected term would still be only 0.1 MeV. We again see the good agreement between the semiclassic and Strutinsky values. These Strutinsky values were obtained by Ross and Bhaduri (1972).

Calculations have also been done for potentials including Coulomb effects as well as for deformed potentials (Jennings et. al. 1975 a,b). In both cases results similar to those quoted were obtained. The computer time needed to complete the calculation of E_{sc}, for axially deformed nuclei at a single deformation, was about 8 sec. on a CDC-6400

computer. In most cases checked the agreement with Strutinsky results was reasonable. The formal relation between these two results will be discussed in chapter 8.

CHAPTER III

THE SPATIAL AND KINETIC ENERGY DENSITIES

III.1 The Spatial Density.

In the last chapter we developed semiclassical expressions for the total energy. It is also of interest to develop expressions for the spatial and kinetic energy densities. We shall start with the spatial density, $\rho(\underset{\sim}{r})$. It is useful for this purpose to define a mixed density $g(\varepsilon,\underset{\sim}{r})$ given by:

$$g(\varepsilon,\underset{\sim}{r}) = \sum_i \psi_i^*(\underset{\sim}{r})\psi_i(\underset{\sim}{r})\delta(\varepsilon-\varepsilon_i) \qquad (1)$$

where $\psi_i(\underset{\sim}{r})$ is the wave function corresponding to ε_i. The normal density of states, $g(\varepsilon)$, of eq. (II.1) may be obtained by integrating $g(\varepsilon,\underset{\sim}{r})$ over all space. The spatial density, $\rho(\underset{\sim}{r})$ is obtained by integrating $g(\varepsilon,\underset{\sim}{r})$ from the bottom of the well to the chemical potential λ. In analogy with the partition function of eq. (II.4) we may define the diagonal Bloch density, $C(\underset{\sim}{r},\beta)$, (March et. al. 1967 p. 13) as the Laplace transform of $g(\varepsilon,\underset{\sim}{r})$. This gives us:

$$C(r,\beta) = \mathcal{L}\, g(\varepsilon,\underset{\sim}{r}) = \int_0^\infty g(\varepsilon,\underset{\sim}{r})e^{-\beta\varepsilon}d\varepsilon$$

$$= \sum_i \psi_i^*(\underset{\sim}{r})\psi_i(\underset{\sim}{r})e^{-\beta\varepsilon_i} \qquad (2)$$

Integrating over $\underset{\sim}{r}$ yields the usual partition function of eq. (II.4). The spatial density is given in terms of $C(r,\beta)$ as:

$$\rho(r) = \mathcal{L}_{\lambda}^{-1}\left[\frac{C(r,\beta)}{\beta}\right] . \tag{3}$$

As in the previous chapter we shall do our expansion in β-space, only here it is $C(r,\beta)$ we must evaluate, not $Z(\beta)$.

It is convenient here to introduce the off-diagonal Bloch density, $C(\underset{\sim}{r},\underset{\sim}{r}',\beta)$ given by:

$$C(\underset{\sim}{r},\underset{\sim}{r}',\beta) = \sum_i \psi_i^*(\underset{\sim}{r})\psi_i(\underset{\sim}{r}')e^{-\beta\varepsilon_i} . \tag{4}$$

The diagonal Bloch density is given in terms of the off-diagonal Bloch density as:

$$C(\underset{\sim}{r},\beta) \equiv C(\underset{\sim}{r},\underset{\sim}{r},\beta) . \tag{5}$$

It is easily seen that $C(\underset{\sim}{r},\underset{\sim}{r}',\beta)$ satisfies the differential equation:

$$\hat{H}_{\underset{\sim}{r}} C(\underset{\sim}{r},\underset{\sim}{r}',\beta) + \frac{\partial C(\underset{\sim}{r},\underset{\sim}{r}',\beta)}{\partial\beta} = 0 \tag{6}$$

with boundary condition:

$$\lim_{\beta\to 0} C(\underset{\sim}{r},\underset{\sim}{r}',\beta) = \delta(\underset{\sim}{r}-\underset{\sim}{r}') \tag{7}$$

The operator $\hat{H}_{\underset{\sim}{r}'}$ is the Hamiltonian acting in $\underset{\sim}{r}'$ space. By direct substitution it can be seen that the solution of eq. (6) with correct boundary condition is:

$$C(\underset{\sim}{r},\underset{\sim}{r}',\beta) = \frac{1}{h^3}\int e^{-i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar}\, e^{-\beta\hat{H}_{\underset{\sim}{r}'}}\, e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}'/\hbar}\, d^3p \qquad (8)$$

The diagonal Bloch density is obtained trivially from eq. (5). We now use the semiclassical results (II.17) and (II.20) to write the diagonal Bloch density as:

$$C_{sc}(\underset{\sim}{r},\beta) = \frac{1}{h^3}\int d^3p\, e^{-\beta H_{Cl}}\,(1 + \hbar w_1 + \hbar^2 w_2 + \text{---}) \quad , \qquad (9)$$

where the w's are given in appendix A. The p-integrations are identical to those done in obtaining $Z_{sc}(\beta)$. The result for the $C(\underset{\sim}{r},\beta)$ after the p-integrations is:

$$C_{sc}(\underset{\sim}{r},\beta) = \frac{1}{4\pi^{3/2}\beta^{3/2}}\left(\frac{2m}{\hbar^2}\right)^{3/2} e^{-\beta V}\Big\{1 - \frac{\hbar^2\beta^2}{12m}\left[\nabla^2 V - \frac{\beta}{2}(\nabla V)^2\right]$$

$$+ \frac{\hbar^4\beta^3}{24m^2}\Big[-\frac{\nabla^4 V}{20} + \frac{\beta}{24}(\nabla^2 V)^2 + \frac{\beta}{15}\nabla V\cdot\nabla\nabla^2 V + \frac{\beta}{60}\nabla^2(\nabla V)^2$$

$$- \frac{\beta^2}{24}(\nabla^2 V)(\nabla V)^2 - \frac{\beta}{40}\nabla V\cdot\nabla(\nabla V)^2 + \frac{\beta^3}{96}(\nabla V)^4\Big] + \text{----}\Big\} \; . \qquad (10)$$

The partition function of eq. (II.22) may be recovered from this expression by integration over $\underset{\sim}{r}$ and using identities such as eq. (II.23). Unfortunately the density cannot be obtained by a straight forward application of eq. (3) because

for most terms in eq. (10) the Laplace inverse does not, strictly speaking, exist. If however we were to multiply $C(\underset{\sim}{r},\beta)$ by $e^{1/4\beta^2\gamma^2}$ the inverse transform will exist. This corresponds to convoluting the mixed density with a Gaussian (see appendix F). If γ is small this should have little effect on the smooth semiclassical density. This procedure is similar in spirit to a technique used by Balian and Bloch (1971) in which they introduced a Lorentzian smoothing in ϵ-space in order to justify their $\hbar$-expansion. The mathematical details of using the Gaussian smoothing are given in appendix F. The final result for the Laplace inversion formula, from eq. (F.8) is:

$$\mathcal{L}_{\lambda}^{-1}\ \beta^{n+1/2}\ e^{-\beta V} = \frac{\theta(\lambda-V)}{\Gamma(-n-1/2)\,(\lambda-V)^{n+3/2}} \qquad (11)$$

which is valid except near the turning point, where $\lambda=V$. For negative n this is just the usual inversion formula (Abramowitz and Stegun 1965, p. 1022) and is valid for all λ. With the use of this formulae the semiclassical expression for ρ_{sc} may be easily obtained from eqs. (3) and (10). The result is:

$$\rho_{sc}(\underset{\sim}{r}) = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(\lambda_{sc}-V)^{3/2} - \frac{1}{24\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}\left\{\right.$$

$$\left.\frac{(\nabla V)^2}{4(\lambda_{sc}-V)^{3/2}} + \frac{\nabla^2 V}{(\lambda_{sc}-V)^{1/2}}\right\} + \frac{1}{480\pi^2}\left(\frac{\hbar^2}{2m}\right)^{1/2}\left\{\frac{\nabla^4 V}{(\lambda_{sc}-V)^{3/2}}\right.$$

Table 3

r	ρ_{TF}	$\rho_{sc}^{(-1)}$	ρ_{st}	ρ
0.000	1.751	1.758	1.758	1.571
0.333	1.730	1.737	1.737	1.694
0.667	1.668	1.674	1.674	1.716
1.000	1.566	1.572	1.572	1.549
1.333	1.426	1.431	1.432	1.443
1.667	1.253	1.258	1.258	1.270
2.000	1.053	1.056	1.057	1.038
2.333	0.831	0.832	0.837	0.848
2.667	0.598	0.596	0.595	0.611
3.000	0.367	0.360	0.340	0.332
3.333	0.157	0.139	0.137	0.129
3.667	0.011	-0.168	0.035	0.036
4.000	0.000	0.000	0.006	0.007
4.333	0.000	0.000	0.001	0.001

Table 3 The smooth spatial density for a three-dimensional harmonic oscillator. The particle number is 112 and units are chosen such that $\hbar\omega=\hbar^2/m=1$. The first column gives the radius at which the densities are evaluated. The remaining give, in order, the following densities; the TF density, ρ_{TF}; the semiclassical density to order h^{-1}, $\rho_{sc}^{(-1)}$, the Strutinsky density, ρ_{st}, and the exact density, ρ.

$$+\frac{1}{4}\frac{1}{(\lambda_{sc}-V)^{5/2}}\left(5(\nabla^2V)^2+8\nabla V\cdot\nabla\nabla^2V+2\nabla^2(\nabla V)^2\right)$$

$$+\frac{5}{8}\frac{1}{(\lambda_{sc}-V)^{7/2}}\left(5(\nabla^2V)(\nabla V)^2+3\nabla V\cdot\nabla(\nabla V)^2\right)$$

$$+\frac{175}{64}\frac{(\nabla V)^4}{(\lambda_{sc}-V)^{9/2}}\Bigg\}, \qquad (12)$$

for $(\lambda_{sc}-V)$ greater than zero and $\rho=0$ otherwise. This expression is not valid near the turning points where it diverges. The leading term in this expansion is just the TF result (Kirzhnits 1967, p. 45). The total expression, to order $\hbar$, has also been obtained by Kirzhnits (1967, p. 53) using completely different methods.

For the harmonic oscillator the density obtained from this semiclassical result is in good agreement with the Strutinsky density, ρ_{st}, (Jennings and Bhaduri 1975), for r inside the classical turning points. This is shown in table 3 where the TF density, ρ_{TF}, and ρ_{sc} to order h^{-1} are compared to both the Strutinsky and the exact ρ.

The semiclassical density was also found for a Woods-Saxon potential with the same parameters as given in the first part of section II.6. For the closed shell case, N=92, both the semiclassical and the exact density are plotted in fig. 1. It may be seen that semiclassical density is quite smooth except near the turning points where it diverges. The exact density oscillates about the semiclassical value.

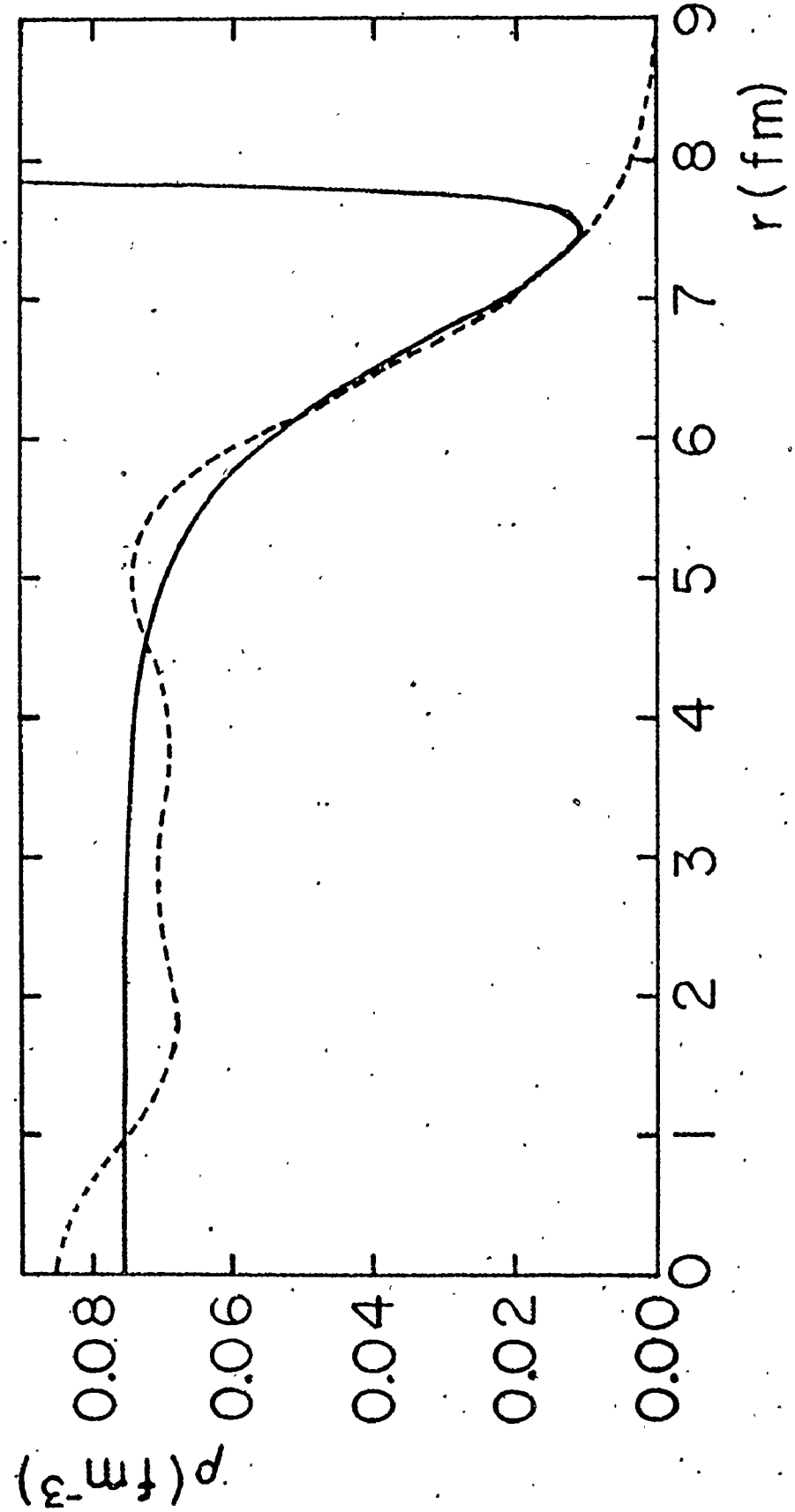

Fig. 1 The semiclassical density (solid line) and exact density (dotted line) for 92 particles in a Woods-Saxon potential as a function of radius, r. The potential parameters are given in text. The density is in units of fm^{-3} and the radius in fm.

The Strutinsky density in a Woods-Saxon well, unlike the semiclassical density, contains oscillations (Brack et. al. 1972, Brack 1976) as a function of $\underset{\sim}{r}$. We believe that these oscillations in the smooth density are spurious and reasons for their presence will be discussed in chapter 6 where the Strutinsky method is dealt with in more detail.

III.2 The Kinetic Energy Density.

The kinetic energy density, $\tau(\underset{\sim}{r},\lambda)$ is defined in terms of the single particle wave functions, $\psi_i(\underset{\sim}{r})$, as

$$\tau(\underset{\sim}{r},\lambda) = \frac{\hbar^2}{2m} \sum_i \nabla\psi_i^* \cdot \nabla\psi_i \; \theta(\lambda-\epsilon_i) \quad , \tag{13}$$

As in previous sections we shall take the Laplace transform. This gives us:

$$\tau(\underset{\sim}{r},\beta) = \mathcal{L}\tau(\underset{\sim}{r},\lambda) = \frac{\hbar^2}{2m} \frac{1}{\beta} \sum_i \nabla\psi_i^* \; \nabla e^{-\beta\hat{H}} \; \psi_i \tag{14}$$

We now wish to express this in the plane wave basis. This can be done by expanding ψ_i in a plane wave basis:

$$\psi_i(\underset{\sim}{r}) = \frac{1}{h^{3/2}} \int d^3p \; \phi_i(\underset{\sim}{p}) e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar} \tag{15}$$

This expression can be used in eq. (14) along with the completeness relation on the $\phi_i(\underset{\sim}{p})$ to yield:

$$\tau(\underset{\sim}{r},\beta)= \frac{\hbar^2}{2m}\ \frac{1}{\beta}\ \frac{1}{h^3}\int d^3p\ e^{-i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar}\left(-\frac{i}{\hbar}\ \underset{\sim}{p}\cdot\nabla\right) e^{-\beta\hat{H}}\ e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar} \tag{16}$$

The semiclassical relation (II.17) and (II.20) can now be used to yield:

$$\tau_{sc}(\underset{\sim}{r},\beta) = \frac{1}{\beta}\ \frac{1}{h^3}\int d^3p\ \left[\ \frac{p^2}{2m} - \frac{i\hbar}{2m}\ \underset{\sim}{p}\cdot\nabla\ \right]\ e^{-\beta H_{Cl}(1+\hbar w_1 + \hbar^2 w_2 + \cdots)} \ . \tag{17}$$

In this equation we have already let the del-operator act on the second plane wave to yield the p^2 term. Using the expressions for the w's from appendix A this equation may be straightforwardly evaluated and with the help of eq. (11) the final result is obtained:

$$\tau_{sc}(r,\lambda) = \left(\frac{2m}{\hbar^2}\right)^{3/2}\ \frac{(\lambda_{sc}-V)^{5/2}}{5\pi^2} + \frac{1}{8\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}\left\{-\frac{5}{3}\ \nabla^2 V(\lambda_{sc}-V)^{1/2}\right.$$

$$\left. + \frac{3}{4}\ \frac{(\nabla V)^2}{(\lambda_{sc}-V)^{1/2}}\right\} - \frac{1}{24\pi^2}\left(\frac{\hbar^2}{2m}\right)^{1/2}\left\{\frac{7}{20}\ \frac{\nabla^4 V}{(\lambda_{sc}-V)^{1/2}} + \frac{7}{48}\ \frac{(\nabla^2 V)^2}{(\lambda_{sc}-V)^{3/2}}\right.$$

$$+ \frac{1}{3}\ \frac{\nabla V\cdot\nabla\nabla^2 V}{(\lambda_{sc}-V)^{3/2}} + \frac{1}{12}\ \frac{\nabla^2(\nabla V)^2}{(\lambda_{sc}-V)^{3/2}} + \frac{11}{32}\ \frac{(\nabla V)^2\nabla^2 V}{(\lambda_{sc}-V)^{5/2}}$$

$$\left. + \frac{39}{160}\ \frac{\nabla V\cdot\nabla(\nabla V)^2}{(\lambda_{sc}-V)^{5/2}} + \frac{75}{256}\ \frac{(\nabla V)^4}{(\lambda_{sc}-V)^{7/2}}\right\} . \tag{18}$$

It is of interest in many applications to have τ in terms of ρ and gradients of ρ rather than in term of $(\lambda-V)$ and gradients of V. Such an expansion may be obtained by inverting eq. (12) to obtain an expression for V in terms of ρ and using the result in eq. (18). This is a straightforward but tedious procedure. The result is:

$$\tau_{sc}(\underset{\sim}{r}) = \frac{\hbar^2}{2m}\left\{\frac{3}{5}(3\pi^2)^{2/3}\rho^{5/3} + \frac{\nabla^2\rho}{3} + \frac{(\nabla\rho)^2}{36\rho}\right.$$

$$\left. \frac{1}{4320(3\pi^2)^{2/3}}\left(24\frac{\nabla^4\rho}{\rho^{2/3}} - 60\frac{\nabla\rho\cdot\nabla\nabla^2\rho}{\rho^{5/3}} - 28\frac{(\nabla^2\rho)^2}{\rho^{5/3}} - 14\frac{\nabla^2(\nabla\rho)^2}{\rho^{5/3}}\right.\right.$$

$$\left.\left. + \frac{280}{3}\frac{(\nabla\rho)^2(\nabla^2\rho)}{\rho^{8/3}} + \frac{184}{3}\frac{\nabla\rho\cdot\nabla(\nabla\rho)^2}{\rho^{8/3}} + \frac{1152}{12}\frac{(\nabla\rho)^4}{\rho^{11/3}}\right)\right\} \qquad (19)$$

The first term is the TF result, the second term vanishes upon $\underset{\sim}{r}$ integration while the third term is the Weizsäcker term with the correct coefficient (Kirzhnits 1967, p. 53). The terms in the last bracket are additional corrections. This expression as derived is only valid when the density used is the semiclassical density. When the semiclassical density is used the expression is not valid near the turning points. In spite of this limitation in the derivation it is interesting to apply the result to a continuous density such as the exact or Strutinsky density. In particular it is interesting to use this type of expression to calculate the total kinetic

energy. When eq. (19) is integrated over all space it can be simplified by using the fact that the integration over a gradient gives zero. Thus eq. (19) becomes:

$$\tau = \frac{\hbar^2}{2m}\int d^3r\left\{\frac{3}{5}(3\pi^2)^{2/3}\rho^{5/3} + \frac{(\nabla\rho)^2}{36\rho} + \frac{\rho^{1/3}}{6480(3\pi^2)^{2/3}}\left[8\left(\frac{\nabla\rho}{\rho}\right)^4\right.\right.$$

$$\left.\left. - 27\left(\frac{\nabla^2\rho}{\rho}\right)\left(\frac{\nabla\rho}{\rho}\right)^2 + 24\left(\frac{\nabla^2\rho}{\rho}\right)^2\right]\right\} \quad . \qquad (20)$$

This expression differs from Kirzhnits (1957) although it agrees with Hodges (1973). We believe this discrepancy is due to an algebraic error in Kirzhnits' result.

Eq. (20) was checked (Brack, 1976) by using the exact density from Woods-Saxon potentials for various particle numbers. The resultant τ was found to differ from the true τ by an amount of the same sign and approximately the same size as the shell correction. This seems to indicate that for this ρ we pick up most of the smooth contribution to the kinetic energy as well as some but not all of the shell correction contribution. The Strutinsky density, for both harmonic oscillator and Woods-Saxon potentials and various particle numbers, was then used (Brack 1976). The τ obtained from eq. (20) was in most cases within one MeV of the Strutinsky smoothed τ_{st}. In a few cases the difference was larger (2-4 MeV). It is believed that the discrepancy in these cases was due to a poor determination of the Strutinsky

density. To indicate the relative size of the various terms in eq. (20) we will consider an isotropic harmonic oscillator with N=90 and $\hbar\omega$ = 7.55 and use the Strutinsky smoothed density. In this case the leading TF term gives 1636.65 MeV; the Weizsacker term gives 21.62 MeV and the remaining term 7.71 MeV for a total of 1665.98 MeV. This compares to the Strutinsky smoothed τ_{sc} of 1667.22. The numbers for Woods-Saxon potentials tend to be similar although the last term is somewhat larger ($\sim$12 MeV for N=82).

We also tested eq. (20) for Woods-Saxon potentials by using a trial density of the form:

$$\rho = \frac{\rho_0}{1 + \exp[(r-R_0)/a]} \tag{21}$$

where ρ_0 was chosen such that the central density was the same as the semiclassical central density. The surface thickness, a, was varied to minimize the total energy and R_0 was chosen to reproduce the correct number of particles. The total energy was then calculated by:

$$E = \tau + \int d^3r\, \rho V \quad , \tag{22}$$

where τ is given by eq. (20). This was then compared to the semiclassical energy. For N=82 we obtained a total energy that was more negative than the semiclassical energy by 5 MeV. Similar results were found for other particle numbers with the

discrepancy increasing slowly with particle number. As there is no strict varational principle for the density, this discrepancy may be due to a poor choice of density.

CHAPTER IV

SEMICLASSICAL ENERGY FOR A CONSTRAINED HAMILTONIAN

IV.1 The General Constrained System.

Recent developments in heavy ion reaction experiments have allowed the production of nuclei with high angular momentum (Johnson and Szymanski 1973). One theoretical method for studying the effects of angular momentum on the binding energy and nuclear stability is a generalization of the Strutinsky method (Bengtsson et. al. 1975, Neergard and Pashkevich 1975). As with the Strutinsky method for the non-rotating case it is necessary to find the smooth energy for a system of noninteracting particles, however here we must use the cranking Hamiltonian. In this chapter we will develop a semiclassical expression for this smooth energy using a generalized Wigner-Kirkwood expansion.

In the Thomas-Fermi approximation the cranking model for noninteracting particles gives the rigid body value for the moment of inertia (Bloch 1954). If corrections to the Thomas-Fermi approximation are considered, however, the moment of inertia is found to deviate from the rigid body value. We will obtain expressions for these deviations and show that they are quite small.

Rather than beginning directly with the rotating case

we shall develop the formalism by considering the more general case of a constrained Hamiltonian. This formalism will then be used for the pushing model (Amado and Bruecker 1959) for linear motion to demonstrate the techniques which have been developed. We shall then consider the cranking model for arbitrarily large angular momentum when the Hamiltonian has no spin-orbit term. The Hamiltonian with spin-orbit interaction will be considered for small angular momentum and the order of magnitude of the corrections to the rigid body moment of inertia will be discussed. In section IV.4 we will discuss the effects of axial symmetry on the moment of inertia.

The formalism we have developed forthe cranking model can be applied with only minor modifications to the problem of determining the magnetic susceptibility of a system of non-interacting electrons in a uniform magnetic field. This will be done in chapter VII.

We will now set up our formalism for the case of a constrained Hamiltonian. We want to find the wave functions that minimize the energy while simultaneously keeping the expectation value,

$$F = \langle \hat{F} \rangle . \tag{1}$$

of some given one-body operator $\hat{F}$ fixed. This may be done by introducing a constrained Hamiltonian:

$$\hat{H}^{\mu} = \hat{H} - \mu \hat{F} , \tag{2}$$

where $\hat{H}$ is the unconstrained Hamiltonian and μ the Lagrange multiplier used to constrain F. The energy is now given by:

$$E = \sum_{i=1}^{N} \varepsilon_i^{\mu} + \mu F \quad , \tag{3}$$

where the ε_i^{μ} are the eigenvalues of the constrained Hamiltonian. The expectation value of $\hat{F}$ now becomes:

$$F = \sum_{i=1}^{N} \int \psi_i^{\mu *}(\underset{\sim}{r})\ \hat{F}\ \psi_i^{\mu}(\underset{\sim}{r}) d^3r = \int_0^{\lambda} g^F(\varepsilon) d\varepsilon \quad , \tag{4}$$

where ψ_i^{μ} is the eigenfunction corresponding to ε_i^{μ}. In the second expression we have again introduced the chemical potential λ. The density g^F is given by:

$$g^F(\varepsilon) = \sum_i \int \psi_i^{\mu *}(\underset{\sim}{r})\ \hat{F}\ \psi_i^{\mu}(\underset{\sim}{r}) \delta(\varepsilon - \varepsilon_i^{\mu}) d^3r. \tag{5}$$

In analogy with eq. (II.1) we introduce a density of states:

$$g^{\mu}(\varepsilon) = \sum_i \delta(\varepsilon - \varepsilon_i^{\mu}) \tag{6}$$

Eqs. (II.2) and (II.3) of chapter II are now replaced by the three equations:

$$N = \int_0^{\lambda} g^{\mu}(\varepsilon) d\varepsilon \tag{7}$$

$$F = \int_0^{\lambda} g^F(\varepsilon)d\varepsilon \tag{8}$$

$$E = \lambda N + \mu F - \int_0^{\lambda} d\varepsilon \int_0^{\varepsilon} g^{\mu}(\varepsilon')d\varepsilon' \tag{9}$$

Continuing as in chapter II we introduce the one-body partition function:

$$Z^{\mu}(\beta) = \int_0^{\infty} g^{\mu}(\varepsilon)e^{-\beta\varepsilon}d\varepsilon = \text{tr } e^{-\beta\hat{H}^{\mu}} \tag{10}$$

In terms of $Z^{\mu}(\beta)$ the two densities given by eqs. (5) and (6) may be expressed as:

$$g^{\mu}(\varepsilon) = \mathcal{L}_{\varepsilon}^{-1}[Z^{\mu}(\beta)] \tag{11}$$

$$g^{F}(\varepsilon) = \mathcal{L}_{\varepsilon}^{-1}\left[\frac{1}{\beta}\frac{\partial}{\partial\mu}Z^{\mu}(\beta)\right] \tag{12}$$

In obtaining eq. (12) we have used the identity:

$$\frac{\partial}{\partial\mu}\text{tr } e^{-\beta(\hat{H}-\mu\hat{F})} = \beta \text{ tr } \hat{F}\, e^{-\beta(\hat{H}-\mu\hat{F})} \tag{13}$$

This identity, which is true even when $\hat{F}$ and $\hat{H}$ do not commute may be easily proved by Taylor expanding the exponentials and using the fact that the order of operators under a trace may be cyclically permuted.

Rewriting eqs. (7)-(9) interms of the partition function, in analogy with eqs. (II.7) and (II.8) we arrive at our final

expressions:

$$N = \mathcal{L}_\lambda^{-1}\left[\frac{Z^\mu(\beta)}{\beta}\right] \tag{14}$$

$$F = \mathcal{L}_\lambda^{-1}\left[\frac{1}{\beta^2}\frac{\partial Z^\mu(\beta)}{\partial \mu}\right] \tag{15}$$

$$E = \lambda N + \mu F - \mathcal{L}_\lambda^{-1}\left[\frac{Z^\mu(\beta)}{\beta^2}\right] \tag{16}$$

For given values of F and N one uses eqs. (14) and (15) to determine λ and μ which are then used in eq. (16) to determine E. By considering dE at constant N it is easy to show that:

$$\left.\frac{dE}{dF}\right|_N = \mu \quad . \tag{17}$$

This is true even if approximate expressions are used for $Z^\mu(\beta)$ in eqs. (14)-(16).

If the expectation value of $\tilde{F}$ is zero for $\mu = 0$ these expressions may be simplified for small μ or F. The partition function may then be expanded as:

$$Z^\mu(\beta) = Z^\mu(\beta)\Big|_{\mu=0} + \mu\left.\frac{\partial Z^\mu(\beta)}{\partial \mu}\right|_{\mu=0} + \frac{\mu^2}{2!}\left.\frac{\partial^2 Z^\mu(\beta)}{\partial \mu^2}\right|_{\mu=0} + \cdots \tag{18}$$

The condition that F is zero at $\mu = 0$ means that the linear term is zero. This then gives us for F:

$$F = \mu \mathcal{L}_{\lambda}^{-1} \left[\frac{1}{\beta^2} \frac{\partial^2 z^{\mu}(\beta)}{\partial \mu^2} \Big|_{\mu=0} \right] = \mu I \qquad (19)$$

where I is independant of μ. Using this result and expanding the partition function in eq. (16) we have:

$$E = \lambda N + \frac{1}{2} \mu F - \mathcal{L}_{\lambda}^{-1} \left[\frac{1}{\beta^2} z^{\mu}(\beta) \Big|_{\mu=0} \right] \qquad (20)$$

The chemical potential, λ, has no term linear in μ and hence by arguments such as given in appendix C we can use the chemical potential determined at $\mu = 0$. It therefore follows that:

$$E - E^0 = \frac{1}{2} \mu F = \frac{1}{2} \mu^2 I = \frac{1}{2} \frac{F^2}{I} \qquad (21)$$

where E^0 is the μ independant energy.

If we wish to obtain the semiclassical energy in the case of a constraint we must replace $z^{\mu}(\beta)$ by its $\hbar$-expansion in the relevant equations. If the constraint operator $\hat{F}$ depends only on the coordinates, the quadrupole operator for example, the $\hbar$-expansion may be obtained by a straight forward application of the Wigner-Kirkwood expansion as given in chapter II. If on the other hand $\hat{F}$ is momentum dependant the Wigner-Kirkwood expansion is nontrivially modified. In the remaining sections of this chapter two such examples will be considered. The first is the pushing model where $\hat{F} = \hat{p}_x$,

the momentum in the x-direction and μ can be identified as the velocity in the x-direction. The second is the cranking model where $\hat{F} = \hat{J}_z$, the angular momentum in the z-direction and μ becomes the angular frequency of rotation.

IV. 2 The Pushing Model.

In this example we put the constraint on the total momentum, P_x, in the x-direction. The $\hat{F}$ of the previous section is taken to be $\hat{p}_x$ and F becomes just P_x. The constrained Hamiltonian is now:

$$\hat{H}^{\mu} = -\frac{\hbar^2\nabla^2}{2m} + V(\underset{\sim}{r}) - \mu\frac{\hbar}{i}\frac{\partial}{\partial x} \quad . \tag{22}$$

We now proceed to develop expressions for the partition function as in section (II.2). Using plane waves to take the trace in eq. (10) we get:

$$Z^{\mu}(\beta) = \frac{1}{h^3}\int e^{-\frac{i}{\hbar}\underset{\sim}{p}\cdot\underset{\sim}{r}} e^{-\beta\hat{H}^{\mu}} e^{\frac{i}{\hbar}\underset{\sim}{p}\cdot\underset{\sim}{r}} d^3r d^3p = \frac{1}{h^3}\int e^{-\beta H^{\mu}_{Cl}} w\, d^3r d^3p \tag{23}$$

where this equation defines w. The classical Hamiltonian, H^{μ}_{Cl} is given by:

$$H^{\mu}_{Cl} = \frac{p^2}{2m} + V(r) - \mu p_x \quad . \tag{24}$$

A differential equation may now be developed for w as in

section (II.2). In this case the differential equation becomes:

$$\frac{\partial w^{\mu}}{\partial \beta} = -i\hbar\left[\frac{\beta}{m}(p\cdot\nabla V)w^{\mu} - \frac{1}{m}(p\cdot\nabla w^{\mu}) - \mu\beta\frac{\partial V}{\partial x}w^{\mu} + \mu\frac{\partial w^{\mu}}{\partial x}\right]$$

$$+ \frac{\hbar^2}{2m}\left[\beta^2(\nabla V)^2 w^{\mu} - \beta(\nabla^2 V)w^{\mu} + \nabla^2 w^{\mu} - 2\beta(\nabla V\cdot\nabla w^{\mu})\right] \qquad (25)$$

This differs from eq. (II.19) by the addition of two terms proportional $\hbar$. We now define a new variable, $\underset{\sim}{p}'$:

$$p_x' = p_x - m\mu \ , \ p_y' = p_y, \ p_z' = p_z \ . \qquad (26)$$

With these variables eq. (25) reduces to eq. (II.19) with the only change being $\underset{\sim}{p}$ is replaced by $\underset{\sim}{p}'$. Hence we have:

$$w^{\mu}(\underset{\sim}{p},\underset{\sim}{r},\beta) = w(\underset{\sim}{p}',\underset{\sim}{r},\beta) \qquad (27)$$

since they both satisfy the same differential equation with the same boundary condition. Eq. (27) holds for the semi-classical w as well as for the exact w. For a semiclassical expansion w is expanded as in eq. (II.20); this is however unnecessary. The partition function may be written using eqs. (23) and (27) as:

$$z^{\mu}(\beta) = \frac{2}{h^3}\int d^3r d^3p \ e^{-\beta H_{Cl}^{\mu}} w(\underset{\sim}{p}',\underset{\sim}{r},\beta) \ . \qquad (28)$$

We now change the p-variable of integration to $\underset{\sim}{p}'$. This

gives us:

$$Z^{\mu}(\beta) = \frac{2}{h^3} e^{\beta m\mu^2/2} \int d^3r d^3p' \; e^{-(\frac{p'^2}{2m}+V(r))} w(\underset{\sim}{p}', \underset{\sim}{r}, \beta)$$

$$= e^{\beta m\mu^2/2} Z^0(\beta) \quad , \tag{29}$$

where $Z^0(\beta)$ is the μ independent partition function. This leads to simplifications in eqs. (14)-(16). In eq. (15) the μ derivative may be done explicitly to yield:

$$P_x = m\mu \mathcal{L}_{\lambda}^{-1} \left[\frac{1}{\beta} Z^{\mu}(\beta) \right] = mN\mu \quad . \tag{30}$$

Using the relation (Abramowitz and Stegun 1965, p. 1021)

$$\mathcal{L}_{\lambda}^{-1} \left[e^{\beta a} Z(\beta) \right] = \mathcal{L}_{\lambda+a}^{-1} \left[Z(\beta) \right] \tag{31}$$

we can see that:

$$\lambda = \lambda^0 - \frac{1}{2} m\mu^2 \quad , \tag{32}$$

where λ^0 is the value of λ at μ equals zero. Using this relation along with eqs. (30), (31) and (16) we have for E:

$$E = \lambda^0 N + \frac{1}{2} mN\mu^2 - \mathcal{L}_{\lambda}^{-1} \left[\frac{Z^0(\beta)}{\beta} \right]$$

$$= E^0 + \frac{1}{2} mN\mu^2 = E^0 + \frac{p_x^2}{2mN} \tag{33}$$

where E^0 is the value of E at μ equals zero. This yields the

total mass, mN, for the mass parameter as it should (Amado and Brueckner, 195). This example illustrates how simply some problems may be solved using the partition function formalism.

IV.3 The Cranking Model.

In this section we will consider a system with a constraint upon the z-component of the angular momentum, $\hat{J}_z$. Note that the operator $\hat{J}_z$ consists of the sum of two parts. The first is the orbital angular momentum $\hat{\ell}_z$ while the second term is the spin angular momentum, $\hbar\sigma_z/2$, expressed here in terms of the Pauli spin matrix, σ_z. The expectation value of $\hat{J}_z$ will be denoted by M which correspond to the F of section (IV.1). The Lagrange multiplier will be denoted by ω in recognition of the fact that it here represents the angular frequency of rotation. The constrained Hamiltonian of eq. (2) becomes:

$$\hat{H}_\omega = -\frac{\hbar^2}{2m}\nabla^2 + V(\underset{\sim}{r}) - \omega\hat{J}_z \qquad (34)$$

In this equation we have not put any restriction on the symmetry of $V(\underset{\sim}{r})$. In particular we have <u>not</u> assumed that it is axially symmetric about the z-axis. The case where it is axially symmetric about the z-axis will be discussed in section IV.5. The effects of a spin-orbit term in the potential will not be

considered in this section. The partition function in the plane wave basis is:

$$Z^{\omega}(\beta) = \frac{1}{h^3} \mathrm{tr}_{\sigma_z} \int d^3r d^3p \, e^{-\frac{i}{\hbar}\underset{\sim}{p}\cdot\underset{\sim}{r}} \, e^{-\beta\hat{H}^{\omega}} \, e^{-\frac{i}{\hbar}\underset{\sim}{p}\cdot\underset{\sim}{r}} \qquad (35)$$

The spin trace, tr_{σ_z}, can be done explicitly to yield a factor of $2\cosh(\beta\hbar\omega/2)$ and the partition function can be rewritten as:

$$Z^{\omega}(\beta) = \cosh\frac{\beta\hbar\omega}{2} \frac{2}{h^3}\int d^3r d^3p \, e^{-\frac{i}{\hbar}\underset{\sim}{p}\cdot\underset{\sim}{r}} \, e^{-\beta(\frac{\hat{p}^2}{2m}+V(\underset{\sim}{r})-\omega\hat{\ell}_z)} \, e^{-\frac{i}{\hbar}\underset{\sim}{p}\cdot\underset{\sim}{r}} \qquad (36)$$

where $\hat{\ell}_z$ is the operator for the orbital part of the angular momentum. It is now necessary to develop an $\hbar$-expansion for this partition function. The cosh factor may be expanded straightforwardly and a modified Wigner-Kirkwood expansion may be used to expand the expression under the integral. As in section (II.2) we define w by:

$$e^{-\beta(\frac{\hat{p}^2}{2m}+V(\underset{\sim}{r})-\omega\hat{\ell}_z)} \, e^{-\frac{i}{\hbar}\underset{\sim}{p}\cdot\underset{\sim}{r}} = e^{-\beta H_{Cl}} \, e^{-\frac{i}{\hbar}\underset{\sim}{p}\cdot\underset{\sim}{r}} \, w \qquad (37)$$

with H_{Cl} denoting the classical Hamiltonian:

$$H_{Cl} = \frac{p^2}{2m} + V(\underset{\sim}{r}) - \omega\ell_z \; . \qquad (38)$$

where ℓ_z is the classical angular momentum. The differential equation for w becomes:

$$\frac{\partial w}{\partial \beta} = -i\hbar\left[\frac{\beta}{m}(\underset{\sim}{p}.\nabla V)w - \frac{1}{m}\underset{\sim}{p}.\nabla w - \omega\beta(x\frac{\partial V}{\partial y} - y\frac{\partial V}{\partial x})\, w\right.$$

$$\left. -\beta\omega^2(xp_x+yp_y)w + \omega(x\frac{\partial w}{\partial y} - y\frac{\partial w}{\partial x})\right]$$

$$+ \frac{\hbar^2}{2m}\left[\beta^2(\nabla V)^2 w - 2\omega\beta^2(p_y\frac{\partial V}{\partial x} - p_y\frac{\partial V}{\partial y})\, w + \beta^2\omega^2(p_x^2+p_y^2)w\right.$$

$$\left. -\beta(\nabla^2 V)w + \nabla^2 w - 2\beta\nabla V.\nabla w + 2\beta\omega(p_y\frac{\partial w}{\partial x} - p_x\frac{\partial w}{\partial y})\right] . \qquad (39)$$

It is now possible to write w in a power series in $\hbar$ as in eq. (II.20) and solve to each order in $\hbar$. This was done to order $\hbar^2$. The term proportional to $\hbar$ is:

$$w_1 = \frac{i}{2}\beta^2\left[-\frac{1}{m}(\underset{\sim}{p}.\nabla V) + \omega(x\frac{\partial V}{\partial y} - y\frac{\partial V}{\partial x}) + \omega^2(xp_x+yp_y)\right] . \qquad (40)$$

The term proportional to $\hbar^2$ contains thirteen terms and is not written down due to its length. The p-integrations may be done as outlined in appendix B if the substitution,

$$p_x = p_x' - m\omega y$$

$$p_y = p_y' + m\omega x \qquad (41)$$

is first made. The partition function correct to order $\hbar^2$ can now be written as:

$$Z_{sc}^{\omega}(\beta) = \frac{1}{4\pi^{3/2}}\left(\frac{2m}{\hbar^2}\right)^{3/2}\frac{1}{\beta^{3/2}}\int d^3r\, e^{-\beta V_{eff}(\underset{\sim}{r})}\left\{1 - \frac{\hbar^2\beta^2}{12m}\left[\nabla^2 V_{eff}\right.\right.$$

$$\left.\left. + \frac{1}{2}m\omega^2 - \frac{\beta}{2}(\nabla V_{eff})^2\right]\right\} , \qquad (42)$$

where V_{eff} is given by:

$$V_{eff} = V - \frac{1}{2} m\omega^2 r_\perp^2 \quad , \tag{43}$$

where $r_\perp^2 = (x^2+y^2)$. With this partition function we can now calculate the expressions for N, M_{sc} and E_{sc}. Before doing this let us rewrite the partition function as:

$$Z_{sc}^{\omega}(\beta) = \frac{1}{4\pi^{3/2}}\left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{1}{\beta^{3/2}} \int d^3r\, e^{-\beta V_{eff}} \left\{1 - \frac{\beta^2\hbar^2}{24m}\left[\nabla^2 V_{eff} + m\omega^2\right]\right\} , \tag{44}$$

where we have used eq. (II.23). Using eqs. (14)-(16) we obtain for N, M_{sc}, and E_{sc}:

$$N = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int d^3r\left\{(\lambda_{sc}-V_{eff})^{3/2} - \frac{\hbar^2}{32m}\frac{\nabla^2 V_{eff}+m\omega^2}{(\lambda_{sc}-V_{eff})^{1/2}}\right\} \tag{45}$$

$$M_{sc} = \frac{m\omega}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int d^3r\left\{(\lambda_{sc}-V_{eff})^{3/2} r_\perp^2 - \frac{\hbar^2}{32m}\frac{(\nabla^2 V_{eff}+m\omega^2)}{(\lambda_{sc}-V_{eff})^{1/2}} r_\perp^2 + \frac{\hbar^2}{8m}(\lambda_{sc}-V_{eff})^{1/2}\right\} \tag{46}$$

$$E_{sc} = \lambda_{sc} N + \omega M - \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int d^3r\left\{\frac{2}{5}(\lambda_{sc}-V_{eff})^{5/2} - \frac{\hbar^2}{16m}(\nabla^2 V_{eff}+m\omega^2)(\lambda_{sc}-V_{eff})^{1/2}\right\} \tag{47}$$

where all integrals are cut off at the turning point, $\underset{\sim}{r}_{sc}$, given by $V_{eff}(\underset{\sim}{r}_{sc}) = \lambda_{sc}$. These equations should be compared with eqs. (II.25) and (II.26) of the nonrotating case.

It is possible in this case also to develop an expression for the density. This is done in strict analogy with section (III.1). The diagonal Bloch density, $C^{\omega}_{sc}(\underset{\sim}{r},\beta)$ is given by same expression as the partition function of eq. (42) with the only difference being that for the Bloch density we do not do the $\underset{\sim}{r}$-integration. The density is obtained by taking the Laplace inverse of the diagonal Bloch density as described in section (III.1). The semiclassical density is given by:

$$\rho^{\omega}_{sc}(\underset{\sim}{r}) = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\left\{(\lambda_{sc}-V_{eff})^{3/2} - \frac{\hbar^2}{16m}\left[\frac{\nabla^2 V_{eff}+\frac{1}{2}m\omega^2}{(\lambda_{sc}-V_{eff})^{1/2}}\right.\right.$$

$$\left.\left. + \frac{(\nabla V_{eff})^2}{4(\lambda_{sc}-V_{eff})^{3/2}}\right]\right\} \qquad (48)$$

for $\underset{\sim}{r}$ inside the turning points. Otherwise ρ^{ω}_{sc} is zero. This expression is, of course, not valid near the turning points.

The expression, eq. (47), for E_{sc} can be rewritten in terms of ρ^{ω}_{sc} in the same way as the kinetic energy of section (III.2). In this case eq. (48) is inverted to find V_{eff} in terms of ρ^{ω}_{sc} and this used in connection with eqs. (46) and (47). Realizing that:

$$\lambda\rho^{\omega} = (\lambda - V_{eff})\rho^{\omega} + V\rho^{\omega} - \frac{1}{2}m\omega^2 r^2 \rho^{\omega} \quad , \qquad (49)$$

and then proceeding in the same way as in section (III.2) we have:

$$E = \int V\rho^{\omega} d^3r + \frac{\hbar^2}{2m} \int d^3r \ \ \frac{3}{5}(3\pi^2)\rho^{\omega^{5/3}} + \frac{(\nabla\rho^{\omega})^2}{36\rho^{\omega}} + \frac{1}{2}\omega M \quad . \tag{50}$$

Due to the singularities of ρ^{ω}_{sc} at the turning points this is not strictly valid, but is only valid in the same sense as eq. (III.20) for τ. The effect of the rotation is to add an extra term $\frac{1}{2}\omega M$, which looks like the classical rotation energy, and to modify the density.

It is possible to define a moment of inertia, I, as:

$$I = \frac{M}{\omega} \quad . \tag{51}$$

We shall also define a rigid-body moment of inertia, I_{rd}, as:

$$I_{rd} = m \int d^3r \ r_{\perp}^2 \rho = \lambda^{-1}\left[\frac{m}{\beta} \int d^3r \ r_{\perp}^2 C(\underset{\sim}{r},\beta)\right] \quad . \tag{52}$$

In the semiclassical approximation the second form of this equation must be used to avoid problems with the density diverging at the turning points. When the Thomas-Fermi results for ρ and M, as given by the leading terms in eqs. (45) and (46), are used we get the well-known result (Bohr and Mottelson 1955) that I reduces to the rigid-body value. For our semiclassical result this is not true. To see this it is

most convenient to use the partition function of eq. (42). Using eqs. (15), (42) and (52) we immediately have:

$$I = I_{rd} - \frac{m}{12\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}\int d^3r(\lambda_{sc}-V_{eff})^{1/2}\ \theta(\lambda_{sc}-V_{eff}) \quad . \tag{53}$$

With a level density defined in analogy with eq. (II.12) we have $I = I_{rd} - \hbar^2\, g^{\omega}_{Cl}(\lambda)/12$. The moment of inertia can also be written in a form consistent with eq. (50) as:

$$I = m\int d^3r\left[r_\perp^2\rho - \frac{\rho^{1/3}}{4(3\pi^2)^{2/3}}\right] \quad . \tag{54}$$

Although there is a correction to the rigid-body value it is quite small. The order of magnitude will be estimated in the next section where we consider the small-ω case.

In ending this section we will just note that eq. (17) in this case reduces to the canonical relation:

$$\frac{dE}{dM} = \omega \tag{55}$$

IV.4 The Cranking Model in the Presence of a Spin-Orbit Force.

In this section we will investigate the effects of a spin-orbit term in the Hamiltonian on the cranking model moment of inertia. We shall only consider the case when ω is small and can be treated perturbatively. From eqs. (18)-(21) we see

that if the term in the partition function proportional to ω is zero the effects of rotation can be easily calculated once the moment of inertia is known. We shall first develop an expansion for the partition function correct to order ω^2. The term proportional to ω will be seen to be zero and the term proportional to ω^2 will yield the moment of inertia.

The constrained Hamiltonian which we will use here is:

$$\hat{H}^{\omega} = -\frac{\hbar^2}{2m}\nabla^2 + V(\underset{\sim}{r}) + i\kappa\frac{\hbar^2}{2m}(\nabla f\times\nabla).\hat{\sigma} - \omega\hat{J}_z \ . \qquad (56)$$

The unconstrained part of the Hamiltonian is as discussed in section (II.4), while the constraint is the same as the one discussed in the last section. The partition function is now:

$$Z^{\omega}(\beta) = \mathrm{tr}\ e^{-\beta\hat{H}^{\omega}} = \mathrm{tr}\ e^{-\beta(\hat{H}_0+\hat{V}_{LS}-\omega\hat{J}_z)} \ , \qquad (57)$$

with the same notation as in section (II.4). We shall proceed to do a perturbative expansion on both κ and ω. In both cases we shall keep only terms to second order. The expansions are done as described in section (II.4). See particularly equations (38) through (41). Doing the ω-expansion we have:

$$\mathrm{tr}\ e^{-\beta(\hat{H}_0+\hat{V}_{LS}-\omega\hat{J}_z)} = \mathrm{tr}\ e^{-\beta(\hat{H}_0+\hat{V}_{LS})}(1 + \omega\beta\hat{J}_z +$$

$$\omega^2\int_0^{\beta}d\beta'\int_0^{\beta'}d\beta''\ e^{\beta'(\hat{H}_0+\hat{V}_{LS})}\hat{J}_z\, e^{-(\beta'-\beta'')(\hat{H}_0+\hat{V}_{LS})}\hat{J}_z\, e^{-\beta''(\hat{H}_0+\hat{V}_{LS})}$$

$$+ \cdots) \qquad (58)$$

The first term is just the partition function of section (II.4) and will not be discussed further here. In obtaining the second term we have used the fact that operators under a trace may be cyclicly permuted. To see that this term is zero let us break $\hat{J}_z$ into two parts; an orbital part and a spin part. The orbital part is just $\hat{\ell}_z$. If we take the trace in plane wave basis the ω term may be written as in eq. (II.44) The only difference is that we will have an extra factor of $(xp_y - yp_x)$ from $\hat{\ell}_z$ acting on the plane wave. The real terms in the resultant expression will have an odd power of p and hence vanish upon p-integration. The imaginary terms must vanish as the partition function is real since it involves only the trace of Hermitian operators. Similar arguments may be used for the spin part. This leaves only the ω^2 term. We shall work out only the leading term in $\hbar$ for both κ and κ^2. The κ-expansion is now done as described in section (II.4). The final result for the partition function is:

$$Z^{\omega}(\beta) = Z^{0}(\beta) + \omega^2 \frac{1}{8\pi^{3/2}} \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{m}{\beta^{1/2}} \int d^3r\, e^{-\beta V} \left\{ r_\perp^2 - \frac{\hbar^2\beta^2}{12m} \right.$$

$$\left[r_\perp^2 \nabla^2 V - \frac{\beta}{2} (\nabla V)^2 r_\perp^2 - \frac{3}{\beta} + \nabla V \cdot \nabla (x^2+y^2) - \frac{6\kappa}{\beta} \left(x \frac{\partial f}{\partial x} + y \frac{\partial f}{\partial y} \right) \right.$$

$$\left. \left. - \frac{6\kappa^2}{\beta} \left((\nabla f)^2 r^2 - \frac{1}{2} \left(x \frac{\partial f}{\partial y} - y \frac{\partial f}{\partial x} \right)^2 \right) \right] \right\}$$

$$= Z^{0}(\beta) + \omega^2 m\beta \int d^3r\, r_\perp^2 C_{sc}(\underset{\sim}{r}, \beta) + \frac{\omega^2 \beta^{1/2}}{96\pi^{3/2}} \cdot \frac{(2m)^{3/2}}{\hbar} \int d^3r\, e^{-\beta V}$$

$$\left\{-1 + 6\kappa\left(x\frac{\partial f}{\partial x} + y\frac{\partial f}{\partial y}\right) + 3\kappa^2\left[(\nabla f)^2 r^2 - \left(x\frac{\partial f}{\partial y} - y\frac{\partial f}{\partial x}\right)^2\right]\right\} \tag{59}$$

In the last expression we have separated the terms that contribute to the rigid-body moment of inertia and have put them in the second term. There is a term in $C_{sc}(\underset{\sim}{r},\beta)$ proportional to κ^2. It is just equal to the first κ^2 term in the last bracket. Using eqs. (19), (51) (52) and (59) we have for the moment of inertia:

$$I = I_{rd} + \frac{1}{24\pi^2}\left(\frac{2m}{\hbar}\right)^{3/2}\int d^3r\,(\lambda_{sc}-V)^{1/2}\left\{-1+6\kappa\left(x\frac{\partial f}{\partial x} + y\frac{\partial f}{\partial y}\right)\right.$$

$$\left. + 3\,\kappa^2\left[(\nabla f)^2 r^2 - \left(x\frac{\partial f}{\partial y} - y\frac{\partial f}{\partial x}\right)^2\right]\right\} \tag{60}$$

Thus we see that the presence of a spin-orbit term in Hamiltonian has an effect on the moment of inertia not only through I_{rd} (there is a κ^2 term in I_{rd}) but also through the presence of additional terms. Unlike the $\omega=0$ case we here have a term proportional κ. We shall investigate the size of the various terms by considering the spherical harmonic oscillator model, with spin-orbit term, given in section (II.5). The Hamiltonian is given by eq. (II.48). It is straightforward to work out the integrals in this case to get:

$$I = \hbar^2\left[\frac{\lambda_{sc}^4}{6\hbar^5\nu^5} + \frac{5}{6}\frac{\kappa^2\lambda_{sc}^4}{\hbar^5\nu^5} - \frac{\lambda_{sc}^2}{12\hbar^3\nu^3}\right] + \hbar^2\left[-\frac{\lambda_{sc}^2}{12\hbar^3\nu^3}\right.$$

$$+\frac{2}{3}\frac{\kappa\lambda_{sc}^{3}}{\hbar^{4}\nu^{4}}+\frac{5}{6}\frac{\kappa^{2}\lambda_{sc}^{4}}{\hbar^{5}\nu^{5}}\Bigg]. \tag{61}$$

We have used ν for the oscillator frequency here in order to avoid confusion with the angular frequency. The terms in the first bracket give the rigid-body value while the second bracket gives the correction terms. Using $\kappa=0.1$, $\hbar\nu=7$ MeV and $\lambda_{sc} = 42$ MeV as in section (II.5) we have,

$$I = \frac{\hbar^{2}}{\text{MeV}}\left[30.86 + 1.54 - 0.43\right] + \frac{\hbar^{2}}{\text{MeV}}\left[-0.43 + 2.06 + 1.54\right] \tag{62}$$

where the numbers correspond to the terms in eq. (61). In the case where $\kappa=0$ the correction to the rigid body value is seen to be the order of a percent. The spin-orbit term is seen to contribute about five percent to the rigid-body moment of inertia, while the correction to rigid-body moment of inertia has increased from one percent to about ten percent. The total effect of the spin-orbit terms is seen to be about fifteen percent. The deviation from the rigid-body value here is larger than the deviation found by Pashkevich and Frauendorf (1975). They investigated the moment of inertia in a Woods-Saxon potential with a spin-orbit term using the Strutinsky method and found that the smooth value of the moment of inertia differed from the rigid-body value by about three percent for heavy nuclei. This difference is probably due to the fact that the density in the harmonic oscillator is concentrated near r=0

giving too small a value of the rigid-body moment of inertia while not similarly decreasing the correction terms.

Other velocity dependent terms in the Hamiltonian can cause still larger deviations from the rigid-body value of the moment of inertia. For example the $\hat{\ell}^2$ term in the Nilsson model (Nilsson et. al. 1969) can easily cause a forty percent deviation (Brack and Jennings 1976).

IV.5 A Further Discussion of the Cranking Model.

In this section we will consider the effect of axially symmetric potentials on the moment of inertia. In the cranking model one usually considers potentials that have a symmetry axis perpendicular to the axis one is cranking about. It is however also possible to constrain the angular momentum along a symmetry axis (Bohr and Mottelson 1975, p. 80) of the potential. In this case the angular momentum is generated by aligning the angular momentum of the individual particles. Although the density is still axially symmetric in the presence of the constraint, the wave function is not. The equations developed in section (IV.1) and used for the cranking model in sections (IV.3) and (IV.4) will still be valid in this case.

We will now consider the case when ω is small and the potential does not necessarily have an axis of symmetry. The partition function will be expanded to second order in ω by using second order perturbation theory to find the ε_i^{ω}. To second

order ε_i^ω is given by:

$$\varepsilon_i^\omega = \varepsilon_i - \omega\langle\psi_i|\hat{J}_z|\psi_i\rangle + \omega^2 \sum_{j\neq i} \frac{|\langle\psi_i|\hat{J}_z|\psi_j\rangle|^2}{\varepsilon_i - \varepsilon_j} \tag{63}$$

The partition function now becomes:

$$Z^\omega(\beta) = \sum_i e^{-\beta\varepsilon_i^\omega} = \sum_i e^{-\beta\varepsilon_i} + \omega\beta\Sigma\langle\psi_i|\hat{J}_z|\psi_i\rangle e^{-\beta\varepsilon_i}$$

$$-\omega^2\beta \sum_i \sum_{j\neq i} \frac{|\langle\psi_i|\hat{J}_z|\psi_j\rangle|^2}{\varepsilon_i - \varepsilon_j} e^{-\beta\varepsilon_i} + \frac{\omega^2\beta^2}{2} \sum_i |\langle\psi_i|\hat{J}_z|\psi_i\rangle|^2 e^{-\beta\varepsilon_i} \tag{64}$$

The first term in this equation is just the ω independent term and is of no interest to us here. The term linear in ω is more difficult to deal with. As we have seen it is zero in the semiclassical partition function, however for the exact partition function it may be finite. It is this term that gives the angular momentum at $\omega=0$ and will be finite if the unconstrained ground state has finite total angular momentum. This term however gives exactly zero contribution to the partition function when the potential is axially symmetric. For simplicity we will consider only cases where it is zero.

There are two terms proportional to ω^2 which we will now use to find the moment of inertia. From eq. (19) we have:

$$I = 2 \sum_{i_{occ}} \sum_{j\neq i} \frac{|\langle\psi_i|J_z|\psi_i\rangle|^2}{\varepsilon_j - \varepsilon_i} + \sum_j |\langle\psi_i|\hat{J}_z|\psi_i\rangle|^2 \delta(\varepsilon_i - \lambda) . \tag{65}$$

The first term is just the usual cranking formulae term (Inglis, 1954). It vanishes if the z-axis is a symmetry axis. The second term is zero if the potential is axially symmetric about an axis perpendicular to the z-axis because the matrix elements are zero. In other cases this term will be zero or infinite depending on the value of λ. This term likely indicates a break-down in the ω-expansion due to the fact that if a degenerate level is not completely filled the angular moment changes discontinuously with ω at $\omega=0$. This discontinuity occurs because as ω goes from slightly positive to slightly negative the occupancy of the degenerate states may change. Despite this problem with the exact moment of inertia the semiclassical moment of inertia is well defined. As we have seen different terms in eq. (65) contribute to the exact moment of inertia depending on the orientation of the symmetry axis of the potential however the Thomas-Fermi result yields the rigid body moment of inertia in all cases and the semiclassical result is only slightly affected by axial symmetry.

CHAPTER V

THE LARGE A-EXPANSION FOR NONINTERACTING PARTICLES

V.1 The Large A-expansion.

In the simplified model where nuclei are assumed to consist of equal numbers of neutrons and protons and Coulomb effects are ignored the smooth part of the binding energy may be expanded as a power series in $A^{1/3}$ of the form:

$$E = C_1 A + C_2 A^{2/3} + C_3 A^{1/3} + C_4 A^0 + \text{---} \qquad (1)$$

where the first three terms are respectively referred to as the volume, surface and curvature terms. This equation has been used (Dworzecka and Moszkowski 1975) to compare the Hartree-Fock and energy-density functional approaches for obtaining the binding energy. In this case they fitted both the Hartree-Fock energy which contains shell effects and the energy-density functional energy which does not contain shell effects to eq. (1) to see if the energy-density functional energy correctly reproduces the smooth part of the Hartree-Fock energy. By consideration of a simplified system of non-interacting particles we investigate how much information can be obtained by using least squared fitted energies that contain shell effects. For this purpose it is only necessary to

consider noninteracting particles since by the Strutinsky energy theorem the shell effects in the Hartree-Fock energy can be reproduced from an independant particle model (Strutinsky 1967, 1968).

The expansion of eq. (1) has also been used by (Siemens and Sobiczewski 1972) in an attempt to obtain the smooth energy of a system of noninteracting particles by considering systems of large A. They were able to obtain the first two coefficients in eq. (1). Using a least square fit we will show that the semiclassical energy gives the same value of these two coefficients and further more that the A-expansion is somewhat slower converging than the $\hbar$-expansion for the cases considered.

We shall first consider a system of noninteracting particles moving in a square well. The square well is used because in that case the A-expansion of the semiclassical energy can be worked out analytically. The coefficients obtained from this expansion will be compared to those obtained by doing a least squares fit of eq. (1) to both the semiclassical and exact energies. To obtain the semiclassical energy we cannot use the expressions developed in chapter II as the gradients of the potential must exist for that expansion to be valid. A semiclassical expression for the single-particle partition function and density of states for this case has however been developed by Bhaduri and Ross (1971).

The semiclassical partition function in this case is:

$$Z_{sc}(\beta) = \frac{1}{4}\left(\frac{2mL^2}{\hbar^2\pi\beta}\right)^{3/2}\left[1-3\hbar\left(\frac{\pi\beta}{2mL^2}\right)^{1/2}+ 3\hbar^2\left(\frac{\pi\beta}{2mL^2}\right)\right.$$

$$\left. - \hbar^3\left(\frac{\pi\beta}{2mL^2}\right)^{3/2} + ---\right] \quad , \tag{2}$$

where L is the length of a side of the square well. For the sake of this discussion we shall take:

$$L = L_0 A^{1/3} \quad , \tag{3}$$

where L_0 is just a proportionality constant. Using the fact that A=2N as well as eqs. (II.7) and (II.8) we have for A and E_{sc}:

$$A = \frac{2}{3\pi^2}\left(\frac{2mL^2}{\hbar^2}\right)^{3/2}\lambda_{sc}^{3/2} - \frac{3}{2\pi}\left(\frac{2mL^2}{\hbar^2}\right)\lambda_{sc}$$

$$+ \frac{3}{\pi}\left(\frac{2mL}{\hbar^2}\right)^{1/2}\lambda_{sc}^{1/2} - \frac{1}{2} \quad , \tag{4}$$

$$E_{sc} = \frac{2}{5\pi^2}\left(\frac{2mL^2}{\hbar^2}\right)^{3/2}\lambda_{sc}^{5/2} - \frac{3}{4\pi}\left(\frac{2mL^2}{\hbar^2}\right) + \frac{1}{\pi}\left(\frac{2mL^2}{\hbar^2}\right)\lambda_{sc}^{3/2} \tag{5}$$

Eq. (4) which determines λ is a cubic equation in $\lambda^{1/2}$ and hence may be solved exactly for λ. It is however easier to define a variable Y as:

$$Y = \left(\frac{2mL^2}{\hbar^2\pi^2}\right)^{1/2}\lambda_{sc}^{1/2} \quad .$$

With this variable eqs. (4) and (5) become:

$$Y^3 - \frac{9}{4} Y^2 + \frac{9}{2\pi} Y - \frac{3}{4\pi} - \frac{3A}{2\pi} = 0 \quad , \tag{6}$$

$$E_{sc} = \frac{\hbar^2\pi^2}{2mL^2} \left(\frac{2\pi}{5} Y^5 - \frac{3\pi}{4} Y^4 + Y^3\right) \quad . \tag{7}$$

It is now relatively easy to solve for Y and obtain E. Keeping terms to order $A^{-1/3}$ we have:

$$E_{sc} = \left(\frac{\hbar^2\pi^2}{2mL_0^2}\right) \left[\frac{3}{5} \left(\frac{3}{2\pi}\right)^{2/3} A + \frac{9}{8} \left(\frac{3}{2\pi}\right)^{1/3} A^{2/3} \right.$$

$$+ \frac{3}{2\pi} \left(\frac{9\pi}{8} - 2\right) A^{1/3} + \left(\frac{3}{2\pi}\right)^{2/3} \left(-4 + \frac{45}{32}\pi\right)$$

$$\left. + A^{-1/3} \left(\frac{3}{2\pi}\right)^{1/3} \left(\frac{9}{2\pi} - 6 + \frac{189\pi}{128}\right) \right] \quad . \tag{8}$$

In getting this equation we have used eq. (3). Thus we now have analytic expressions for the coefficients in the A expansion. These coefficients may now be compared with those obtained by least square fitting both the semiclassical energy obtained directly from eqs. (4) and (5) and the exact energy calculated using the eigenvalues:

$$\varepsilon = \left(\frac{\hbar^2\pi^2}{2mL^2}\right) \left(n_x^2 + n_y^2 + n_z^2\right) \quad ,$$

where the n_x, n_y and n_z are positive integers. In the fitting we used A from 4 to 400 in steps of 4. For the purpose of

Table 4

	C_1	C_2	C_3	C_4	C_5
	23.04	55.26	46.04	16.04	3.50
Sc	23.04	55.16	46.75	13.77	6.71
Ex	9.97	274.80	-1227.28	3013.19	-2376.09
Sc	22.99	55.98	42.39	23.05	
Ex	28.54	-16.01	317.97	-273.94	
Sc	23.55	49.25	65.70		
Ex	21.88	63.95	40.93		
Sc	19.01	88.07			
Ex	19.05	88.13			
Sc		53.29	59.58		
Ex		54.87	54.71		
Sc		55.45	44.14	21.40	
Ex		46.68	113.35	-81.28	
Sc		55.24	46.34	14.60	6.12
Ex		77.58	219.47	945.12	-924.71

Table 4. The coefficients of the A-expansion for a square well. All numbers are in MeV. The parameters of the well are as described in the text. The columns are respectively the coefficients of A, $A^{2/3}$, $A^{1/3}$, A^0 and $A^{-1/3}$. The first row gives the coefficients as determined from eq. (8). The remaining rows give the coefficients as determined by least square fitting the semiclassical energies (marked as Sc) and the exact energy (marked as Ex). Coefficients not fitted are left blank. When C_1 is not given it is fixed at 23.04 MeV.

this comparison we have taken $\hbar^2/2m$ to be 20.747 and $L_0 = 1.805$. It was found that with the five coefficients given by eq. (8) the semiclassical energy was reproduced within .5 MeV for A greater than 4, while with only four coefficients the error is 1.5 MeV for A=20 and increases as A decreases. The fourth term itself gives 16 MeV for all particle numbers. This means that four terms are sufficient to reproduce the semiclassical energy for medium and heavy nuclei. The coefficients obtained from the least squared fitting as well as those given by eq. (8) are given in table 4. The fitting has been done using 2 to 5 terms in the A-expansion. It has also been done with the volume term fixed at the value taken from eq. (8). With the semiclassical energy four terms were necessary to obtain a good fit although the coefficients obtained in the five parameter fit agreed more closely with those of eq. (8). With less than four terms the agreement deteriorated somewhat. By fitting the exact energies we could not reproduce the smooth energies. However when only the first three terms of eq. (1) were used reasonable values of the coefficients were obtained. This was particularly true when the volume term was fixed and only two coefficients fitted. This indicates that as more freedom is allowed in the fit one starts to fit the shell fluctuations rather than reproducing the smooth energy. It is interesting that Dworzecka and Moszkowski (1975) in their comparison fitted C_2 and C_3 of

eq. (1) with C_1 fixed, for as we have seen above fitting these two coefficients gives the best results.

We have also looked at the A-dependance of the semiclassical energy for a Woods-Saxon potential without a spin-orbit term. The same parameters as given in the first part of section (II.6) were used. In this case it is impossible to obtain analytic expressions for all the coefficients in the A-expansion. However the first two coefficients have been obtained by Siemens and Sobiczewski (1972) by considering the limit of large A. In least square fitting the semiclassical energy we found that five terms were necessary to obtain a good fit. The coefficients are given by: $C_1 = -26.10$ MeV, $C_2 = 37.65$ MeV, $C_3 = -7.13$ MeV, $C_4 = -80.48$ and $C_5 = 94.46$. The first two terms are in good agreement with those given by Siemans and Sobiczewski (1972). In this case it can be seen that the A-expansion converges slower than the $\hbar$-expansion which requires only three terms.

In the case of the square well potential the leading $\hbar$-term in eq. (2) gives only the volume term while the higher order terms in $\hbar$ give the remaining terms in the A-expansion. A similar result is true for the harmonic oscillator where the leading term in the $\hbar$-expansion, the Thomas-Fermi term, gives just the volume term. The $A^{2/3}$ term or surface term for the harmonic oscillator is zero and the corrections to the Thomas-Fermi term first contribute to order $A^{1/3}$. The results are however quite different for more realistic

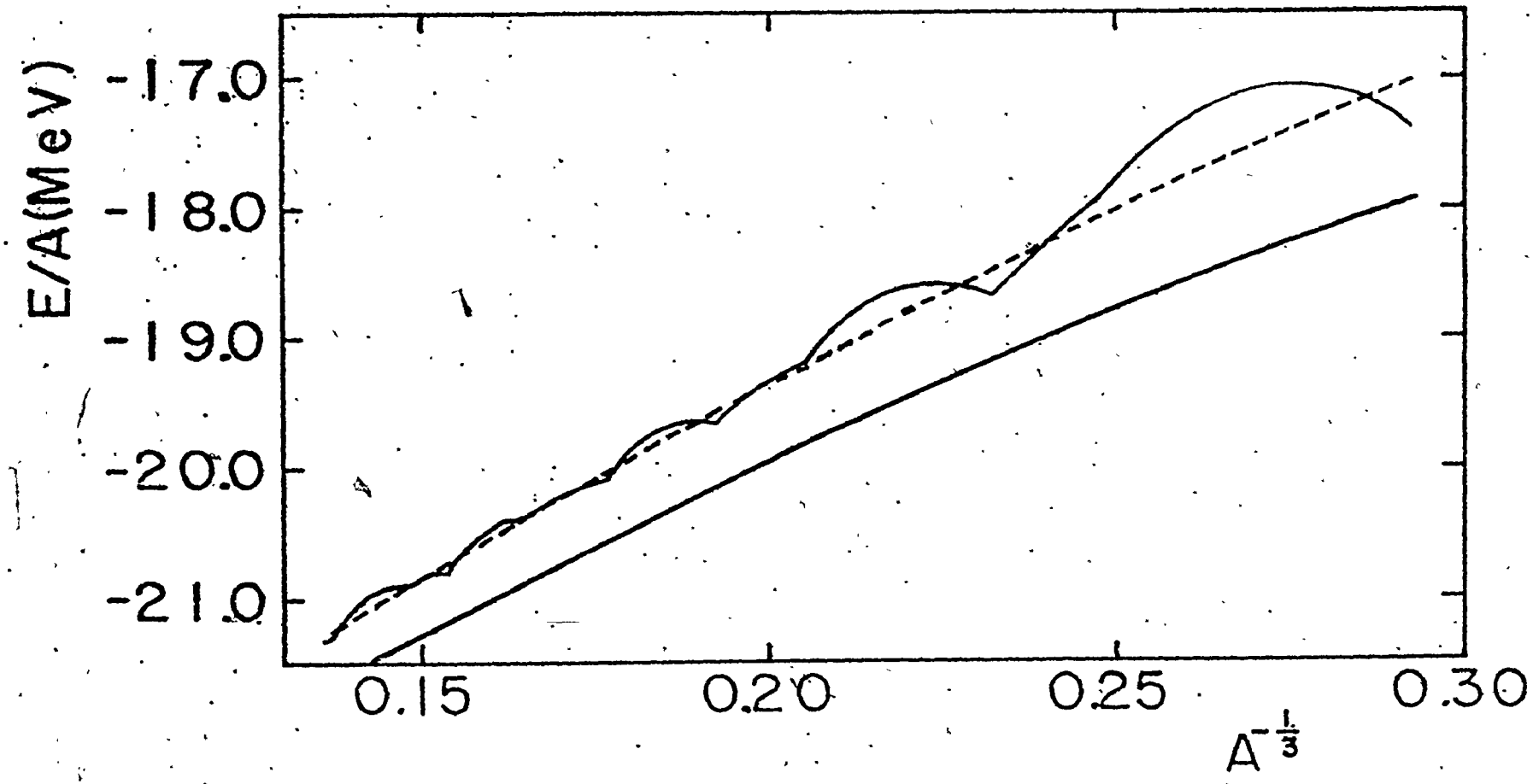

Fig. 2 The binding energy as a function of A. The binding energy per particle as calculated exactly (thin line), semiclassically (dashed line) and from Thomas-Fermi (lower thick line) is plotted as a function of $A^{-1/3}$ for noninteracting particles in a Woods-Saxon potential. The parameters of the well are given in the first part of section (II.6). All energies are in MeV.

potentials like the Woods-Saxon potential discussed above. In that case the Thomas-Fermi gives not only the volume term but also makes substantial contributions to higher order terms. To show this we have fitted the Thomas-Fermi energy from eqs. (II.13) and (II.14) to eq. (1). The coefficients are C_1 = -26.10 MeV, C_2 = 34.81 MeV, C_3 = -7.83 MeV, C_4 = -81.75 MeV and C_5 = 94.85. It is seen that all coefficients are close to those obtained by fitting the semiclassical energy. The fact that the Thomas-Fermi result contains more than just the volume term can also be seen by looking at fig. 2 where we have plotted the energy per particle as a function of $A^{-1/3}$ for the exact energy, the semiclassical energy and the Thomas-Fermi energy. If the Thomas-Fermi term gave only the volume contribution it would be a horizontal straight line. It can also be seen that in contrast to the harmonic oscillator potential the surface term is nonzero.

Another important point can be seen from the graph. Namely that the difference between the exact and the semiclassical result does not average to zero if it is averaged over a large range of A. This means that the shell correction obtained using the semiclassical energy will similarly not be zero when averaged. If the smooth energy were obtained by a least squared fitting this average would be zero. This feature of the semiclassical energy, which is shared (Strutinsky and Ivanjuk 1975) by the usual Strutinsky smoothed

energy, is not to be looked on as a fault in the method. In fitting the liquid drop mass parameters it is necessary to first extract a theoretical shell correction from experimental binding energies (Myers and Swiatecki 1966) and hence when using the liquid drop mass parameters the main point is to use a shell correction that is consistant with the one used in obtaining the liquid drop parameters. Also in deriving the expressions that are fitted one uses semi-classical arguments (Myers and Swiatecki 1966) that are very much in the spirit of an extended Thomas-Fermi theory such as used here.

CHAPTER VI

A DERIVATION OF THE STRUTINSKY SMOOTHING PROCEDURE

VI.1 Introduction.

The smooth energy used to obtain shell corrections is usually found (Brack et. al. 1972) by using the Strutinsky smoothing procedure. In this chapter we shall derive the Strutinsky smoothing procedure as an approximate method for finding the semiclassical energy. To do this it is necessary to consider the exact partition function and to see what properties of the exact partition function give rise to shell effects. By studying these properties of the partition function and using analytic properties of the Laplace transform it is possible to derive the Strutinsky smoothing procedure including the form of the curvature corrections. This derivation of the Strutinsky smoothing procedure gives new insight into the smoothing procedure. For example the reasons why the Strutinsky smoothing method works better for the harmonic oscillator than the square well potential or why the plateau deteriorates for very large deformations can be easily seen in this derivation.

Another method which has been proposed for finding the smooth energy is the temperature averaging method (Ramamurthy et. al. 1970, Ramamurthy and Kapoor 1972). In this method one

uses the fact that at high temperatures the smooth Fermi occupation factors for the single particle states should make shell effects disappear. The energy (or other appropriate thermodynamic function) is evaluated at temperatures high enough to have washed out shell effects and then the smooth part, thus obtained, is extrapolated back to zero temperature. As this method of obtaining the smooth energy is equivalent to the Strutinsky method (Bhaduri and Das Gupta 1973) we will only discuss the Strutinsky method here.

For the harmonic oscillator potential it is possible to obtain explicit expressions not only for the smooth part of the density of states but also for the oscillating part. This makes the harmonic oscillator especially useful as an explicit example and it will be used extensively as such in the present chapter. However our derivation of the Strutinsky method is valid for quite general potentials.

As we will be discussing the Strutinsky method extensively a brief description of it will be presented here to fix the notation and to show the reader the type of expression we are trying to derive. Details of the method will be given later as they are derived. In the Strutinsky method one convolutes a smoothing function, $S(\epsilon)$, with the exact density of states to obtain a Strutinsky smoothed density of states $g_{st}(\epsilon)$,

$$g_{st}(\epsilon) = \int_0^\infty \frac{1}{\gamma} S\left(\frac{\epsilon-\epsilon'}{\gamma}\right) g(\epsilon') d\epsilon'$$

$$= \sum_i \frac{1}{\gamma} S\left(\frac{\epsilon-\epsilon_i}{\gamma}\right) . \qquad (1)$$

The second line follows immediately using the fact that $g(\varepsilon)$ is a sum of delta functions (eq. (II.1)). In this equation γ is the smoothing parameter and has been introduced explicitly here to simplify the notation that will be used throughout this chapter. The energy is obtained from the smoothed density of states through eqs. (II.2) and (II.3). The smoothing function that is usually used is (Strutinsky 1967, 1968),

$$S(\varepsilon) = \frac{e^{-\varepsilon^2}}{\sqrt{\pi}} L_n^{1/2}(\varepsilon^2) \qquad (2)$$

where $L_n^{1/2}(\varepsilon)$ is the associated Laguerre polynomial (Abramowitz and Stegun 1965, p. 775) and n is the curvature order. The $L_n^{1/2}(\varepsilon^2)$ in this context is often referred to as the curvature correction and their significance will become clear in later parts of this chapter. Other forms of the smoothing function have been proposed (Brack and Pauli 1973) although none are in common use. The parameter γ and n of eqs. (1) and (2) are determined from the condition that they have values in a region where the energy is insensitive to the actual value chosen.

In this chapter we shall start by considering in detail the partition function of the three-dimensional harmonic osciallator to gain more insight into the separation of the energy into a smooth and an oscillating part. We will then derive the Strutinsky method. In this derivation we will first discuss smoothing the density of states in detail and then at the end extend the results to physically interesting

properties such as the total energy or the spatial density. Finally we shall discuss the modifications necessary in the case of a finite well.

VI.2 Oscillating Terms in the Density of States of the Harmonic Oscillator.

For simple potentials such as the harmonic oscillator potential it is possible to find explicit expressions not only for the smooth part of energy but also for the oscillating contributions. In this section we will consider only the three dimensional harmonic oscillator although the analysis is easily extended to the harmonic oscillator in other dimensions or to the harmonic oscillator in the presence of the spin-orbit term of section (II.5).

The partition function for the three dimensional harmonic oscillator is given by (Bhaduri and Ross 1971) as:

$$Z(\beta) = \frac{1}{4}\,\mathrm{csch}^3\left(\frac{\beta\hbar\omega}{2}\right) \quad . \tag{3}$$

The corresponding semiclassical expansion is given by eq. (II.55) and it is easy to see that the semiclassical partition function is just the first few terms of the Laurent series for the exact partition function about $\beta=0$ so the exact and semiclassical partition functions will agree for small β. They differ however far from $\beta=0$ and in particular the exact partition function has poles along the imaginary β-axis. We shall now show that it is these poles that give rise to

oscillating terms (shell effects) in the density of states. Using an explicit form of the Laplace inversion formula (van der Pol and Bremmer 1955 p. 16) we have from eq. (II.6):

$$g(\varepsilon) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{\beta\varepsilon} Z(\beta) d\beta \quad , \tag{4}$$

where c is an arbitary positive constant. For the partition function of eq. (3) this integral may be done by contour integration after closing the contour to the left or to the right. For ε negative the contour is closed to the right and the integral gives zero. For ε positive the contour is closed to the left and we get contributions from each pole of the partition function. Thus we have the density of states given by the sum of the residues. Hence we must find the residues of $\exp(\beta\varepsilon)$ times the partition function. The poles are given by:

$$\beta = \frac{2\pi i n}{\hbar\omega} \tag{5}$$

for n running through all the integers both negative and positive. The corresponding residues, R_n, are given by:

$$R_n = (-1)^n e^{2\pi i n\varepsilon/\hbar\omega} \left(\frac{\varepsilon^2}{(\hbar\omega)^2} - \frac{1}{4\hbar\omega} \right) . \tag{6}$$

The density of states is now obtained by summing over n. It can be immediately seen that the n=0 term gives the first two

and (II.55). The terms with $n \neq 0$ give oscillating contributions. Summing over n we have:

$$g(\varepsilon) = \left(\frac{\varepsilon^2}{(\hbar\omega)^3} - \frac{1}{4\hbar\omega}\right)\left[1+2\sum_{n=1}^{\infty}(-1)^n \cos(2\pi n\varepsilon/\hbar\omega)\right]\theta(\varepsilon) \qquad (7)$$

In this expression we have combined the contributions from n and $-n$. The step function arises because as we have noted above $g(\varepsilon)$ is zero for ε negative. Eq. (7) can now be used with eq. (II.3) to obtain an expression for the energy. This gives us:

$$E = \lambda N - \int_0^{\lambda} d\varepsilon \int_0^{\varepsilon} d\varepsilon' \left(\frac{\varepsilon'^2}{(\hbar\omega)^3} - \frac{1}{4\hbar\omega}\right)\left[1+2\sum_{n=1}^{\infty}(-1)^n \cos(2\pi n\varepsilon'/\hbar\omega)\right]$$

$$= \lambda N - \frac{\lambda^4}{12(\hbar\omega)^4} + \frac{\lambda^2}{8\hbar\omega} + \frac{1}{2}\sum_{n=1}^{\infty}\frac{(-1)^n\hbar\omega}{(2\pi n)^2} + 12\sum_{n=1}^{\infty}\frac{(-1)^n\hbar\omega}{(2\pi n)^4}$$

$$+ \text{oscillating terms.} \qquad (8)$$

The terms containing the n-sums come from integrating the terms containing cos factors and looking at the contribution from the lower limit on the ε integral. The oscillating terms contain explicit factors of $\cos(2\pi n\lambda/\hbar\omega)$ and give rise to the shell effects. The sums over n may be done (Gradshteyn and Ryzhik 1965, p. 7) to yield a combined total of $-17\hbar\omega/960$. Eq. (II.57) for the semiclassical energy gives exactly the nonoscillating terms of eq. (8) when the spin-orbit effects are not included in eq. (II.57).

Using the relation (van der Pol and Bremmer 1955, p. 102),

$$\sum_{n=-\infty}^{\infty} e^{2\pi i n x} = \sum_{n=-\infty}^{\infty} \delta(x-n) \quad , \tag{9}$$

eq. (7) for the density of states reduces to:

$$g(\varepsilon) = \left(\frac{\varepsilon^2}{(\hbar\omega)^3} - \frac{1}{4\hbar\omega}\right)\left[\sum_{n=-\infty}^{\infty} \delta\left(\frac{\varepsilon}{\hbar\omega} - (n+\tfrac{1}{2})\right)\right]\theta(\varepsilon)$$

$$= \sum_{n=1}^{\infty} n(n+1)\,\delta(\varepsilon-(n+\tfrac{1}{2})\hbar\omega) \quad , \tag{10}$$

which is just the usual expression for the density of states of the harmonic oscillator.

The oscillating terms in the density of states arising from the poles of the one-body partition function give rise to effects in other physical situations as well. A prime example of this is the de Haas-van Alphen effect (Pathria 1972, p. 231) for electrons in a magnetic field. In this case the magnetic susceptibility oscillates as a function of applied magnetic field. These oscillations can be traced directly to the poles of the one-body partition function (Sondheimer and Wilson, 1951).

VI.3 Smoothing and the Partition Function.

In the previous parts of this thesis we have obtained the smooth part of the energy by doing an $\hbar$-expansion of the partition function. Such an expansion is expected to reproduce

the exact partition function when β is small (Uhlenbeck and Beth 1936). Thus we expect that the smooth part of the energy can be obtained by looking at the partition function for small β. In the last section we have shown that, for the three-dimensional harmonic oscillator, the smooth or semiclassical terms in the density of states come from the β=0 singularity of the partition function while oscillating terms come from singularities off the real axis. Although this is shown only for the harmonic oscillator similar results are expected for other potentials. This means that it is possible to reproduce the semiclassical results by multiplying the exact partition function by a function, $f(\gamma\beta)$, that is one near β=0 and goes to zero when the imaginary part of β becomes large. The parameter γ determines how fast $f(\gamma\beta)$ falls off as the imaginary part of β increases. One choice of $f(\beta\gamma)$ would be:

$$f(\gamma\beta) = e^{\beta^2\gamma^2/4} . \qquad (11)$$

We will show shortly that this choice of $f(\beta)$ give the Strutinsky smoothing of eqs. (1) and (2) with n=0 and γ being the smoothing parameter. The corresponding density of states, which we will call, anticipating our results, the Strutinsky density of states, is given by:

$$g_{st}(\varepsilon) = \mathcal{L}_{\varepsilon}^{-1}[Z(\beta)f(\beta\gamma)]$$

$$= \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\beta e^{\beta\varepsilon} Z(\beta)f(\beta\gamma) , \qquad (12)$$

where c is a positive constant. In getting the second expression we have used the explicit form of the Laplace inversion formulae (van der Pol and Bremmer 1955, p. 16). Using the convolution theorem (van der Pol and Bremmer 1955, p. 39) we have from eq. (12):

$$g_{st}(\varepsilon) = \int_0^\infty g(\varepsilon') \mathcal{L}^{-1}_{\varepsilon-\varepsilon'} [f(\beta\gamma)] \, d\varepsilon'$$

$$= \sum_i \mathcal{L}^{-1}_{\varepsilon-\varepsilon_i} [f(\beta\gamma)] \quad , \tag{13}$$

where we have used explicitly the fact that $g(\varepsilon)$ is a sum of delta functions. This equation is already in the same form as eq. (1) for Strutinsky smoothed density of states.

We now investigate the conditions on $f(\beta\gamma)$ more carefully. The behaviour of $f(\beta\gamma)$ far from the imaginary axis is of little interest as the line of integration can be taken arbitrarily close to the imaginary axis. We now impose two conditions on $f(\beta\gamma)$ for the sake of mathematical simplicity. First we insist that $f(\beta\gamma)$ be analytic function in a strip of the imaginary β plane parallel to and including the imaginary β-axis. The imaginary β-axis cannot lie on the boundary of this strip but must be actually inside the strip. The second condition is that $f(\beta\gamma)$ is an even function of β. This condition is purely for convenience and can be relaxed at the cost of losing some simplicity.

As the imaginary part of β increases $f(\beta\gamma)$ must

decrease fast enough to be close to zero once we are outside the region where the semiclassical and exact partition functions agree. To make this more precise let us again consider the harmonic oscillator. In this case the partition function has singularities at $\beta = \pm 2\pi i n/\hbar\omega$ and hence the exact and semiclassical partition functions can only agree for the absolute value of β less than $2\pi/\hbar\omega$. The $f(\beta\gamma)$ must already be quite small for the above value of β. For the $f(\beta\gamma)$ given by eq. (11) this means $\exp(-\pi^2\gamma^2/\hbar^2\omega^2)$ must be small which implies γ must be the order of $\hbar\omega$ or larger. This will cause $f(\beta\gamma)$ to be down by five order of magnitude at the first singularity. This is reasonable as the smooth energy must be known to at least four figures to obtain the shell corrections for heavy nuclei. If one were to consider a deformed harmonic oscillator the location of the pole nearest $\beta=0$ is determined by the largest frequency and not an average frequency. Hence the smoothing parameter γ must increase as the deformation increases if one keeps the product of the three frequencies constant for volume conservation. If the same effect holds true for other potentials it would account for the deterioration of the plateau in the Strutinsky smoothed energy for Woods-Saxon potentials with very large deformation (Brack 1976). If these conditions on $f(\beta\gamma)$ are satisfied the exact partition function in eq. (12) may be replaced by the semiclassical one. This gives us:

$$g_{st}(\varepsilon) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\beta\, e^{\beta\varepsilon} Z_{sc}(\beta) f(\beta\gamma) \quad . \qquad (14)$$

We would like the semiclassical and Strutinsky densities of states to agree for all ε. However this is too strong a condition and we will only impose the condition that the two become equal asymptotically for large ε. To see what condition this imposes on $f(\beta\gamma)$ let us look at the equation:

$$\int_{-\infty}^{\infty}\left[g_{sc}(\varepsilon)- g_{st}(\varepsilon)\right]e^{-\beta\varepsilon}d\varepsilon = Z_{sc}(\beta)-Z_{sc}(\beta)f(\beta\gamma) \ , \tag{15}$$

where the second term on the left side of this equation follows immediately from eq. (14). The integral over ε is taken from $-\infty$ to $+\infty$ because we have no guarantee that $g_{st}(\varepsilon)$ will be zero for negative ε. In fact it will in general not be zero. This means we are working with the two-sided Laplace transform (van der Pol and Bremmer, 1955). For the sake of simplicity we shall write:

$$D(\varepsilon) = g_{sc}(\varepsilon) - g_{st}(\varepsilon) \ . \tag{16}$$

With this notation eq. (15) becomes:

$$\mathcal{L}[D(\varepsilon)] = \int_{-\infty}^{\infty} d\varepsilon\, D(\varepsilon)\ e^{-\beta\varepsilon} = Z_{sc}(\beta)[1-f(\beta\gamma)] \ . \tag{17}$$

The condition on the Strutinsky density of states given above means $D(\varepsilon)$ must go to zero for large ε. This in turn implies that as β goes to zero $Z_{sc}(\beta)[1-f(\beta\gamma)]$ must diverge slower than β^{-1}. Hence $[1-f(\beta\gamma)]$ must go to zero fast enough to cancel out part of the divergence of $Z_{sc}(\beta)$. For the harmonic

oscillator $Z_{sc}(\beta)$ diverges as β^{-3} (eq. (II.55)) and hence $[1-f(\beta\gamma)]$ must go to zero faster than β^2. It does not do this for the $f(\beta\gamma)$ of eq. (11). However if we replace $f(\beta\gamma)$ by the function $f_m(\beta\gamma)$ defined by:

$$f_m(\beta\gamma) = f(\beta\gamma) \sum_{n=0}^{m} \frac{(\beta\gamma)^{2n}}{(2n)!} \left[\frac{\partial^{2n}}{\partial(\beta\gamma)^{2n}} \frac{1}{f(\beta\gamma)}\right]_{\beta=0} \tag{18}$$

the new function $[1-f_m(\beta\gamma)]$ can be made to go to zero as rapidly as we like by increasing m. For the harmonic oscillator m must be equal to or greater than one. Note that the series in eq. (18) is just the first m terms in the Maclaurin series for $1/f(\beta\gamma)$; hence $f_m(\beta\gamma)$ will reduce to one as m goes to infinity. The odd terms in β are zero because $f(\beta\gamma)$ is an even function of β. Thus $f_m(\beta\gamma)$ is the function we must multiply the exact partition by in order to extract the smooth density. For $f_m(\beta\gamma)$ to fall off as the imaginary part of β becomes large $f(\beta\gamma)$ must fall off faster than β^{-2n}. The Strutinsky density of states now becomes, in analogy with eq. (13),

$$g_{st}(\varepsilon) = \int_0^\infty g(\varepsilon') \mathcal{L}^{-1}_{\varepsilon-\varepsilon'}[f_m(\beta\gamma)]d\varepsilon' \tag{19}$$

This is in the same form as eq. (1) with,

$$S(\varepsilon) = \mathcal{L}^{-1}_{\varepsilon}[f_m(\beta)] \tag{20}$$

$$= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta\ e^{\beta\varepsilon} f(\beta) \sum_{n=0}^{m} \frac{\beta^{2n}}{(2n)!} \left[\frac{\partial^{2n}}{\partial\beta^{2n}} \frac{1}{f(\beta)}\right]_{\beta=0}$$

We have thus derived the Strutinsky smoothing procedure for the density of states with the generalized smoothing function as given by eq. (20). We will now look at the properties of this function in ε-space. In particular we will show that our generalized smoothing function, $S(\varepsilon)$, is very similar to the one discussed by Brack and Pauli (1973) and that for the choice of $f(\beta\gamma)$ given by eq. (11) we get the usual Gaussian smoothing of eq. (2).

As $f(\beta\gamma)$ or equivalently $f_m(\beta\gamma)$ is analytic in a strip of the complex β-plane including the imaginary axis, $S(\varepsilon)$ of eq. (20) must fall off at least exponentially for ε large negative or large positive. This may be seen by looking at the interval of convergence of the Laplace transform integral. The analytic properties of $f_m(\beta\gamma)$ also means that the c in eq. (20) may be zero. By replacing β by -β in eq. (20) one can see that because $f_m(\beta\gamma)$ is an even function of β, $S(\varepsilon)$ is an even function of ε. This implies that the odd moments, b_{2n+1}, of $S(\varepsilon)$ given by:

$$b_{2n+1} = \int_{-\infty}^{\infty} \varepsilon^{2n+1} S(\varepsilon) d\varepsilon \qquad (21)$$

will be zero. The even moments will be nonzero and are equal to:

$$b_{2n} = \frac{\partial^{2n} f(\beta)}{\partial \beta^{2n}} \bigg|_{\beta=0} \qquad (22)$$

This equation is derived by differentiating the Laplace transform integral. None of the moments diverge because $S(\varepsilon)$ falls

off at least exponentially. By looking at either the Laplace transform integral or the Laplace inversion integral with c=0 we see that $f_m(\beta)$ along the imaginary β-axis is just the Fourier transform of $S(\varepsilon)$. Since $f_m(\beta)$ goes to zero for the imaginary part of β large, the higher Fourier components of $S(\varepsilon)$ must be small and $S(\varepsilon)$ must be in some sense smooth. We will now explicitly take the Laplace inverse in eq. (20). Using eq. (II.28) we have:

$$S(\varepsilon) = \sum_{n=0}^{m} \frac{1}{(2n)!} \frac{\partial^{2n}}{\partial \beta^{2n}} \frac{1}{f(\beta)} \Bigg|_{\beta=0} \frac{\partial^{2n} S_0(\varepsilon)}{\partial \varepsilon^{2n}} \qquad (23)$$

where $S_0(\varepsilon)$ is the Laplace inverse of $f(\beta)$. The coefficients may be expressed in terms of the moments of eq. (22) if one takes the β-derivatives explicitly and uses eq. (22) to express the derivatives of $f(\beta)$ at β=0 in terms of the moments b_{2n}.

The smoothing function of eq. (23) corresponds closely to the one discussed by Brack and Pauli (1973). The main difference is that they do not explicitly impose the smoothness condition discussed above. They do however insist that $S_0(\varepsilon)$ is continuous and that all derivatives exist. To get the coefficients of the curvature corrections they say that terms to order $\partial^{2m} S_0(\varepsilon)/\partial \varepsilon^{2m}$ in:

$$\sum_{n=0}^{\infty} \frac{b_{2n}}{(2n)!} \frac{\partial^{2n} S(\varepsilon)}{\partial \varepsilon^{2n}}$$

must be zero. Using eq. (22) it is easy to see that this is satisfied for $S(\varepsilon)$ given by eq. (23) and hence our coefficients agree with theirs.

The function $f(\beta)$ may take on many different explicit forms besides the one given by eq. (11). Each of these will results in different forms of the smoothing function $S(\varepsilon)$. The value of $g_{st}(\varepsilon)$ will not depend on the form of $f(\beta)$, at least for large ε, if $f_m(\beta)$ satisfies the above conditions. Various forms of $S(\varepsilon)$ are discussed by Brack and Pauli (1973).

We will now work out the form of the smoothing function when $f(\beta)$ is given by eq. (11). In this case $S_0(\varepsilon)$ is given analytically by:

$$S_0(\varepsilon) = \frac{e^{-\varepsilon^2}}{\sqrt{\pi}} \quad . \tag{24}$$

This may be shown by explicitly taking the Laplace transform of eq. (24). The coefficients in eq. (23) may be worked out and this equation becomes:

$$S(\varepsilon) = \frac{1}{\sqrt{\pi}} \sum_{n=0}^{m} \frac{(-1)^n}{n!} \frac{1}{2^{2n}} \frac{\partial^{2n} e^{-\varepsilon^2}}{\partial \varepsilon^{2n}} \tag{25}$$

This may be further simplified using the three relations (Abramowitz and Stegun, 1965, chapter 22)

$$\frac{\partial^n}{\partial \varepsilon^n} e^{-\varepsilon^2} = (-1)^n H_n(\varepsilon) e^{-\varepsilon^2} \quad , \tag{26}$$

$$L_n^{-\frac{1}{2}}(\varepsilon^2) = \frac{(-1)^n}{n!\,2^{2n}} H_{2n}(\varepsilon) \quad , \tag{27}$$

$$L_m^{\frac{1}{2}}(\varepsilon^2) = \sum_{n=0}^{m} L_n^{-\frac{1}{2}}(\varepsilon^2) \quad , \tag{28}$$

where $H_n(\varepsilon)$ is the Hermite polynomial and $L_m^{\frac{1}{2}}$ the generalized Laguerre polynomial. Eq. (25) now becomes identical to eq. (2) which gives the usual Strutinsky smoothing function. Thus we have derived the usual Strutinsky smoothing procedure for the density of states.

An interesting difference arises when we compare Strutinsky smoothing in a square well with Strutinsky smoothing in a harmonic oscillator well. The difference between the semiclassical and Strutinsky density of states as we have seen can be written as:

$$D(\varepsilon) = \mathcal{L}_{\varepsilon}^{-1}\left[Z_{sc}(\beta)\,[1-f_m(\beta)]\right] \quad . \tag{29}$$

For the harmonic oscillator the function we are taking the Laplace inverse will be analytic at $\beta=0$ if m is greater than one. On the other hand for the square well $Z_{sc}(\beta)$ goes like $\beta^{-3/2}$, see eq. (V.2), and the function we are taking the Laplace inverse of in eq. (29) will never be analytic at $\beta=0$ for any finite m. To see the significance of this let us look at eq. (17). The integral in this equation will converge for negative β if and only if $D(\varepsilon)$ falls off exponentially or

faster for large ε. In this case the integral will be an analytic function of β along the imaginary β-axis. If on the other hand D(ε) falls off slower than exponentially the integral will diverge for negative β and there must be at least one singularity on the imaginary β-axis (van der Pol and Bremmer, 1955 p. 104). Thus the presence of a singularity on the imaginary β-axis gives us information on the behaviour of D(ε) for large ε. Hence we see D(ε) must fall off exponentially or faster for the harmonic oscillator while it must fall off slower than exponentially for the square well. In this discussion we have ignored the error due to using eq. (14) rather than eq. (12) which should be negligible. This difference between the two potentials accounts for the fact that the Strutinsky procedure works better for the harmonic oscillator than the square well (Bhaduri and Ross 1971, Brack and Pauli 1973) as well as the fact that for the square well the Strutinsky results although poor for small particle numbers improve for large particle numbers.

Since S(ε) falls off at least exponential for large ε we see from eqs. (19) and (2) that the Strutinsky density of states evaluated at ε depends only on the exact density of states near ε. Hence from a practical point of view it will be only the behaviour of g(ε) near ε that will be important in determining the conditions on $f_m(\beta\gamma)$. If the conditions on $f_m(\beta\gamma)$ discussed above are met the value of $g_{st}(\varepsilon)$ will not depend on the precise form of $f_m(\beta\gamma)$. In particular if we take

$f_m(\beta\gamma)$ from eq. (11) the result should not depend on γ or m for certain ranges of these variables. This leads to the plateau condition (Strutinsky 1967, 1968) that γ and m should be chosen in a region where the Strutinsky density of states is insensitive to the actual values chosen.

So far we have just discussed the smoothed density of states but we are in fact interested in the smooth energy. This means we must use the above arguments on eqs. (II.7) and (II.8) which determine λ and E. The only difference is that these equations have respectively one and two more factors of β in their denominators. This means we must take m larger by one when determining the energy. If this condition on m is met one can then use the Strutinsky density of states given by eq. (19) or equivalently eq. (1) in eqs. (II.2) and (II.3) to determine the energy as is usually done (Brack et. al. 1972). In the case of the harmonic oscillator m must be greater than or equal to two. The above arguments can also be used when working with the constrained Hamiltonian of chapter IV. The procedure of multiplying the partition function by an appropriate function in that case tells us to Strutinsky-smooth not only the density of states given by eq. (IV.6) but also the subsidiary density given by eq. (IV.5). These two densities are then used in eqs. (IV.7)-(IV.9) to determine the energy. It is necessary to smooth two densities as one alone is not enough to determine the energy. This is done in actual numerical calculations (Bengtsson et. al. 1975). The

value of m required in this case is determined by the same arguments as in the unconstrained case. Even when using Strutinsky smoothed quantities the canonical relation given by eq. (IV.17) or eq. (IV.55) is still satisfied.

If one is smoothing quantities other than the density of states one must be careful that the conditions on $f_m(\beta\gamma)$ have not changed. This happens as we have noted when we determined the energy. In that case we saw that m had to be taken larger. The conditions on $f_m(\beta\gamma)$ also changes when we want to find the smoothed spatial density given by:

$$\rho_{st}(\underset{\sim}{r}) = \mathcal{L}_\lambda^{-1}\left[\frac{1}{\beta} C(r,\beta) f_m(\beta\gamma)\right] . \qquad (30)$$

In this case $f_m(\beta\gamma)$ must fall off more quickly as β goes off the real axis. To see why this is so let us again consider the spherical harmonic oscillator. In this case the lowest frequency in the density of states is given by $1/\hbar\omega$ (Section VI.5). It is this frequency that causes the singularity in the partition function at $\beta=2\pi i/\hbar\omega$. For the spatial density the lowest frequency is half this value. This is particularly obvious for r=0 where the density is zero for alternating shells implying a period of $2\hbar\omega$ or a frequency of $1/2\hbar\omega$. This implies that the smoothing parameter, γ, must be twice as large when one is smoothing the density. This we saw when we obtained the Strutinsky smoothed density for the harmonic oscillator in Chapter III. It also accounts for the spatial oscillations in density for the Woods-Saxons potential

discussed in Chapter III.

In the arguments given above we have assumed that the one-body potential is infinite. In a finite well the smoothing function extends above the top of the well and into the continuum. This means that even if we are working at energies below the top of well we are sensitive to contributions from the continuum (Balian and Bloch 1974). We must therefore apply the Strutinsky smoothing to a density of states that is well behaved even above the top of the well. Such a density of states is provided by eq. (II.29) where we include the effects of the resonances in the continuum. The smooth or semiclassical part of this density is, as shown in section (II.3), well defined and continuous for energies above the top of the potential well if the volume integral of the potential is finite. It is then even continuous at the top of the well. The partition function of eq. (II.31) corresponding to this density of states is the natural extension (Huang 1963, p. 309) of the partition function for finite wells. Thus it is reasonable to use the resonances in the Strutinsky smoothing procedure. In fact numerical calculations (Ross and Bhaduri 1972) using the resonances yield results in good agreement with the samiclassical results (see section II.6). It is worth noting again that this is only valid if the volume integral of the potential is finite.

The procedure described above is not the one usually

used in doing Strutinsky calculations in finite wells. The usual procedure (Bolsterli et. al. 1972, Brack and Pauli 1973) involves using a set of artificial states generated in the continuum by diagonalizing the Hamiltonian in a finite basis. This procedure is different from the one described above in that it works even when the volume integral of the potential is infinite. This indicates that the artificial states are not to be looked on as approximating the resonances (see also Bolsterli et. al. 1972) but only as an artificial means of continuing the density of states in a smooth manner into the continuum region.

CHAPTER VII

SURFACE CORRECTIONS TO THE LANDAU DIAMAGNETIC SUSCEPTIBILITY

VII.1 Introduction.

By considering a system of free electrons confined in a large box and neglecting surface effects due to the walls of the box, Landau (1930) obtained the diamagnetic susceptibility of the electron gas. In the weak field limit, simple expressions for this quantity are obtained for both the zero temperature degenerate gas (Pathria 1972, p. 227) and the high temperature Boltzmann gas (Haung 1963, p. 243). These expressions give the so-called Landau values. We are not concerned, here, about that part of the orbital susceptibility which oscillates with a varying field and shows up at low temperatures as the de Haas-van Alphen effect. This oscillation in the susceptibility comes from oscillating terms in the single-particle density of states (Pathria 1972, p. 231) and hence are similar to nuclear shell effects (section VI.2.). We however are concerned only with the smooth part of the magnetic susceptibility. One may then ask as to how the steady value of the susceptibility is affected by the presence of a surface. Since the electrons are confined by some sort of a potential barrier, one may expect changes from the Landau values as the classical radius of gyration of the electron becomes comparable

to the confinement size. Since the radius of gyration of an electron is inversely proportional to the applied magnetic field strength, one may expect surface effects to be important in the weak field limit. This question has been investigated by Friedman (1964) and Thomas (1973) who considered explicit forms for the constraining potential and worked out the susceptibility by considering the eigenspectrum in the presence of a magnetic field.

In this chapter we will develop semiclassical expressions for the susceptibility, in the weak field limit, that are valid for quite general potentials. To do this the susceptibility is first expressed in terms of the single particle electronic partition function. This partition function may then be expanded in a power series in $\hbar$ using exactly the same techniques as used in chapter IV for the cranking model partition function. It is possible by this method to get general expressions because we do not deal directly with the eigenspectrum. The general semiclassical expressions for the susceptibility will then be evaluated for specific constraining potentials and the results compared with those obtained by Friedman (1964) and Thomas (1973).

VII.2 Semiclassical Expressions for the Magnetic Susceptibility.

Consider an electron gas, in which each electron moves independently of the others, but in a one-body potential $V(\underline{r})$

whose form need not be specified. A magnetic field $\underset{\sim}{B}$ will couple with the orbital as well as the spin angular momentum of the electron. The spin coupling will give rise to paramagnetism, and is not important in the present context. We shall therefore regard the electrons as spinless in what follows. For completeness the modification due to the inclusion of spin will be given in appendix G. The orbital Hamiltonian of an electron in a magnetic field $\underset{\sim}{B}$ is:

$$\hat{H}^B = \frac{1}{2m} (\hat{\underset{\sim}{p}} + \frac{e}{c} \underset{\sim}{A})^2 + V(r) \qquad (1)$$

where -e is the charge and m the mass of the electron. For a uniform magnetic field, the vector potential $\underset{\sim}{A} = \frac{1}{2} (\underset{\sim}{B} \times \underset{\sim}{r})$. The above Hamiltonian may be simplified by taking the z-axis along the direction of the magnetic field. This gives us:

$$\hat{H}^B = - \frac{\hbar^2}{2m} \nabla^2 + V(r) + \frac{e^2 B^2}{8mc^2} r_\perp^2 + \frac{eB}{2mc} \hat{\ell}_z \qquad (2)$$

with the same notation as in section IV.3. This Hamiltonian is very similar to the cranking Hamiltonian of eq. (II.34). The only differences are the absence of the spin term here and the presence of term proportional to $r_\perp^2$. The ω of that case can be identified with the eB/2mc in this case. The one-body partition function can now be defined, as in previous chapters (see eq. (IV.10)), by:

$$Z^B(\beta) = \text{tr } e^{-\beta \hat{H}^B} \qquad (3)$$

The magnetic susceptibility is completely determined in terms of $Z^B(\beta)$, both in the zero and the high temperature limits. The magnetization, M, at a temperature T is given by (Pathria 1972, p. 228):

$$M = kT \left(\frac{\partial}{\partial B} \ln Q\right)_{\lambda,T} \tag{4}$$

where Q is the grand-canonical partition function and λ the chemical potential. In the high temperature limit we may use Boltzmann statistics instead of Fermi-Dirac statistics (Reif 1965, p. 352). For noninteracting particles the grand-canonical partition function becomes (Pathria 1972, p. 104):

$$\ln Q = e^{\beta\lambda} Z^B(\beta) \tag{5}$$

where we are for the first time in this thesis using β as the reciprocal of the temperature, i.e. $\beta=1/kT$ where k is the Boltzmann constant and T the temperature. In this case $N=\ln Q$ so the magnetization per particle can be written, using eqs. (4) and (5) as:

$$\frac{M}{N} = \frac{1}{\beta} \frac{1}{Z^B(\beta)} \frac{\partial Z^B(\beta)}{\partial B} \tag{6}$$

In the weak field limit it is only necessary to evaluate $Z^B(\beta)$ to order B^2. The field-independent susceptibility, given by $\chi = M/B$ (Pathria 1972, p. 223) in this case

becomes:

$$\frac{\chi}{N} = \frac{M}{NB} = \frac{1}{\beta B} \frac{1}{Z^0(\beta)} \frac{\partial Z^B(\beta)}{\partial B}\bigg|_{B=0} \tag{7}$$

where $Z^0(\beta)$ is the partition function for B=0.

To express the zero-temperature susceptibility of a degenerate gas in terms of $Z^B(\beta)$ we again use eq. (4). In the low temperature case we must use Fermi-Dirac statistics. The grand-canonical partition is then (Pathria 1972, p. 228),

$$\ln Q = \int_0^\infty g^B(\varepsilon) \ln(1+e^{(\lambda-\varepsilon)/kT}) \, d\varepsilon \tag{8}$$

where $g^B(\varepsilon)$ is the density of states obtained by taking the Laplace inverse of $Z^B(\beta)$. For a degenerate gas, in the zero temperature limit, this reduces to:

$$kT \ln Q = \int_0^\lambda g^B(\varepsilon)(\lambda-\varepsilon) d\varepsilon$$

$$= \int_0^\lambda d\varepsilon \int_0^{\varepsilon'} g^B(\varepsilon') d\varepsilon' \tag{9}$$

where the second expression has been obtained by integrating by parts. As in chapter II we may express $g^B(\varepsilon)$ in terms of the one-body partition function and write in analogy with eq. (II.8):

$$kT \ln Q = \mathcal{L}_\lambda^{-1} \left[\frac{Z^B(\beta)}{\beta^2}\right] \tag{10}$$

Substituting this in eq. (4) we get the zero temperature magnetization:

$$M = \mathcal{L}_\lambda^{-1}\left[\frac{1}{\beta^2}\frac{\partial Z^B(\beta)}{\partial B}\right] . \tag{11}$$

The weak-field susceptibility λ of a degenerate gas at zero temperature is thus:

$$\chi = \frac{M}{B} = \frac{1}{B}\ \mathcal{L}_\lambda^{-1}\left[\frac{1}{\beta^2}\frac{\partial Z^B(\beta)}{\partial B}\right] . \tag{12}$$

Note that again here β is just a dummy variable as in chapter II. To examine the behaviour of χ in the zero or high temperature limits, it is only necessary to evaluate the one-body partition function to order B^2.

We now want the semiclassical expansion for the exact partition function:

$$Z^B(\beta) = \mathrm{tr}\ e^{-\beta\left(-\frac{\hbar^2\nabla^2}{2m}+V+\frac{e^2B^2}{2mc^2}r^2+\frac{eB}{2mc}\hat{\ell}_z\right)} \tag{13}$$

As the semiclassical expansion for very similar partition functions has been done in section (IV.3) and (IV.4) we will not repeat the details here but refer the reader to those sections. The partition function to order $\hbar$ and B^2 is given by:

$$Z^B_{sc}(\beta) = Z^0_{sc}(\beta) - \frac{e^2B^2\hbar^2}{24m^2c^2}\beta^2\left\{\frac{1}{4\pi^{3/2}\beta^{3/2}}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int d^3r\ e^{-\beta V}\left[1 - \frac{\beta^2\hbar^2}{24m}\nabla^2V - \frac{\beta^2\hbar^2}{30m}\left(\frac{\partial^2V}{\partial x^2}+\frac{\partial^2V}{\partial y^2}\right)\right]\right\} \tag{14}$$

where $Z^0_{sc}(\beta)$ is the B independent partition function of eq. (II.22). This equation may be rewritten, using eq. (II.22) as

$$Z^B_{sc}(\beta) = Z^0_{sc}(\beta) - \frac{e^2B^2\hbar^2}{24m^2c^2}\beta^2 Z^0_{sc}(\beta) + \frac{e^2B^2\hbar^2}{24m^2c^2}\beta^4 \frac{\hbar^2}{60m}\left\langle\left(\frac{\partial^2V}{\partial x^2} + \frac{\partial^2V}{\partial y^2}\right)\right\rangle Z^0_{sc}(\beta) \quad , \quad (15)$$

where:

$$\left\langle\left(\frac{\partial^2V}{\partial x^2} + \frac{\partial^2V}{\partial y^2}\right)\right\rangle = \int d^3r\, e^{-\beta V}\left(\frac{\partial^2V}{\partial x^2} + \frac{\partial^2V}{\partial y^2}\right) \Big/ \int d^3r\, e^{-\beta V} \quad . \quad (16)$$

Eq. (15) differs from eq. (14) in terms of order higher than $\hbar$. This is not important as eq. (14) is only accurate to order $\hbar$ anyway. The above expression for $Z^B_{sc}(\beta)$ may now be used in eq. (7) or eq. (12) to determine the magnetic susceptibility. The high-temperature susceptibility per particle is:

$$\frac{\chi}{N} = -\frac{e^2\hbar^2}{12m^2c^2}\frac{1}{kT} + \frac{e^2\hbar^2}{12m^2c^2}\frac{1}{(kT)^3}\frac{\hbar^2}{60m}\left\langle\left(\frac{\partial^2V}{\partial x^2} + \frac{\partial^2V}{\partial y^2}\right)\right\rangle \quad (17)$$

where the first term is just the Landau value, and the second term the sought after correction.

Eqs. (11) and (15) may be used to obtain the zero temperature susceptibility of the degenerate gas. The Laplace inverse here is done in the same manner as the Laplace inverse

used in determining $g_{sc}(\varepsilon)$ in chapter II. See in particular eq. (II.28). The result for the susceptibility is:

$$\chi = -\frac{e^2\hbar^2}{12m^2c^2}\left[g^0_{sc}(\lambda) - \frac{1}{8\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}\frac{1}{30}\frac{\partial}{\partial\lambda}\int d^3r\left(\frac{\partial^2 V}{\partial x^2}+\frac{\partial^2 V}{\partial y^2}\right)\right.$$

$$\left.\times\ \frac{\theta(\lambda-V)}{\sqrt{\lambda-V}}\right] , \qquad (18)$$

where $g^0_{sc}(\lambda)$ is the density of states, eq. (II.27), for an electron in the absence of any magnetic field evaluated at the Fermi energy λ. Again the first term is the well-known Landau term, while the next term is the sought after correction term.

VII.3 Magnetic Susceptibility for Specific Examples.

In this section, we shall apply the formulae (17) and (18) to evaluate the diamagnetic susceptibility for some simple potential barriers. In the first example we will consider a one-dimensional harmonic barrier. In this case, $V = \frac{1}{2}m\Omega^2y^2$, where Ω is the oscillator "frequency". We then have;

$$\frac{\partial^2 V}{\partial x^2} = 0 \quad , \quad \frac{\partial^2 V}{\partial y^2} = m\Omega^2 \quad , \qquad (19)$$

and hence

$$\left\langle\left(\frac{\partial^2 V}{\partial x^2}+\frac{\partial^2 V}{\partial y^2}\right)\right\rangle = m\Omega^2 \qquad (20)$$

Substituting this in eq. (17), we get for the Boltzmann gas:

$$\frac{\chi}{N} = \chi_L\left(1 - \frac{\hbar^2\Omega^2}{60(kT)^2}\right) \quad , \tag{21}$$

where

$$\chi_L = -\frac{e^2h^2}{12m^2c^2}\frac{1}{kT} \tag{22}$$

is the Landau value. Hence the correction term to the Landau value goes to zero at high temperatures irrespective of the parameter Ω. This is in agreement with eq. (4.10) of Thomas (1973).

To calculate the zero-temperature susceptibility of a degenerate gas for the same potential, we use eq. (18). In this case it is necessary to evaluate the integral:

$$I = \int dy\, m\Omega^2 \frac{\theta(\lambda - \frac{1}{2}m\Omega^2y^2)}{\sqrt{\lambda - \frac{1}{2}m\Omega^2y^2}} \tag{23}$$

and then take its derivative with respect to λ. Because of the step function, the y-integration is cut off at $y=\pm(2\lambda/m\Omega^2)^{1/2}$. The result now becomes (Gradshteyn and Ryzhik 1965, p. 86):

$$I = \pi\sqrt{2m\Omega^2} \quad . \tag{24}$$

Since this is independent of λ, the derivative with respect

to λ is zero and hence the correction to the Landau value of the susceptibility at zero temperature vanishes to this order in $\hbar$.

We will now consider the case where:

$$V = \frac{1}{2} m\Omega^2 r^2 \quad . \tag{25}$$

Using eq. (17) it is straightforward to show that the high-temperature susceptibility is:

$$\frac{\chi}{N} = \chi_L \left(1 - \frac{\hbar^2 \Omega^2}{30 (kT)^2}\right) \quad . \tag{26}$$

Again the correction to the Landau value vanishes at high temperature.

To evaluate the correction at zero temperature it is necessary to evaluate the integral:

$$I = 2m\Omega^2 \int d^3r \left(\lambda - \frac{1}{2} m\Omega^2 r^2\right)^{-1/2} \theta\left(\lambda - \frac{1}{2} m\Omega^2 r^2\right) \quad . \tag{27}$$

This may be done in a manner similar to that used in the last case. The result is:

$$I = 2^{5/2} \frac{\pi^2 \lambda}{(m\Omega^2)^{1/2}} \quad . \tag{28}$$

Substituting this in eq. (18), we get for the zero temperature

susceptibility:

$$\chi = - \frac{e^2\hbar^2}{12m^2c^2} \left[g^0_{sc}(\lambda) - \frac{1}{30\hbar\Omega} \right] \quad . \tag{29}$$

As the semiclassical density of states for a harmonic oscillator potential, without spin degeneracy, is (Bhaduri and Ross 1971):

$$g^0_{sc}(\varepsilon) = \frac{\lambda^2}{2(\hbar\Omega)^3} - \frac{1}{8\hbar\Omega} \tag{30}$$

we see that the correction to the Landau term is very small.

Lastly we shall evaluate the high temperature susceptibility for the potential:

$$V = \frac{1}{2} m\Omega^2 y^2 + V_0 b_4 y^4 \quad , \tag{31}$$

discussed by Thomas (1973). Here we have:

$$\left\langle \left(\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} \right) \right\rangle = m\Omega^2 + 12 V_0 b_4 I \tag{32}$$

with:

$$I = \frac{\int_{-\infty}^{\infty} y^2 e^{-\beta \left(\frac{1}{2} m\Omega^2 y^2 + V_0 b_4 y^4 \right)} dy}{\int_{-\infty}^{\infty} e^{-\beta \left(\frac{1}{2} m\Omega^2 y^2 + V_0 b_4 y^4 \right)} dy}$$

$$= - \frac{2}{\beta\Omega^2} \frac{\partial}{\partial m} \ell n \left(\int_{-\infty}^{\infty} e^{-\beta \left(\frac{1}{2} m\Omega^2 y^2 + V_0 b_4 y^4 \right)} dy \right) . \tag{33}$$

The integral may be expressed in terms of the modified Bessel function $K_{1/4}$ as (see Gradshteyn and Ryzhik 1965 p. 339 and p. 952):

$$\int_{-\infty}^{\infty} e^{-\beta(\frac{1}{2}m\Omega^2 y^2 + V_0 b_4 y^4)}\, dy = \frac{1}{2}\sqrt{\frac{m\Omega^2}{2V_0 b_4}}\ \exp\left(\frac{\beta}{32}\frac{m^2\Omega^4}{V_0 b_4}\right) \times K_{1/4}\left(\frac{\beta}{32}\frac{m^2\Omega^4}{V_0 b_4}\right) \quad . \tag{34}$$

Using eq. (34) and the identity (op. cit, p. 970):

$$\frac{d}{dx} K_\nu(x) = -\frac{\nu}{x} K_\nu(x) - K_{\nu-1}(x) \tag{35}$$

we immediately obtain:

$$I = \frac{m\Omega^2}{8V_0 b_4}\left[-1 + K_{3/4}\left(\frac{\beta}{32}\frac{m^2\Omega^4}{V_0 b_4}\right)/K_{1/4}\left(\frac{\beta}{32}\frac{m^2\Omega^4}{V_0 b_4}\right)\right] \quad . \tag{36}$$

To take the proper high temperature limit of this, we assume the parameters of the potential V to be fixed and let $\beta \to 0$. Using the relation (Abramowitz and Stegun 1965, p. 375)

$$\lim_{x\to 0} K_\nu(x) = \frac{1}{2}\Gamma(\nu)\left(\frac{x}{2}\right)^{-\nu} \tag{37}$$

we can simplify eq. (36) in the limit

$$\frac{1}{32}\beta\frac{m^2\Omega^4}{V_0 b_4} \ll 1 \quad . \tag{38}$$

We then get:

$$I \sim \frac{\Gamma(3/4)}{\Gamma(1/4)} \frac{1}{(\beta V_0 b_4)^{1/2}} \tag{39}$$

The high temperature susceptibility can now be immediately written down using eqs. (17), (32) and (39). It is:

$$\frac{\chi}{N} = \chi_L \left[1 - \frac{\hbar^2}{5m} \frac{\Gamma(3/4)}{\Gamma(1/4)} \frac{1}{(kT)^{3/2}} (V_0 b_4)^{1/2}\right] , \tag{40}$$

where we have neglected terms of order $(kT)^{-2}$. This expression again reduces to the Landau value at high temperature. We emphasize that eq. (40) was not obtained by Thomas (1973), since he did not evaluate χ in the high temperature limit. Rather, he used a perturbation formalism and allowed the strength of the y^4 term in V to be adjustable at high temperatures, so that the condition

$$\frac{V_0 b_4}{m^2 \Omega^4} \ll \beta \tag{41}$$

is satisfied. This is actually the opposite condition to eq. (38). Using the asymptotic relation (Abramowitz and Stegun 1965, p. 378):

$$K_{-\nu}(x) \sim \sqrt{\frac{\pi}{2x}}\, e^{-x}\left(1 + \frac{4\nu^2 - 1}{8x}\right) \tag{42}$$

valid for large x, eq. (36) for I reduces to:

$$I \sim \frac{1}{\beta m \Omega^2} \quad . \tag{43}$$

Using this in eqs. (17) and (32) we get:

$$\frac{\chi}{N} = \chi_L \left(1 - \frac{\hbar^2\Omega^2}{60(kT)^2} - \frac{\hbar^2\Omega^2}{5(kT)} \frac{V_0 b^4}{m^2\Omega^4}\right) \quad . \tag{44}$$

This is the same result as obtained by Thomas (1973), after minor algebraic errors in his paper are corrected.

To summarize, we have used the semiclassical partition to derive expressions for the weak field susceptibility for both the Boltzmann and degenerate electron gas subject to a smooth potential barrier of arbitrary shape. Even in this weak field limit, when surface effects should be most effective, we find that the corrections to the Landau values of the susceptibility are unimportant.

CHAPTER VIII

CONCLUSION

An expression for the smooth part of the energy of a system of noninteracting particles has been developed as an expansion in $\hbar$. This expansion, which is valid for finite or infinite potentials, gives to leading order just the Thomas-Fermi result. The final expression can therefore be regarded as an extended Thomas-Fermi expression. It is to be stressed that although we have used the one-body partition function the result is an $\hbar$-expansion and not a thermodynamic result. In fact the same results, to a lower order in $\hbar$ have been derived by both Balian and Bloch (1971) and Gross (1972) using methods that made no use of the partition function or thermodynamics. We have used the partition function only as an analytic tool to simplify the mathematics. The effects of a spin-orbit term in the Hamiltonian are included explicitly in our formalism. The $\hbar$-expansion was shown to converge rapidly for realistic potentials by considering specific examples.

The analysis was then extended to the case of a constrained Hamiltonian. In particular the pushing and cranking models were considered. In the cranking model the moment of inertia was calculated. It was found that although the moment of inertia takes on the rigid body value in the Thomas-Fermi

approximation, small corrections to this value arise when higher terms in the $\hbar$-expansion are considered. The corrections to the rigid body value were found to become more important when the one-body potential contained momentum dependant terms.

The semiclassical expansion was also used to obtain expressions for the spatial and kinetic energy densities. These expressions were not valid near the classical turning points where they diverged. An expression was then obtained for the kinetic energy density in terms of spatial density. The first term in this expression was the usual Thomas-Fermi $\rho^{5/3}$ term while the second term was the Wiezsacker term with the correct coefficient. Higher order terms were also obtained.

The semiclassical results for the energy were compared to the Strutinsky smoothed energy. It was found both numerically and analytically the two energies were the same. In fact the Strutinsky smoothing method may be regarded as a practical numerical method for finding the semiclassical energy.

The semiclassical expansion was compared with the A-expansion. It was found that the semiclassical expansion converged somewhat faster. The volume and surface terms found by least square fitting the semiclassical energies for a Woods-Saxon well are in good with the values obtained analytically by Siemans and Sobiczewski (1972). It was also

observed that the shell correction obtained using the semi-classical energy did not average to zero when averaged over a large region of A. This is not a disadvantage as it merely causes a slight change in the liquid drop mass formula parameters.

The formalism developed for the cranking model was applied to, the formally very similar problem, of non-interacting particles in a magnetic field. In particular surface effects on the diamagnetic susceptibility were investigated. It was found that at high temperatures the diamagnetic susceptibility reduced to the Landau value while at zero temperature small effects remained.

APPENDIX A

THE EXPRESSIONS FOR w

In this appendix we will give the expressions for w_1 through w_4 as required by eq. (II.19). They are:

$$w_1 = -\frac{i\beta^2}{2m}\, \underset{\sim}{p}.\nabla V \quad ,$$

$$w_2 = -\frac{\beta^2}{4m}\nabla^2 V + \frac{\beta^3}{6m}(\nabla V)^2 - \frac{\beta^4}{8m^2}(\underset{\sim}{p}.\nabla V)^2 + \frac{\beta^3}{6m^2}(\underset{\sim}{p}.\nabla)^2 V \quad ,$$

$$w_3 = -\frac{i\beta^3}{6m^2}(\underset{\sim}{p}.\nabla)\nabla^2 V + \frac{i\beta^4}{4m^2}\left[\frac{(\nabla^2 V)}{2}\,(\underset{\sim}{p}.\nabla V)\right.$$

$$\left. + \frac{5}{12}\,(\underset{\sim}{p}.\nabla)(\nabla V)^2 + \frac{(\underset{\sim}{p}.\nabla)^3}{6m}\, V\right]$$

$$- \frac{i\beta^5}{4m^2}\left[\frac{(\nabla V)^2}{3}\,\underset{\sim}{p}.\nabla V + \frac{1}{6m}\,(\underset{\sim}{p}.\nabla)(\underset{\sim}{p}.\nabla V)^2\right]$$

$$+ \frac{i\beta^6}{48m^3}\,(\underset{\sim}{p}.\nabla V)^3 \quad ,$$

$$w_4 = -\frac{\beta^3}{24m^2}\nabla^4 V + \frac{\beta^4}{4m^2}\left[\frac{1}{8}\,(\nabla^2 V)^2 + \frac{1}{4}\,\nabla V.\nabla\nabla^2 V\right.$$

$$\left. + \frac{1}{12}\,\nabla^2(\nabla V)^2 + \frac{1}{4m}\,(\underset{\sim}{p}.\nabla)^2\nabla^2 V\right] - \frac{\beta^5}{4m^2}\left[\frac{1}{6}\,(\nabla^2 V)(\nabla V)^2\right.$$

$$\left. + \frac{2}{15}\,\nabla V.\nabla(\nabla V)^2 + \frac{1}{6m}\,(\nabla^2 V)(\underset{\sim}{p}.\nabla)^2 V + \frac{1}{30m}\,\nabla V.\nabla(\underset{\sim}{p}.\nabla)^2 V\right.$$

$$+ \frac{1}{3m} (\underset{\sim}{p}.\nabla V)\nabla^2(\underset{\sim}{p}.\nabla V) + \frac{2}{15m} (\underset{\sim}{p}.\nabla)^2(\nabla V)^2$$

$$+ \frac{1}{30m^2} (\underset{\sim}{p}.\nabla)^4 V\Big] + \frac{\beta^6}{4m^2}\Big[\frac{(\nabla V)^4}{18} + \frac{1}{9m} (\nabla V)^2(\underset{\sim}{p}.\nabla)^2 V$$

$$+ \frac{1}{8m} (\nabla^2 V)(\underset{\sim}{p}.\nabla V)^2 + \frac{5}{24m} (\underset{\sim}{p}.\nabla V)\ \underset{\sim}{p}.\nabla\ (\nabla V)^2$$

$$+ \frac{1}{12m^2} (\underset{\sim}{p}.\nabla V)(\underset{\sim}{p}.\nabla)^3 V + \frac{1}{18m^2} [(\underset{\sim}{p}.\nabla)^2 V]^2\Big]$$

$$- \frac{\beta^7}{8m^3}\Big[\frac{1}{6} (\nabla V)^2(\underset{\sim}{p}.\nabla V)^2 + \frac{1}{6m} (\underset{\sim}{p}.\nabla V)^2(\underset{\sim}{p}.\nabla)^2 V\Big]$$

$$+ \frac{\beta^8}{384m^4} (\underset{\sim}{p}.\nabla V)^4$$

APPENDIX B

THE p-INTEGRATIONS

In order to obtain the semiclassical partition function it is necessary to do integrations of the form:

$$I = \int d^3p\, e^{-\beta p^2/2m}\, \underset{\sim}{p}.\underset{\sim}{A}\ \underset{\sim}{p}.\underset{\sim}{B} \cdots \underset{\sim}{p}.\underset{\sim}{C}\ , \qquad (1)$$

where the $\underset{\sim}{A}$, $\underset{\sim}{B}$ and $\underset{\sim}{C}$'s are either ordinary vectors or vector operators. Although integrals such as this may be done in cartesian coordinates, it is much easier to use the following rules, which may be easily verified by using cartesian coordinates. The rules are:

1) the integral is zero if there are an odd number of p's.
2) there is always a factor of $\pi^{3/2}$
3) if there are 2n p's there is an overall factor of $(2m/\beta)^{n+3/2}/2^n$,
4) the $\underset{\sim}{A}$, $\underset{\sim}{B}$ and $\underset{\sim}{C}$'s are taken in all possible scalar combinations as often as they occur,
5) a factor of p^2 is written as $\underset{\sim}{p}.\underset{\sim}{i}\underset{\sim}{p}.\underset{\sim}{i}+\underset{\sim}{p}.\underset{\sim}{j}\underset{\sim}{p}.\underset{\sim}{j}+\underset{\sim}{p}.\underset{\sim}{\kappa}\underset{\sim}{p}.\underset{\sim}{\kappa}$, where $\underset{\sim}{i}$, $\underset{\sim}{j}$ and $\underset{\sim}{\kappa}$ are the three cartesian coordinate basis.

If any of the $\underset{\sim}{A}$, $\underset{\sim}{B}$ or $\underset{\sim}{C}$'s are operators care must be taken to see that they act on the same factor in both the intergrand the result. As an example let us consider the integral:

$$I = \int d^3p\, e^{-\beta\frac{p^2}{2m}}\, p^2 (\underset{\sim}{p}.\nabla V)^2 (\underset{\sim}{p}.\nabla)^2 V \qquad (2)$$

This may be written using rule (5) :

$$I = \int d^3p\, e^{-\beta\frac{p^2}{2m}} (\underset{\sim}{p}.\underset{\sim}{i}\underset{\sim}{p}.\underset{\sim}{i}+\underset{\sim}{p}.\underset{\sim}{j}\underset{\sim}{p}.\underset{\sim}{j}+\underset{\sim}{p}.\underset{\sim}{\kappa}\underset{\sim}{p}.\underset{\sim}{\kappa})\,(\underset{\sim}{p}.\nabla V)^2 (\underset{\sim}{p}.\nabla)^2 V \qquad (3)$$

Using rules (2), (3) and (4) we get:

$$I = \pi^{3/2}\left(\frac{2m}{\beta}\right)^{9/2} \frac{1}{2^3}\Big[(\underset{\sim}{i}.\underset{\sim}{i}+\underset{\sim}{j}.\underset{\sim}{j}+\underset{\sim}{\kappa}.\underset{\sim}{\kappa})\,(\nabla V)^2(\nabla^2 V)$$

$$+2(\underset{\sim}{i}.\underset{\sim}{i}+\underset{\sim}{j}.\underset{\sim}{j}+\underset{\sim}{\kappa}.\underset{\sim}{\kappa})\nabla V.(\nabla V.\nabla)\nabla V + 2(\underset{\sim}{i}.\nabla V\underset{\sim}{i}.\nabla V+\underset{\sim}{j}.\nabla V\underset{\sim}{j}.\nabla V$$

$$+\underset{\sim}{\kappa}.\nabla V\underset{\sim}{\kappa}.\nabla V)\nabla^2 V + 2(\nabla V)^2(\underset{\sim}{i}.(\underset{\sim}{i}.\nabla)\nabla V + \underset{\sim}{j}.(\underset{\sim}{j}.\nabla)\nabla V + \underset{\sim}{\kappa}.(\underset{\sim}{\kappa}.\nabla)\nabla V)$$

$$+8\nabla V.(\underset{\sim}{i}.\nabla V\underset{\sim}{i}.\nabla + \underset{\sim}{j}.\nabla V\underset{\sim}{j}.\nabla + \underset{\sim}{\kappa}.\nabla V\underset{\sim}{\kappa}.\nabla)\nabla V\Big]. \qquad (4)$$

This reduces to:

$$I = \pi^{3/2}\left(\frac{2m}{\beta}\right)^{9/3} \frac{1}{8}\Big[(3+2+2)\,(\nabla V)^2(\nabla^2 V)+(6+8)\,\nabla V.(\nabla V.\nabla)\nabla V\Big]$$

$$= \pi^{3/2}\left(\frac{2m}{\beta}\right)^{9/3} \frac{7}{8}\Big[(\nabla V)^2(\nabla^2 V) + \nabla V.\nabla(\nabla V)^2\Big]. \qquad (5)$$

APPENDIX C

The semiclassical energy, E_{sc}, may be written as:

$$E_{sc} = \lambda_{sc} N - \int_0^{\lambda_{sc}} n(\varepsilon) d\varepsilon \quad , \tag{1}$$

where:

$$n(\varepsilon) = \int_0^{\varepsilon} g_{sc}(\varepsilon) d\varepsilon \tag{2}$$

In $g_{sc}(\varepsilon)$, obtained by using eq. (II.22) in eq. (II.6), we include the leading term of order $\hbar^{-3}$ and correction terms of order $\hbar^{-1}$ and $\hbar$, so that $n(\varepsilon)$ is correct to order $\hbar$. The quantity λ_{sc} is determined from the equation:

$$N = n(\lambda_{sc}) \tag{3}$$

If, however, we use in eq. (1) an approximate Fermi energy, $\lambda'_{sc} = \lambda_{sc} + \delta\lambda$, obtained through the equation:

$$n'(\lambda'_{sc}) = N \quad , \tag{4}$$

where n' is correct only to order $\hbar^{-1}$, we get:

$$E'_{sc} = \lambda'_{sc} N - \int_0^{\lambda'_{sc}} n(\varepsilon) d\varepsilon \quad . \tag{5}$$

Note that in eq. (5), the integrand of the second term still

contains $n(\varepsilon)$. It is easy to see that:

$$E'_{sc} - E = \frac{1}{2} (\delta\lambda)^2 g(\lambda_{sc}) \quad . \tag{6}$$

From eq. (3) and (4), we obtain:

$$\delta\lambda \approx \frac{n(\lambda_{sc}) - n'(\lambda_{sc})}{g'(\lambda_{sc})} \quad . \tag{7}$$

Since the numerator of the above equation is of order $\hbar$, and the denominator is of order $\hbar^{-3}$, $\delta\lambda$ is of order $\hbar^4$. Hence $E'_{sc} - E_{sc}$, from eq. (6), is of order $\hbar^5$. It then follows that eq. (4), rather than eq. (3), may be used to determine λ_{sc}.

APPENDIX D

The expression for $I(\underset{\sim}{r},\underset{\sim}{p},\beta)$ as needed in eq. (II.44) is:

$$\sum_{\sigma} I(\underset{\sim}{r},\underset{\sim}{p},\beta) = \frac{\beta^2\kappa^2\hbar^2}{(2m)^2}\left\{p^2(\nabla f)^2 - (\underset{\sim}{p}.\nabla f)^2\right\}$$

$$+ i\,\beta^2\,\frac{\kappa^2\hbar}{(2m)^2}\Big\{-\frac{1}{2}\,\underset{\sim}{p}.\nabla(\nabla f)^2 + (\underset{\sim}{p}.\nabla f)\nabla^2 f + \frac{\beta}{3}\,(\nabla f)^2(\underset{\sim}{p}.\nabla V)$$

$$- \frac{\beta}{3}\,(p.\nabla f)(\nabla f.\nabla V) - \beta\,\frac{p^2}{3m}\,\nabla f.\nabla(p.\nabla f) + \frac{\beta}{3m}(\underset{\sim}{p}.\nabla)^2 f\;\underset{\sim}{p}.\nabla f\Big\}$$

$$+ \beta^3\kappa^2\,\frac{\hbar^4}{(2m)^3}\Big\{\frac{p^2}{3}\,\nabla f.\nabla\nabla^2 f + \frac{1}{3}(\underset{\sim}{p}.\nabla\nabla^2 f)\underset{\sim}{p}.\nabla f + \frac{2}{3}(p.\nabla)^2 f\;\nabla^2 f$$

$$- \frac{1}{3}\,p^2\nabla^2(\nabla f)^2 - \beta\,\frac{p^2}{6m}\,\nabla f.\nabla(\underset{\sim}{p}.\nabla)^2 f + \frac{\beta}{6m}\,(\underset{\sim}{p}.\nabla)^3 f\;\underset{\sim}{p}.\nabla f$$

$$+ \frac{\beta}{6}\,\underset{\sim}{p}.\nabla(\nabla f)^2\underset{\sim}{p}.\nabla V - \frac{\beta}{3}\,(\underset{\sim}{p}.\nabla)^2 f\;\nabla f.\nabla V + \frac{\beta}{6}(\nabla f)^2(\underset{\sim}{p}.\nabla)^2 V$$

$$- \frac{\beta}{6}(\underset{\sim}{p}.\nabla f)\nabla f.\nabla(\underset{\sim}{p}.\nabla V) + \frac{\beta p^2}{12}\,\nabla V.\nabla(\nabla f)^2 - \frac{\beta}{6}\,\nabla V.\nabla(\underset{\sim}{p}.\nabla f)(\underset{\sim}{p}.\nabla f)\Big\}$$

$$+ \frac{\kappa^3\beta^3}{3}\,\frac{\hbar^4}{(2m)^3}\,(\nabla f\times\underset{\sim}{p})\times(\nabla f\times\nabla).(\nabla f\times\underset{\sim}{p})$$

$$+ \frac{\beta^4\kappa^4}{12}\,\frac{\hbar^4}{(2m)^4}\,[(\nabla f)^2p^2 - (p.\nabla f)^2]^2$$

APPENDIX E

The expression for E_{sc} in the case of spherical symmetry reduces to:

$$E_{sc} = \lambda_{sc} N - \frac{8}{15\pi} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^{r_{sc}} dr\, r^2 (\lambda_{sc} - V)^{5/2}$$

$$+ \frac{1}{6\pi} \left(\frac{2m}{\hbar^2}\right)^{1/2} \int_0^{r_{sc}} dr\, r^2 (\lambda_{sc} - V)^{1/2} \left(\frac{d^2V}{dr^2} + \frac{2}{r}\frac{dV}{dr}\right)$$

$$- \frac{1}{120\pi} \left(\frac{\hbar^2}{2m}\right)^{1/2} \int_0^{r_{sc}} dr\, r^2 (\lambda_{sc} - V)^{-1/2} \left\{\frac{11}{3}\frac{1}{r^2}\frac{d^2V}{dr^2} - \frac{5}{12}\frac{d^4V}{dr^4}\right.$$

$$\left. + \frac{7}{6}\frac{1}{r}\left(\frac{d^2V}{dr^2}\right)^2 \left(\frac{dV}{dr}\right)^{-1} + \frac{7}{6}\frac{d^2V}{dr^2}\frac{d^3V}{dr^3}\left(\frac{dV}{dr}\right)^{-1} - \frac{7}{12}\left(\frac{d^2V}{dr^2}\right)^3 \left(\frac{dV}{dr}\right)^{-2}\right\}$$

$$- \frac{2\kappa^2}{3\pi} \left(\frac{2m}{\hbar^2}\right)^{1/2} \int_0^{r_{sc}} dr\, r^2 (\lambda_{sc} - V)^{3/2} \left(\frac{df}{dr}\right)^2$$

$$+ \frac{\kappa^2}{24\pi} \left(\frac{\hbar^2}{2m}\right)^{1/2} \int_0^{r_{sc}} dr\, r^2 (\lambda_{sc} - V)^{-1/2} \left(\frac{df}{dr}\right)^2 \frac{d^2V}{dr^2}$$

$$- \frac{1}{3\pi} \left(\frac{\hbar^2}{2m}\right)^{1/2} \int_0^{r_{sc}} dr\, r^2 (\lambda_{sc} - V)^{1/2} \left[\left\{\kappa^2 \frac{1}{2}\frac{df}{dr}\frac{d^3f}{dr^3}\right.\right.$$

$$\left.\left. - \frac{1}{r}\frac{df}{dr}\frac{d^2f}{dr^2} - \frac{2}{r^3}\left(\frac{df}{dr}\right)^2\right\} - \kappa^3 \frac{1}{r}\left(\frac{df}{dr}\right)^3 + \frac{\kappa^4}{2}\left(\frac{df}{dr}\right)^4\right],$$

where r_{sc} is the turning point given by $V(r_{sc}) = \lambda_{sc}$.

APPENDIX F

In order to obtain expressions for the semiclassical density it is useful to define a "smoothed" mixed density:

$$g_\gamma(\varepsilon,\underset{\sim}{r}) = \int_0^\infty g(\varepsilon',\underset{\sim}{r})\ \frac{e^{(\varepsilon-\varepsilon')^2/\gamma^2}}{\gamma\sqrt{\pi}}\ d\varepsilon' \qquad (1)$$

where γ is a small but finite smoothing parameter. The factor of $\gamma\sqrt{\pi}$ is needed to insure proper normalization. In the limit $\gamma\to 0$, the Gaussian becomes a delta function and $g_\gamma(\varepsilon,\underset{\sim}{r})$ reduces to $g(\varepsilon,\underset{\sim}{r})$. This means that for small γ the smoothing has little effect. In taking the Laplace transform of $g_\gamma(\varepsilon,\underset{\sim}{r})$ we must deal explicitly with the two sided Laplace transform (van der Pol and Bremmer 1955):

$$C_\gamma(\underset{\sim}{r},\beta) = \int_{-\infty}^{\infty} g_\gamma(\varepsilon,r)\ e^{-\beta\varepsilon}\ d\varepsilon \quad . \qquad (2)$$

Using the convolution theorem for Laplace transforms (van der Pol and Bremmer 1955 p. 39) we obtain:

$$C_\gamma(\underset{\sim}{r},\beta) = C(\underset{\sim}{r},\beta)\int_{-\infty}^{\infty} \frac{e^{-\varepsilon^2/\gamma^2}}{\gamma\sqrt{\pi}}\ e^{-\beta\varepsilon}\ d\varepsilon \quad . \qquad (3)$$

The integral may be done by completing the square to yield:

$$C_\gamma(\underset{\sim}{r},\beta) = C(\underset{\sim}{r},\beta)\ e^{\beta^2\gamma^2/4} \quad . \qquad (4)$$

This equation may now be used in connection with eqs. (III.3)

and (III.10) to obtain a semiclassical density $\rho_{sc\gamma}(\underset{\sim}{r})$. In doing this we need to take Laplace inverses of the form:

$$I = \mathcal{L}_{\lambda}^{-1}\ \beta^{n+1/2}\ e^{-\beta V}\ e^{\beta^2\gamma^2/4} \qquad (5)$$

where n is an integer. Using the explicit form of the inversion formulae (van der Pol and Bremmer 1955, p. 16) we have:

$$I = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \beta^{n+1/2}\ e^{-\beta V}\ e^{\beta^2\gamma^2/4}\ e^{\beta\lambda}\ d\beta\ , \qquad (6)$$

where c is a positive constant. By making the change of variable $x = \beta\gamma/\sqrt{2}$ we get:

$$I = \frac{1}{2\pi i}\frac{2^{\frac{n}{2}+3/4}}{\gamma^{n+3/2}}\int_{c-i\infty}^{c+i\infty} x^{n+1/2}\ e^{\frac{\sqrt{2}x}{\gamma}(\lambda-V)}\ e^{\frac{x^2}{2}}\ dx \qquad (7)$$

The integral may now be recognized as an integral representation (Abramowitz and Stegun 1965, p. 688) of the parabolic cylinder function $U(a,x)$. Hence we have:

$$I = \frac{2^{\frac{n}{2}+1/4}}{\sqrt{\pi}\gamma^{n+3/2}}\ e^{-(\lambda-V)^2/2\gamma^2}\ U(-n-1,-\sqrt{2}(\lambda-V)/\gamma) \qquad (8)$$

As we are only interested in γ small we may use the asymtotic form of $U(a,x)$ for large x (Gradshteyn and Ryzhik 1965, p. 1065 and p. 1066). This gives us:

$$I = \frac{\theta(\lambda-V)}{\Gamma(-n-1/2)\,(\lambda-V)^{n+3/2}} \qquad (9)$$

This should be valid except near the turning points where $\lambda=V$. Due to the fact that γ is small the convolution of eq. (1) should not effect the value of the semiclassical result, it only serves to validate the mathematics. A similar analysis for the Laplace inverse of β^n yield the usual result (van der Pol and Bremmer 1955 p. 385) of the n plus first derivative of the delta function. This tends to lend credence to the method.

APPENDIX G

THE EFFECTS OF SPIN ON THE MAGNETIC SUSCEPTIBILITY

The effects of spin on the weak field magnetic susceptibility is easily included in the formalism of chapter VII. The Hamiltonian in this case becomes:

$$\hat{H}^B = \frac{1}{2m}\left(\underset{\sim}{p} + \frac{e}{c}A\right)^2 + V(r) - B\cdot\mu_s \quad , \tag{1}$$

where:

$$\mu_s = -\frac{e\hbar}{2mc}\underset{\sim}{\sigma} \quad .$$

As in chapter VII we take B along the z-axis. The Hamiltonian then reduces to:

$$\hat{H}^B = -\frac{\hbar^2}{2m}\nabla^2 + V(r) + \frac{e^2B^2}{8mc^2}r_\perp^2 + \frac{eB}{2mc}(\hat{\ell}_z + \hbar\hat{\sigma}_z) \quad . \tag{2}$$

Notice that in this case the orbital term, $\hat{\ell}_z$, and the spin term, $\hbar\hat{\sigma}$, come with the same coefficient. In the cranking Hamiltonian the $\hbar\hat{\sigma}\hat{\ell}_z$ term had a relative one-half. The partition function may be written in analogy with eq. (IV.10) as:

$$Z^B(\beta) = \mathrm{tr}\, e^{-\beta\hat{H}^B} \tag{3}$$

The spin part of the trace may be done using the eigenfunctions of $\hat{\sigma}_z$ as a basis. The partition function is then:

$$Z^B(\beta) = 2 \cosh(\frac{e\beta\hbar}{2mc}) \ tr_0 \ e^{-\beta \hat{H}_0^B} , \qquad (4)$$

where $\hat{H}_0^B$ is the Hamiltonian of eq. (VII.2) which contains only the orbital part of the interaction with the magnetic field. The trace in eq. (4) is the same as in eq. (VII.3) and does not include the sum over spin variables. As we are only interested in small values of B the cosh factor may be expanded to yield:

$$Z^B(\beta) = 2 \ tr_0 \ e^{-\beta \hat{H}_0^B} + (\frac{eB\hbar\beta}{2mc})^2 \ 2 \ tr_0 \ e^{-\beta \hat{H}^0} . \qquad (5)$$

The first term here is just the partition function of eq. (VII.3) with an overall factor of two which arises from the spin degeneracy. As this term was discussed in chapter VII it will not be discussed here. The second term will give the contribution to the susceptibility from the spin. The B independant Hamiltonian, $\hat{H}^0$, can be used in this term because we are only interested in the partition function to order B^2. The contribution to the susceptibility from this term can be found from eq. (VII.7) or eq. (VII.12). In the zero temperature limit eq. (VII.12) gives the additional contribution:

$$\chi_s = \mathcal{L}_\lambda^{-1} \left[(\frac{e\hbar}{2mc})^2 \ 2 \ tr_0 \ e^{-\beta \hat{H}^0} \right] , \qquad (6)$$

where χ_s is the contribution to susceptibility due to spin. The $2\ tr_0\ e^{-\beta\hat{H}^0}$ is just the partition function of chapter II, complete with a factor of two due to spin degeneracy. Eq. (6) therefore reduces to:

$$\chi_s = \frac{e^2\hbar^2}{4m^2c^2}\ g(\lambda) \quad , \tag{7}$$

where $g(\lambda)$ is the density of states (see eq. (II.6)) in the absence of a magnetic field. This is just the expression for the well known Pauli paramagnetic susceptibility (Pauli 1926) and should be added to eq. (VII.18) to obtain the complete expression for the susceptibility.

In the high temperature limit we similarly get an additional term. From eq. (VII.7) it is

$$\frac{\chi_s}{N} = \frac{1}{(kT)}\ \frac{e^2\hbar^2}{4m^2c^2} \quad . \tag{8}$$

The complete expression for the susceptibility is found by adding this term to eq. (VII.17).

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