Semiclassical expansions for confined N fermion systems

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Abstract

A new derivation of the Wigner Kirkwood expansion for N-fermion systems is presented, showing explicitly the connection to the WKB approximation for a single level. This allows to study separately the two ansatz required to obtain the semiclassical expansions : the asymptotic expansions in powers of $\hbar$ and the smoothing of quantal effects . We discuss the one dimensional and three dimensional, with spherical symmetry, cases. Applications for standard potentials used in nuclear physics are described in detail.

1 Introduction

Semiclassical approximations were introduced already in the early days of quantum mechanics. Although it might appear that their interest for practical applications has been reduced by the wide availability of computers, they are still a very useful tool in the derivation of analytical expressions appropriate to clarify the physical interpretation of many problems. Contrary to other approximate methods used in quantum mechanics, the semiclassical approaches exploit explicitly the "smallness" of $\hbar$: these approximations work when the magnitudes of the typical actions of the problem are much larger than $\hbar$. However it should also be remarked that the expressions derived for the observables are divergent power series expansions in $\hbar$ that converge only asymptotically. Nevertheless the numerical accuracy of such expansions truncated after a few terms is often surprisingly good.

In the present work we want to discuss more specifically semiclassical approximations for confined N fermion systems , having in mind their application to condensed matter, atomic and nuclear physics. Although most of the results presented will apply only to the ground states, in their derivation use will be made of expressions for e.g. level densities with a larger domain of application (statistical theories of reaction processes, ...). Even though in the end the most simple form of our results will coincide with the already well known Wigner-Kirkwood expansion [1,2,3], we shall obtain them with what we believe is a new derivation whose main merit is to show the deep and direct connection of these expansions to the standard WKB approximation. The various derivations already available in the literature [2,3,4,5] use apparently rather different physical ideas and mathematical formulations. It was not obvious a priori to us, that starting from the WKB method one could obtain the same results. In this sense what we pretend to achieve is to present a more unified view of the semiclassical formulations for the one and the N particle problems.

The main practical interest of our derivation of the Wigner Kirkwood expansion is twofold:

a) since we show in a clear way every one of the several steps where explicit use is made of the above stated assumption of the "smallness" of $\hbar$, the accuracy of each approximation can be tested independently. This will be illustrated for some simple examples at the end of this work.

b) we give explicit expressions for the neglected terms, thus these can be included in a systematic way to improve on the standard semiclassical results, adding for instance oscillating contributions.

The plan of the article is as follows : in Section 2 we give a reminder of the WKB method for the one dimensional case. We follow a recent review by Montroll [6] based on the rigorous treatment proposed by Dunham [7] many years ago. After the reminder proper we focus our discussion on the properties of the single particle level density, which plays a central role in our formulation and discuss its series expansion in powers of $\hbar$. We then derive expressions for the expectation values of one body operators following a method due to Dagens [8]. We show that they can be reduced to series expansions whose terms are combinations of derivatives with respect to the energy of integrals on the real axis, and are thus free of the divergences at the turning points encountered in the standard formulations.

In Section 3 we derive the expansions for non-interacting N fermion systems in a potential well. We use the power series expansion of the level density to approximate sums over discrete levels by integrations over continuously variable energies. The Wigner Kirkwood expansion is then recovered. Using Dagens prescription for the computation of expectation values, we recover also the Wigner Kirkwood result for the matter density .

In Section 4 the previous results are extended to the three dimensional case (with spherical symmetry) using Langer's method . An additional summation has to be performed over the discrete values of the angular momenta : use of the Euler Mc Laurin formula allows us to replace it by an integration plus correction terms, and this leads to the Wigner Kirkwood expansion.

In Section 5 we present numerical results illustrating the accuracy of the approximations discussed in this work for typical potentials encountered in nuclear physics : the harmonic oscillator and the Woods Saxon well. In particular, for the total energies our results improve on the pioneering work of March and Plaskett [16], allowing to include in a consistent way all the $\hbar^2$ contributions . Finally, Section 6 contains the summary and conclusions of our work.

2 The one dimensional problem

2.1. *A reminder of the standard W.K.B. approximation for the energy*

We shall discuss first the determination of the eigenenergies of the Schrödinger equation following the method of Ref.[6]. We consider the one dimensional equation for one particle in the potential $U(x)$:

$$-\frac{\hbar^2}{2m}\varphi_n''(x) + (U(x) - E_n)\varphi_n(x) = 0 \tag{2.1}$$

and assume for simplicity that the spectrum is discrete, so that $\{\varphi_n(x), E_n, n = 0, ...\infty\}$ are the eigenfunctions and eigenvalues, and also that for each level the potential is such that there are only two turning points : x_n^-, x_n^+. Then, as is well known, all the zeros of $\varphi_n(x)$ lie in the interval $[x_n^-, x_n^+]$ and from Cauchy's theorem it follows that :

$$\frac{1}{2\pi i}\oint \frac{\varphi_n'(z)}{\varphi_n(z)}dz = n \qquad (n = 0, 1, 2..,) \tag{2.2}$$

where the integration contour in the complex z plane encloses the segment of real axis between the turning points. The only additional requirement for (2.2) to hold is that $\varphi_n(z)$ is analytic in the complex plane and does not have other zeros inside the contour of integration. We shall assume that the potential is well behaved to guarantee that the φ_n of interest fulfil these conditions, at least for contours sufficiently close to the real axis. Since the path of integration can be chosen at our convenience, we shall assume also that it is such that $\varphi_n(z)$ never vanishes on it, so that we can define an auxiliary function through the relation :

$$\varphi(z) = exp\left\{\frac{i}{\hbar}\int^z \chi(z)dz\right\} \tag{2.3}$$

When this is substituted into (2.1) the following Ricatti type equation is obtained for χ :

$$-i\hbar\chi'(z) = \varepsilon - V(z) - \chi^2(z) \tag{2.4}$$

where for simplicity we have set V = 2mU, $\varepsilon = 2$mE and omitted the index n. In addition, eq.(2.2) takes the simple form :

$$\oint \chi(z)dz = nh. \tag{2.5}$$

An alternative derivation of the previous equation has been given by Dunham [7], requiring the single valuedness of $\varphi(z)$ as defined by (2.3). We now go back to (2.4) and assume that ϵ is known and with its value fixed we consider the solutions of that equation when $\hbar$ is taken as a parameter. This determines a family of solutions

$$\chi = \chi(\varepsilon; V; \hbar; z). \tag{2.6}$$

The semiclassical W.K.B. approximation is obtained by assuming that χ admits a power series expansion :

$$\chi = \chi_o + (\hbar/i)\chi_1 + ... + (\hbar/i)^j \chi_j + ... \tag{2.7}$$

and substituting in condition (2.5). The explicit form of each term in the series is obtained by requiring that the Ricatti equation for χ, eq.(2.4), be satisfied for all values of $\hbar$. Then the $\chi_j(\varepsilon; V; z)$ are given in implicit form by the recurrence relation :

$$\chi'_{j-1}(z) = -\sum_{k=0}^{j} \chi_{j-k}(z)\chi_k(z) \tag{2.8}$$

and the choice :

$$\chi_o(z) = (\varepsilon - V(z))^{1/2} \tag{2.9}$$

where the branch cut is taken between the turning points on the real axis.
These completely determine the W.K.B. expansion : truncation of the series at a given order and use of (2.5) determines the W.K.B. eigenenergy to that order of approximation. Since from (2.8) : $\chi_1 = -\frac{1}{2} d\log\chi_o/dz$, we get

$$\frac{1}{2\pi i}\oint \chi_1(z)dz = -1/2. \tag{2.10}$$

It can be proved [6 and Refs. therein] that for a very general class of potentials all the integrals of the same form as (2.10) with $\chi_1(z)$ replaced by $\chi_j(z)$ vanish when j is odd and greater than one. Therefore it is useful to introduce a new function,

$$S[\varepsilon;V;\hbar] \equiv \oint (\chi + i\hbar\chi_1)dz \tag{2.11}$$

whose series expansion is thus :

$$\begin{aligned} S[\varepsilon;V;\hbar] &= \sum_{m=0}^{\infty} (i\hbar)^{2m} S_m[\varepsilon;V] \\ &= \sum_{m=0}^{\infty} (i\hbar)^{2m} \oint \chi_{2m}(z)dz \ . \end{aligned} \tag{2.12}$$

Then from (2.5) and (2.10), the eigenvalues ε_n satisfy :

$$S[\varepsilon_n;V;\hbar] = (n+1/2)h \ . \tag{2.13}$$

It is a simple exercise to derive from (2.8), (2.9) and (2.12) the explicit form of the S_m. We give only the first two terms of the series :

$$S_o[\varepsilon;V] = \oint (\varepsilon - V)^{1/2}dz \tag{2.14a}$$

$$S_1[\varepsilon;V] = \frac{1}{24}\frac{d}{d\varepsilon}\oint \frac{V''}{(\varepsilon - V)^{1/2}}dz \ . \tag{2.14b}$$

The above results are a summary of the standard derivation of the semiclassical equations for the energy of a level. For a more careful derivation of these results see Ref.[7,9,10]. The assumptions about the behaviour of the potential and of the solutions of the Schrödinger equation that have been made are fulfilled in a large number of physical problems. It can be proved [11] for instance that if the potential U(x) is determined selfconsistently (Hartree or Hartree-Fock method), U(x) is indefinitely differentiable even for discontinuous two body interactions. The only specific assumption required until here concerns the meaning of the series expansion introduced in (2.7). It is easy to check, by

looking at eq.(2.4), that χ has a singularity when $\hbar \to 0$, and therefore the series expansion, (2.7), can at best be asymptotic. Therefore all the expansions derived from (2.7), such as (2.12) and those that will be given later for expectation values and level densities will also be only asymptotically convergent. It is this fact that makes the study of the convergence of the semiclassical approximations non-trivial.

2.2. *The semiclassical expansion for the level density*

The quantal level density for the eigenstates of eq.(2.1) is the distribution defined by :

$$g(E) = \sum_{n=0}^{\infty} \delta(E - E_n) \ , \tag{2.15a}$$

but to simplify our expressions it will be more useful to introduce :

$$g(\varepsilon) = \sum_{n=0}^{\infty} \delta(\varepsilon - \varepsilon_n) \ . \tag{2.15b}$$

Both are trivially connected : $g(E) = 2mg(\varepsilon)$. This quantity can be related to the function S(ε;V;$\hbar$) introduced above. Since in fact (2.11) allows one to determine S for an arbitrary value of ε, we can interpret eq.(2.13) as defining the integer n as a function of the continuous variable ε :

$$n(\varepsilon) = \sum_{k=1}^{\infty} \theta \left[-\frac{1}{2} + \frac{1}{h} S[\varepsilon; V; \hbar] - k \right] \tag{2.16}$$

where θ is Heaviside's function and we have used the identity : Integer part of $x = \sum_{k=1}^{\infty} \theta(x-k)$. The number of states, $N(\varepsilon)$, is also given by (2.16) but with k running from zero to infinity. Then it can be easily checked that :

$$g(\varepsilon) = \frac{dN(\varepsilon)}{d\varepsilon} \tag{2.17}$$

The proof requires only using the well known identity for the delta distribution :

$$\delta(f(x)) = \sum_{\{x_i\}} \frac{1}{|f'(x_i)|} \delta(x - x_i) \tag{2.18}$$

where the x_i are the values of x for which f(x) vanishes. Differentiating (2.16) with respect to ϵ, one gets

$$g(\epsilon) = \frac{dN}{d\epsilon} = \frac{1}{h}\frac{\partial S}{\partial \epsilon}\sum_{k=0}^{\infty} \delta\left[-\frac{1}{2} + \frac{1}{h}S[\epsilon; V; \hbar] - k\right], \tag{2.19}$$

and applying (2.18) one recovers eq.(2.15).

Until here we did not introduce any approximations, and therefore the level density and its primitive, $N(\epsilon)$, have the characteristic discontinuous behaviour due to the quantization of the eigenvalues of (2.1). We will now discuss two prescriptions to smoothen out these discontinuities by expanding (2.19) and truncating the series : they are based on the Euler McLaurin and the Poisson formulae.

i) *The Euler McLaurin expansion* : Our starting point is the well known summation formula as given e.g. in Abramowitz and Stegun [14], eq.(23.1.32):

$$\begin{aligned}\sum_{k=o}^{s} F(k) &= \int_{-\frac{1}{2}}^{s+\frac{1}{2}} F(t)\, dt \\ &+ \sum_{k=1}^{p} \frac{B_k(\frac{1}{2})}{k!}\,(F^{(k-1)}(s+\frac{1}{2}) - F^{(k-1)}(-\frac{1}{2})) \\ &+ remainder\end{aligned} \tag{2.20}$$

which is valid for an arbitrary, regular, function F, and therefore letting $p \to \infty$ to suppress the remainder, and noticing that $B_{2k+1}(\frac{1}{2}) = 0$, one gets for the sum of delta distributions

$$\begin{aligned}\sum_{k=o}^{\infty} \delta(x - (k+\frac{1}{2})) &= \theta(x) + \sum_{k=1}^{\infty} \frac{B_{2k}(\frac{1}{2})}{(2k)!}\,\delta^{(2k-1)}(x) \\ &= \theta(x) - \frac{1}{24}\delta'(x) + ...\end{aligned} \tag{2.21}$$

Therefore (2.19) takes the form

$$g(\varepsilon) = \frac{1}{h}\frac{\partial S}{\partial \varepsilon}\theta(\varepsilon - \varepsilon_m) - \frac{h}{24}\left(\frac{\partial S}{\partial \varepsilon}\right)^{-1}_{\varepsilon=\varepsilon_m} \delta'(\varepsilon - \varepsilon_m) + ... \qquad (2.22)$$

where ε_m is defined by the condition :

$$S(\varepsilon_m) = 0 \qquad (2.23)$$

and expanding S as in (2.12) there is a corresponding expansion for ε_m :

$$\varepsilon_m = \varepsilon_m^o \; + \; \hbar^2 \varepsilon_m^1 \; + \; ...$$

whose terms are given by :

$$S_o(\varepsilon_m^o) = 0$$

$$-\hbar^2 \; S_1(\varepsilon_m^o) \; + \; \hbar^2 \; \varepsilon_m^1 \left(\frac{\partial S_o}{\partial \varepsilon}\right)_{\varepsilon=\varepsilon_m^o} = 0$$

$$..... \qquad (2.24)$$

Notice that this expansion for $g(\varepsilon)$ is justified only when S is indefinitely differentiable. This is not necessarily the case when it is replaced by its asymptotic expansion (2.12) at $\varepsilon = \varepsilon_m$. Combining the above results , $g(\varepsilon)$ can be explicitly written as an $\hbar^2$ asymptotic power series :

$$g(\varepsilon) = g^{(o)}(\varepsilon) \; + \; \hbar^2 \; g^{(2)}(\varepsilon) + ... \qquad (2.25)$$

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where

$$g^{(o)}(\varepsilon) = \frac{1}{h}\frac{\partial S_o}{\partial \varepsilon}\theta(\varepsilon - \varepsilon_m^o)$$

$$g^{(2)}(\varepsilon) = -\frac{1}{h}\left(\frac{\partial S_1}{\partial \varepsilon}\theta(\varepsilon - \varepsilon_m^o) + S_1(\varepsilon_m^o)\,\delta(\varepsilon - \varepsilon_m^o)\right.$$

$$\left. + \frac{\pi^2}{6}\left(\frac{\partial S_o}{\partial \varepsilon}\right)^{-1}_{\varepsilon=\varepsilon_m^o}\delta'(\varepsilon - \varepsilon_m^o)\right)$$

$$+ \ldots \qquad (2.26)$$

ii) *The Poisson formula* : Using the expansion

$$\sum_{k=0}^{\infty}\delta(x-k) = Y(x-1/2)\left(1 + 2\sum_{p\neq 0}\cos 2\pi p x\right), \qquad (2.27)$$

where $Y(x)$ is any regular function such that

$$Y(x) = 1 \quad \text{if } x \geq \frac{1}{2}$$

and

$$Y(0) = 0 \quad \text{if} \quad x \leq -\frac{1}{2},$$

we rewrite the r.h.s. of (2.19) as :

$$g(\varepsilon) = \frac{1}{h}Y\left(\frac{1}{h}S[\varepsilon;V;\hbar]\right)\left(1 + 2\sum_{p\neq 0}\cos 2\pi p\left[\frac{1}{h}S[\varepsilon;V;\hbar] - \frac{1}{2}\right]\right)\frac{\partial S}{\partial \varepsilon}. \qquad (2.28)$$

This is still an exact expression for $g(\varepsilon)$: when ε coincides with some ε_n the argument of the cosine functions vanishes, so that the sum over p diverges, as it should if it has to reproduce the $\delta(\varepsilon - \varepsilon_n)$ term in $g(\varepsilon)$.

The second step in introducing a semiclassical approximation is the suppression of the discontinuities in $g(\varepsilon)$. Accordingly , we now *define the smoothed level density* , $\tilde{g}(\varepsilon)$ as :

$$\tilde{g}(\varepsilon) = \frac{1}{h}\frac{\partial S}{\partial \varepsilon}\theta(\varepsilon - \varepsilon_m^o) \qquad (2.29a)$$

and its $\hbar^2$-expansion as *the semiclassical level density* :

$$g_{sc}(\varepsilon) = \frac{1}{h}\left(\frac{\partial S_o}{\partial \varepsilon} + (i\hbar)^2\frac{\partial S_1}{\partial \varepsilon} + ...\right)\theta(\varepsilon - \varepsilon_m^o) \qquad (2.29b)$$

comparison with eq.(2.26) shows that we have dropped all the $\delta^{(k)}$ terms, and kept only those proportionnal to the θ functions, whereas if we compare to eq. (2.28), we see that only the first term in the series has been kept and what has been dropped are the terms that are rapidly oscillating when $\hbar$ is small compared to S. Notice however that when ε is close to ε_m the ratio S/h is not large anymore, and more terms in the Poisson series will be "smooth". Under these conditions $g_{sc}(\varepsilon)$ as defined above is expected to be a poor approximation even for the slowly varying part of the level density.

Although the Poisson series is not a proper $\hbar^2$ expansion (and therefore will not be used in the three dimensional case), it is very useful to examine the role of the terms neglected in the derivation of (2.29) : For illustration, we show in Fig. 1 the particle number $N(\varepsilon)$ for the quartic oscillator ($V = x^4$). The step function corresponds to the exact spectrum, while the two continuous curves to adding one and six terms of the Poisson formula to the semiclassical term. A similar application to the matter density is presented in Ref [12].

Finally, the explicit form of the semiclassical level density in terms of the potential is obtained from eqs. (2.29), (2.12) and (2.14):

$$g_{sc}(\varepsilon) = \frac{1}{2h}\left(\oint \frac{dx}{\sqrt{\varepsilon - V(x)}} - \frac{\hbar^2}{24}\frac{\partial^2}{\partial \varepsilon^2}\oint \frac{V''dx}{\sqrt{\varepsilon - V}} + ...\right)\theta(\varepsilon - \varepsilon_m^o) \qquad (2.30)$$

There is no special difficulty in deriving the $O(\hbar^4)$ term, however higher order contributions become very involved to work out.

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This result is the basis for the semiclassical expansions of other quantities like expectation values of one body operators, total energies, matter densities, etc., that will be explicitly given in the next section. The same formula has been derived using the somewhat more involved techniques based on the smoothing via Laplace transforms presented in Refs.[5]. We prefer however the derivation outlined above because the two main approximations : smoothing and asymptotic expansions are clearly separated, and in this way the role of the terms neglected in the Poisson formula ,which are the only ones responsible for the oscillations of $g(\varepsilon)$, can be easily studied.

An important remark is here in order : $g_{sc}(\varepsilon)$ is an asymptotic $\hbar^2$ expansion of $\tilde{g}(\varepsilon)$, this means that for a given $\hbar$ (or conversely for a given $1/\sqrt{\varepsilon - V}$) there is an optimum number of terms for the series (2.29b), and that going further can make it even infinite. In general this number is not known, all what can be said is that it increases when the "small" parameter (here either $\hbar$ or $1/\sqrt{\varepsilon - V}$) decreases. For $\varepsilon \approx \varepsilon_m$ it turns out that the optimum number is 1. This situation is very frequent when dealing with asymptotic expansions : see for instance the Stirling expansion of $\Gamma(x)$ which gives infinity when $x = 1$, unless it is truncated after the first term. For this reason when in Sec. 3 we compute integrals over ε between the limits ε_m and ε_F (the Fermi level) of quantities containing the expansion (2.29b), the contribution of the lower limit will be truncated after the first term.

2.3. *The determination of expectation values*

The above approximations do not allow to derive an explicit semiclassical expansion for the wavefunction, they only determine the energy eigenvalues. Therefore to obtain semiclassical expansions for expectation values without introducing wave functions one has to find a way to relate them to the eigenenergies. Here we follow the method of Dagens [8], who uses elementary results from first order perturbation theory : given an operator $F(x)$ we change the potential in (2.4) to $V(x) + \lambda F(x)$ where λ is the small

parameter (we assume F sufficiently well behaved so that perturbation theory holds). Then the expectation value of F is given by :

$$< F >_\varepsilon = \lim_{\lambda \to 0} \frac{1}{\lambda}(\varepsilon[V + \lambda F] - \varepsilon[V]) \equiv \delta\varepsilon[F] \tag{2.31}$$

where $\varepsilon[V + \lambda F]$ is the exact eigenvalue of (2.4) when the term λF is added to the potential, and the subscript ε on $< F >$ specifies the level for which this expectation value is computed. With that expression as a starting point we can now introduce the semiclassical expansion using the W.K.B. determination of the eigenenergies. We start from eq.(2.13) and consider the variations induced by the above change in the potential when λ is small :

$$\frac{\partial S}{\partial \varepsilon}\lambda\delta\varepsilon[F] + S[\varepsilon; V + \lambda F] - S[\varepsilon; V] = 0 \tag{2.32}$$

So that, defining in analogy with (2.31) :

$$\delta S[F; \varepsilon] = \lim_{\lambda \to 0}(S[\varepsilon; V + \lambda F] - S[\varepsilon; V])/\lambda \tag{2.33}$$

we find :

$$< F >_\varepsilon = \delta\varepsilon[F] = -\frac{\delta S[F; \varepsilon]}{\partial S/\partial \varepsilon} \tag{2.34}$$

Since ε and V always appear as $\varepsilon - V$ in the Schrödinger equation ,

$$S(\varepsilon, V + \lambda.1) \equiv S(\varepsilon - \lambda, V)$$

and therefore :

$$\delta S[1; \varepsilon] = -\frac{\partial S}{\partial \varepsilon} \tag{2.35}$$

which insures that $< 1 >_\varepsilon$ as given by this method is indeed 1. We encountered already this quantity in dealing with the level density $g(\varepsilon)$, so that it is immediate to derive its semiclassical expansion. More generally, we write from (2.12) :

$$\delta S[F; \varepsilon] = \sum_{m=0}^{\infty} (i\hbar)^{2m} \delta S_m[F; \varepsilon] \tag{2.36}$$

At this point it is necessary to realize that when ε is an eigenvalue, it can be also written as a power series in $\hbar^2$: i.e. solving (2.13) with a truncated series in the l.h.s. determines ε_n only to the corresponding order of appproximation in $\hbar^2$. One then writes, dropping the index n for simplicity :

$$\varepsilon = \varepsilon_o + \hbar^2 \varepsilon_1 + ... \tag{2.37}$$

and it is easy to see that from (2.13) :

$$\varepsilon_1 = S_1[\varepsilon_o, V] \Big/ \left[\frac{\partial S_o[\varepsilon_o, V]}{\partial \varepsilon_o}\right] \tag{2.38}$$

Therefore, replacing (2.37) in (2.36) one finds :

$$\begin{aligned} \delta S[F;\varepsilon] = \delta S_o[F,\varepsilon_o] + \hbar^2 \varepsilon_1 \frac{\partial}{\partial \varepsilon_o} \delta S_o[F,\varepsilon_o] \\ - \hbar^2 \delta S_1[F,\varepsilon_o] + O(\hbar^4) \quad , \end{aligned} \tag{2.39}$$

which can be evaluated more explicitly for $F = 1$ using the expression for ε_1. Differentiating (2.38) with respect to ε_o :

$$-\frac{\partial S_1[\varepsilon_o, V]}{\partial \varepsilon_o} + \varepsilon_1 \frac{\partial}{\partial \varepsilon_o}\left(\frac{\partial S_o[\varepsilon_o, V]}{\partial \varepsilon_o}\right) + \frac{\partial \varepsilon_1}{\partial \varepsilon_o} \frac{\partial S_o[\varepsilon_o, V]}{\partial \varepsilon_o} = 0 \tag{2.40}$$

and therefore, combining (2.35), (2.12) and (2.36) :

$$\delta S_1[1;\varepsilon_o] - \varepsilon_1 \frac{\partial}{\partial \varepsilon_o} \delta S_o[1;\varepsilon_o] - \frac{\partial \varepsilon_1}{\partial \varepsilon_o} \delta S_o[1;\varepsilon_o] = 0$$

which when replaced in (2.39) (with $F = 1$), leads to

$$\delta S[1;\varepsilon] = \left(1 - \hbar^2 \frac{\partial \varepsilon_1}{\partial \varepsilon_o}\right) \delta S_o[1;\varepsilon_o] + O(\hbar^4) \ . \tag{2.41}$$

Finally, combining (2.34), (2.39) and (2.41) one gets :

$$< F >_\varepsilon = \frac{\delta S[F;\varepsilon]}{\delta S[1;\varepsilon]} = \frac{\delta S_o[F;\varepsilon_o]}{\delta S_o[1;\varepsilon_o]} + \\ -\hbar^2 \left\{ \frac{\delta S_1[F;\varepsilon_o] - \frac{d}{d\varepsilon_o}(\varepsilon_1 \delta S_o[F;\varepsilon_o])}{\delta S_o[1;\varepsilon_o]} \right\} + O(\hbar^4) \qquad (2.42)$$

which is the semiclassical expansion for the expectation value of a one body operator. From the definition (2.33) and expressions (2.14) we find

$$\delta S_o = -\frac{1}{2} \oint \frac{F}{\sqrt{\varepsilon - V}} dz \qquad (2.43a)$$

$$\delta S_1 = \frac{1}{32} \left\{ 2 \oint \frac{V'F'}{(\varepsilon - V)^{5/2}} dz + \frac{5}{2} \oint \frac{V'^2 F}{(\varepsilon - V)^{7/2}} dz \right\} \qquad (2.43b)$$

so that after integration by parts eq.(2.42) can be rewritten as :

$$< F >_\varepsilon = \frac{\oint \frac{F}{\sqrt{\varepsilon_o - V}} dz}{\oint \frac{1}{\sqrt{\varepsilon_o - V}} dz}$$

$$-\hbar^2 \left\{ \frac{\frac{1}{24} \frac{\partial^2}{\partial \varepsilon_o^2} \left[\oint \frac{2V''F}{\sqrt{\varepsilon_o - V}} dz - \frac{\partial}{\partial \varepsilon_o} \oint \frac{V'^2 F}{\sqrt{\varepsilon_o - V}} dz \right] + \frac{1}{2} \frac{d}{d\varepsilon_o} \left(\varepsilon_1 \oint \frac{F}{\sqrt{\varepsilon_o - V}} dz \right)}{\oint \frac{1}{\sqrt{\varepsilon_o - V}} dz} \right\}$$

$$+ O(\hbar^4) \qquad (2.44)$$

And now all the contour integrations can be reduced to integrals on the real axis with the replacement

$$\oint \quad dz \quad \text{by} \quad 2 \int_{x_-}^{x_+} dx = 2 \int \; dx \; \theta[\varepsilon_o - V] \quad .$$

The use of contour integration [17] in the complex plane gives therefore an elegant and powerful method to avoid the problems related to the divergencies at the turning points encountered in conventional treatments. However when the integrals are taken along the real axis between the turning points care should be taken not to interchange the integrations with the differentiation with respect to the energy.

Perhaps the most distinctive feature of these results is that only the values of the different functions, in particular of the potential, between the turning points appear. Thus these expressions are entirely different from those that would give the conventional WKB approach where the wavefunctions are explicitly constructed using suitable connection formulae. In that case the expectation values are determined by integrals extended to all values of x. In practice we have found that the latter are always very cumbersome to use , while there is no a priori reason why they should have a better accuracy. In addition they are untractable for any further development along the lines of this paper.

2.4. *The semiclassical expansion for the matter density*

The quantal matter density $\rho(x)$ is defined as the expectation value of the operator $\delta(x-x')$. This operator does not satisfy the regularity conditions assumed to hold in the last subsection and one cannot apply directly to it the preceeding results. Therefore , following ref.[8] we define the semiclassical one body density ρ^{ε}_{sc} by requiring it to satisfy for any arbitrary , regular, function F

$$< F >_{\varepsilon} = \int \rho^{\varepsilon}_{sc}(x)F(x)dx =< \rho^{\varepsilon}_{sc},\ F > \tag{2.45}$$

with $< F >_{\varepsilon}$ given by its semiclassical expansion (2.42). The above equation allows then to obtain the power series expansion for ρ^{ε}_{sc} writing

$$\rho^{\varepsilon}_{sc}(x) = \rho^{\varepsilon}_{o}(x) + \hbar^2\rho^{\varepsilon}_{1}(x) + ... + \hbar^{2k}\rho^{\varepsilon}_{k}(x) + ... \tag{2.46}$$

and equating with the term of corresponding order in (2.44) :

$$< F >^{k}_{\varepsilon} =< \rho^{\varepsilon}_{k}, F > \tag{2.47}$$

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By looking at eq.(2.44) it is clear that, when $k = 0$, eq.(2.47) is fulfilled by a function, $\rho_o(x) \sim (\varepsilon_0 - V)^{-1/2}\theta(\varepsilon_0 - V)$ which is the Thomas-Fermi density, but that for $k \geq 1$ eq.(2.47) can only be satisfied if the ρ_k^ε are distributions, and that therefore $\rho_{sc}^\varepsilon(x)$ as defined by the expansion (2.46) has only a meaning also as a distribution. The semiclassical expressions sometimes found in the literature, see e.g. eq.(13.44) in Ref.[3], should only be employed in the argument of integrals over x and taking also proper care of not interchanging the order between integrations over x and differentiation with respect to the energy.

res onsible for that chan e and b lookin at 2.14b it can be seen that t e valu

3. The N-fermion system in the one dimensional case

3.1. *Expectation values of operators*

As discussed in Sect.(2.2), one of the essential requirements for the derivation of semiclassical expansions is the smoothing of the discontinuous behaviour with respect to the energy variable. For the ground state of the N fermion system this leads then very naturally to a second approximation of the same kind , consisting of the replacement of the sums over levels by integrals whose upper limit is the Fermi energy, ε_F. We first discuss the particularly simple example of the energy moments. These are defined as (we neglect the trivial difference between $g(E)$ and $g(\varepsilon)$ defined in eqs.(2.15)) :

$$\mu_\kappa = < \varepsilon^\kappa > \equiv \int_{-\infty}^{\varepsilon_F} \varepsilon^\kappa g(\varepsilon) d\varepsilon \ . \tag{3.1}$$

The most relevant are μ_o : the number of fermions, and μ_1, the total energy. The Fermi energy, ε_F, is fixed by requiring μ_o to equal the chosen number of particles N, and then all the other μ_κ are determined. The semiclassical expansions for these quantities are easily obtained replacing $g(\varepsilon)$ by $g_{sc}(\varepsilon)$ in (3.1).

The same applies also to the expectation values of one body operators : we replace again sums over discrete levels by integration over ε with $g(\varepsilon)$ as weighting function. Therefore we define :

$$< F > = \int_{-\infty}^{\varepsilon_F} < F >_\varepsilon \, g(\varepsilon) d\varepsilon \tag{3.2}$$

where we have used the fact that (2.11) defines $S[\varepsilon; V; \hbar]$ for any arbitrary value of ε, and that correspondingly $< F >_\varepsilon$ can also be constructed for all ε. We now notice that ε plays in these expressions the role of a dummy variable, and that this simplifies considerably the computation of $< F >$ since, contrarily to the case of $< F >_\varepsilon$ in the previous section, the energy eigenvalue does not need to be determined through (2.13) and therefore we do not need to know explicitly its $\hbar^2$ expansion. By looking at the expression for $< F >_\varepsilon$, eq.(2.34) , we see that (3.2) can be rewritten as :

Expectation values : In Table 1.b. we present the same com arison for the ex ectation

$$< F >= -\int_{-\infty}^{\epsilon_F} \frac{\delta S[F;\varepsilon]}{\frac{\partial S}{\partial \varepsilon}} g(\varepsilon) d\varepsilon \ . \tag{3.3}$$

The semiclassical expansion of (3.3) is obtained replacing $g(\varepsilon)$ by $\tilde{g}(\varepsilon) = \frac{1}{h}\frac{\partial S}{\partial \varepsilon}\theta(\varepsilon - \varepsilon_m^o)$. Using eq.(2.43) and performing elementary integrations one finds :

$$\begin{aligned} < F >_{sc} = & \frac{1}{h}\oint F\sqrt{\varepsilon_F - V}dx \\ & - \frac{\hbar}{48\pi}\left\{\frac{d}{d\varepsilon_F}\oint \frac{2FV''}{\sqrt{\varepsilon_F - V}}dx - \frac{d^2}{d\varepsilon_F^2}\oint \frac{FV'^2}{\sqrt{\varepsilon_F - V}}dx\right\} + ... \end{aligned} \tag{3.4}$$

To derive (3.4) we have put to zero the contribution of the integrand of (3.3) for $\varepsilon = \varepsilon_m$ because , as explained in Sec. 2.2, when $\varepsilon \sim \varepsilon_m$ only the first term of $g_{sc}(\varepsilon)$ has to be kept (the formula (3.4) supposes consequently $\varepsilon_F \gg \varepsilon_m$). Here again the integration contour in the complex z plane can be replaced by one on the real axis without problem since all the integrals in (3.4) are well defined on that segment. These expressions will be applied in Sec. 5 to explicit examples of well behaved one body operators, for whom we will study the accuracy of these series expansions. In the following subsections we will however discuss their applicability to two particular cases of operators : that of the matter density, already studied in the previous section, and that of the kinetic energy.

3.2. *The semiclassical expression of the matter density*

We use eq.(2.45) to define the one body density :

$$\tilde{\rho}_o(x) = \frac{1}{\pi\hbar}\sqrt{\varepsilon_F - V}\ \theta(\varepsilon_F - V) \tag{3.5a}$$

$$\tilde{\rho}_1(x) = -\frac{1}{24\hbar\pi}\left(\frac{d}{d\varepsilon_F}.\frac{2V''}{\sqrt{\varepsilon_F - V}} - \frac{d^2}{d\varepsilon_F^2}.\frac{V'^2}{\sqrt{\varepsilon_F - V}}\right)\ \theta(\varepsilon_F - V)\ , \tag{3.5b}$$

but we stress again that these semiclassical expansions cannot be used to determine r-space densities whose shapes improve on the Thomas-Fermi predictions, because the "functions" $\tilde{\rho}_n(x)$ are distributions in the mathematical sense and can only be used in the

computation of expectation values of one body operators. In this process, the derivation with respect to ε_F must be done after the $x-$ integration. This is the price to pay to have smooth level densities or more generally for using everywhere continuous functions of the energy. Formally we could have derived eqs.(3.5) by simply replacing F by $\delta(x-x')$ in eq.(3.4), but this (incorrect) procedure would have made misleading the meaning of eq.(3.5b).

3.3. *The semiclassical expression of the kinetic energy*

The kinetic energy is the expectation value of the operator p^2. From the Schrödinger equation

$$p^2\varphi = (\varepsilon - V)\varphi \tag{3.6}$$

one gets

$$< p^2 >_\varepsilon = < \varepsilon - V >_\varepsilon \ . \tag{3.7}$$

$$< p^2 > = \int_{-\infty}^{\varepsilon_F} < p^2 >_\varepsilon \, g(\varepsilon) d\varepsilon \ . \tag{3.8}$$

So that the expectation value for the N-fermion system can be easily computed from (3.3) with $F = (\varepsilon - V)$. Using again (2.43) and making suitable integrations by parts, one is left with

$$< p^2 > = \frac{1}{6\pi\hbar} \oint (\varepsilon_F - V)^{3/2} dx + \frac{\hbar}{96\pi} \oint \frac{V''}{\sqrt{\varepsilon_F - V}} dx + \ldots \tag{3.9}$$

which do not coincide with the total quantal ener contraril to what ha ens in

4 The three dimensional problem

We consider only the spherically symmetric case. Since we have used the Langer prescription [13] for the single particle levels to derive the WKB expansion, we start with a short summary of this method. Afterwards we give a quick derivation of the results analogous to those of Sections 2 and 3, stressing only the aspects specific to the three dimensional case, in particular those related to the new quantum number, the angular momentum ℓ . Due to the summation over ℓ , the δ contributions (eq.(2.26)) suppressed in the definition of the one dimensional semiclassical level density give now a smooth contribution which is therefore kept in this case.

4.1 Langer's method

The wave function for a spherically symmetric potential writes as

$$\Psi(\vec{r}) = \frac{u(r)}{r} Y_{\ell m}(\Omega) \ , \tag{4.1}$$

substitution into the three dimensional Schrödinger equation leads to the well known equation for the radial part, $u(r)$, entirely analogous to (2.1) but which contains an additional centrifugal term. The boundary conditions are however now different :

$$u(r=0) = 0 \quad \text{and} \quad u(r \to \infty) = 0 \ . \tag{4.2}$$

To make them look as in the one dimensional case, Langer introduced the change of variable

$$x = \ln r \ , \tag{4.3}$$

to make x vary from $-\infty$ to $+\infty$, and defined a new effective wave function $\tilde{\varphi}(x)$ by

$$\tilde{\varphi}(x) = e^{-x/2} u(x) \ , \tag{4.4}$$

arriving at the differential equation :

$$-\hbar^2 \, \tilde{\varphi}''_{n\ell}(x) + \left[e^{2x} \left(V(x) - \epsilon_{n\ell} \right) + \hbar^2 \, (\ell + \frac{1}{2})^2 \right] \tilde{\varphi}_{n\ell}(x) = 0 \tag{4.5}$$

The analytic form is the same already given in (5.1) but now for the three dimensional

where the derivatives are taken with respect to x. Notice that the $\ell(\ell+1)$ term in the usual Schrödinger equation has been replaced by $(\ell+\frac{1}{2})^2$ without making any approximations and that furthermore the new $\tilde{\varphi}(x)$ satisfies the same boundary conditions as in the one dimensional case. Following now closely Section 2 we make again the change of function (2.3) and get the Riccati equation :

$$-i\hbar\tilde{\chi}' = p^2 - \tilde{\chi}^2 \ , \tag{4.6}$$

with

$$p^2 = r^2[\varepsilon - \bar{V}] \tag{4.7}$$

and

$$\bar{V} = V(r) + \frac{\hbar^2}{r^2}(\ell+\frac{1}{2})^2 \ . \tag{4.8}$$

Clearly then eq. (2.5) is again the quantization condition, but now with n counting only the number of zeroes of the radial function. Expanding $\tilde{\chi}$ as in (2.7), one easily gets

$$\tilde{\chi}_0 = p = r[\varepsilon - \bar{V}]^{1/2} \tag{4.9}$$

$$\tilde{\chi}_1 = -\frac{1}{2}\frac{\frac{d}{dz}\tilde{\chi}_0}{\tilde{\chi}_0} = -\frac{1}{2}[1 - \frac{r\bar{V}'}{2(\varepsilon-\bar{V})}] \ . \tag{4.10}$$

An important remark is here in order : although $\hbar^2$ appears twice in eq.(4.5), the asymptotic expansion of $\tilde{\chi}$ has to be performed considering only the coefficient of $\tilde{\varphi}''$ as the small parameter, as in Section 2. We have to proceed in this way because it is "this" $\hbar^2$ which makes the differential eq.(4.5) singular when $\hbar$ goes to zero. The other term proportional to $\hbar^2$ is not small for high values of the angular momentum : $\frac{\hbar^2(\ell+1/2)^2}{r^2}$ is of the same order of magnitude as the potential. This double standard in dealing with terms in $\hbar^2$ has to be carefully taken into account in the derivation of the $\hbar^2$-expansion.

4.2 The first order term and the Thomas Fermi limit.

There is an action integral for each ℓ, which in lowest order is :

$$S_{0,\ell} = \oint \tilde{\chi}_0 dz = 2\int (\varepsilon - \bar{V})^{1/2}\theta(\varepsilon - \bar{V})dr \tag{4.11}$$

so that the total action integral S_0 is

$$S_0 = \sum_{\ell=0}^{\infty}(2l+1)S_{0,\ell}\ ; \tag{4.12}$$

in fact ℓ runs only from zero to an upper limit ℓ_m , the maximum ℓ for which there are values of r such that $\varepsilon - \bar{V}(r) > 0$. ($\ell$ has to be integer). Replacing the discrete sum over ℓ in (4.12) by an integral, writing $(\ell+1/2)^2 = t$ and changing the order of integration one gets the Thomas Fermi action :

$$S_{TF} = 2\int dr \int_0^{t_m} (\varepsilon - V - t\frac{\hbar^2}{r^2})^{1/2}\, dt \tag{4.13}$$

where t_m is the maximum value of t such that $(\varepsilon - V - t\frac{\hbar^2}{r^2}) > 0$. The integration over t is elementary and one finds

$$S_{TF} = \frac{1}{3\pi\hbar^2}\int (\varepsilon - V)^{3/2}\theta(\varepsilon - V)d\vec{r}\ . \tag{4.14}$$

The level density is

$$g_{TF}(\varepsilon) = \frac{\nu}{h}\frac{\partial S_{TF}}{\partial \varepsilon} = \frac{\nu}{(2\pi)^2\hbar^3}\int [\varepsilon - V(r)]^{1/2}\theta[\varepsilon - V(r)]d\vec{r} \tag{4.15}$$

which is the usual Thomas Fermi expression and where we have introduced a factor ν to account for the spin-isospin degeneracy.

Similarly, the first order matter density distribution is defined for every ℓ using (3.5a) :

$$\rho_{\ell,TF}(r) = \frac{1}{\pi\hbar}\sqrt{\varepsilon_F - \bar{V}(r)}\ , \tag{4.16}$$

and replacing again the discrete sum by an integral over ℓ one recovers the Thomas Fermi matter density

$$\rho_{TF}(r) = \frac{\nu}{6\pi^2\hbar^3}[\varepsilon_F - V(r)]^{3/2}\ . \tag{4.17}$$

In summary the Thomas Fermi results can be derived from the lowest order WKB expression replacing the discrete sums over the energies and angular momenta by integrals.

4.3 The second order terms.

The calculation is now more involved because the $\hbar_2$ error due to the summation over ℓ has to be taken into account. A clarifying example of what happens is that of the harmonic oscillator, presented in Sec. 5.2.1 .In that case the ℓ- dependence of the action allows to perform an exact summation.

We start applying to each separate ℓ the same asymptotic $\hbar^2$ expansion of the level density introduced for the one dimensional case, eq.(2.25), (2.26). Then define the total level density as:

$$g(\varepsilon) = \sum_{\ell=0}^{\infty}(2\ell+1)\; g_\ell(\varepsilon) \tag{4.18}$$

Since the g_ℓ contain an additional sum over n , we see that a double summation over two different quantum numbers has to be performed now. In the one dimensional case the sum over n was replaced by an $\hbar^2$ expansion using the Euler McLaurin summation formula, eq. (2.21). We will now use it again to perform also the sum over ℓ. In the one dimensional case there were two different kinds of $O(\hbar^2)$ terms in $g(\varepsilon)$, eq.(2.26): a) those due to the expansion of S: the S_1 terms, b) those due to the first order Euler McLaurin term in the summation over n: the third term in $g^{(2)}(\varepsilon)$. Now there is a third $O(\hbar^2)$ contribution due to the analogous expansion of the sum over ℓ; therefore we write the expansion for the level density as :

$$g(\varepsilon) = g_{TF}(\varepsilon) + \hbar^2(g_a^{(2)}(\varepsilon) + g_b^{(2)}(\varepsilon) + g_c^{(2)}(\varepsilon)) + ..., \tag{4.19}$$

where from eq. (2.26) and (4.18)

$$g_a^{(2)}(\varepsilon) = -\sum_{\ell}(2\ell+1)\frac{\partial}{\partial\varepsilon}(\frac{1}{h}S_{1,\ell}(\varepsilon)\theta(\varepsilon-\varepsilon^0_{m,\ell})) \tag{4.20}$$

$$g_b^{(2)}(\varepsilon) = -\sum_{\ell}(2\ell+1)(\frac{\pi^2}{6h}\left(\frac{\partial S_{0,\ell}}{\partial\varepsilon}\right)^{-1}_{\varepsilon=\varepsilon^0_{m,\ell}}\;\delta\,'(\varepsilon-\varepsilon^0_{m,\ell})) \tag{4.21}$$

and, as shown in Appendix A, the third contribution is:

$$g_c^{(2)}(\varepsilon) = \frac{1}{24\hbar^2}\left[\frac{\partial}{\partial\ell}\left((2\ell+1)\frac{1}{h}\frac{\partial S_{0,\ell}}{\partial\varepsilon}\theta(\varepsilon-\varepsilon^0_{m,\ell})\right)\right]_{\ell=-1/2} \tag{4.22}$$

which after a little algebra becomes:

$$g_c^{(2)}(\varepsilon) = \frac{1}{24\pi\hbar^3}\int(\varepsilon-V)^{-1/2}\theta(\varepsilon-V)dr \tag{4.23}$$

(For simplicity the factor $\theta(\varepsilon - V)$ has been suppressed from now on in the expressions). Since we are only interested in the $O(\hbar^2)$ contributions, in the first two terms in $g^{(2)}(\varepsilon)$ the sums over ℓ can be replaced by the corresponding integrals over ℓ . As shown in Appendix A, these can then be easily computed. The results are :

$$g_a^{(2)}(\varepsilon) = -\frac{1}{24\pi\hbar^3}\frac{\partial}{\partial\varepsilon}\left[2\int(\varepsilon - V)^{1/2}dr + \int \triangle V(\varepsilon - V)^{-1/2}r^2 dr - \pi\sqrt{2}r_m^2\sqrt{\overline{V}''_m}\right] \quad (4.24)$$

(where r_m and $\overline{V}''_m$ are determined by eqs. (A.3) and (A.4)), and

$$g_b^{(2)}(\varepsilon) = -\frac{\sqrt{2}}{24\hbar^3}\frac{\partial}{\partial\varepsilon}\left[r_m^2\sqrt{\overline{V}''_m}\right] \quad (4.25)$$

Adding now (4.23),(4.24) and (4.25) it is seen that the two contributions from the S_0 terms cancel exactly the first and third terms in the S_1 contribution and that the total $g^{(2)}(\varepsilon)$ takes the simpler form

$$g^{(2)}(\varepsilon) = -\frac{\nu}{96\pi^2\hbar^3}\frac{\partial}{\partial\varepsilon}\int \triangle V(\varepsilon - V)^{-1/2}d\vec{r} \quad (4.26)$$

(with ν accounting for the spin-isospin degeneracy), which is the already well known expression given by the Wigner Kirkwood expansion [4, 15]. Notice that, contrarily to the one dimensional case, where one had to neglect the δ terms in (2.26), here the second order contribution to the level density is already smooth i. e.: now we can define directly $g_{sc}^{(2)}(\varepsilon) = g^{(2)}(\varepsilon)$. The replacement of the sum over ℓ by an integration in going from (4.20), (4.21) to (4.24),(4.25) is responsible for that result . Clearly however the delta distributions remain in the higher order terms . It can be remarked that for a harmonic potential $g_a^{(2)}(\varepsilon)$ vanishes, therefore $g^{(2)}(\varepsilon)$ reduces to $g_b^{(2)}(\varepsilon) + g_c^{(2)}(\varepsilon)$. For the potentials currently used in nuclear physics, as will be shown in Sec. 5.2.2. , the contribution of $g_a^{(2)}(\varepsilon)$, generated by the anharmonic part of the potential has been found to be weak.

To complete our derivation, we finally define the semiclassical action for the three dimensional case by requiring , in analogy with eq. (2.29), that

$$g_{sc}^{(2n)}(\varepsilon) = \frac{(-1)^n}{h}\frac{\partial S_{n,sc}}{\partial\varepsilon} \quad (4.27)$$

Therefore then $S_{0,sc}$ is just S_{TF} and from eq.(4.26)

$$S_{1,sc} = \frac{\nu}{48\pi\hbar^2} \int \triangle V (\varepsilon - V)^{-1/2} d\vec{r} \tag{4.28}$$

4.4 Kinetic energy

The calculation is similar to that of section 3.3 : eq.(3.7) still holds but now p^2 is not given by the radial Schrödinger equation (4.5) : therefore V and $\bar{V}$ appear simultaneously. For instance now eq.(2.43a) becomes

$$\delta S_0 = -\frac{1}{2} \oint \sum (2\ell + 1) \frac{\varepsilon - V}{\sqrt{\varepsilon - \bar{V}}} dr \tag{4.29}$$

Replacing the discrete summation by the integral over $t = (\ell + \frac{1}{2})^2$ one gets

$$\delta S_{TF} = -2 \int \frac{r^2}{\hbar^2} (\varepsilon - V)^{3/2} \theta(\varepsilon - V) dr \tag{4.30}$$

Using (3.8)

$$< p^2 >_{TF} = \frac{2}{5\pi\hbar^3} \int r^2 (\varepsilon - V)^{5/2} \theta(\varepsilon - V) dr \tag{4.31}$$

or

$$< p^2 >_{TF} = \int \tau_{TF} d\vec{r} \tag{4.32}$$

one recovers the well known formula.

$$\tau_{TF} = \nu \frac{[\varepsilon - V]^{5/2}}{10\pi^2\hbar^3} \tag{4.33}$$

The calculation of the second order term is straigthforward : from (4.26) we obtain

$$< p^2 > = < p^2 >_{TF} + \frac{\nu}{96\pi^2\hbar} \int \Delta V [\varepsilon - V(r)]^{1/2} d\vec{r} + O(\hbar) \tag{4.34}$$

which is the already known result of the Wigner-Kirkwood expansion.

5 Results for simple potentials

To illustrate quantitatively the accuracy of the different approximations discussed in the previous Sections we shall consider now simple but realistic examples of application in nuclear physics problems. We shall present results for two simple potentials: the harmonic oscillator and the Woods Saxon well. The latter is widely used as a simple parametrization for the mean field that describes the single particle properties of the nucleons in the ground state of atomic nuclei, the former is a bit less realistic but allows to derive many analytical results. We will use it for its simplicity and as a reference to estimate the effect of the shape of the well. We shall also start our discussion with the one dimensional case, to gain understanding on the behaviour of the results, and afterwards treat the three dimensional case.

The particular forms of the equations given in the previous sections appropriate for these wells are derived in the Appendix B ; we shall use freely from those expressions in this section.

To simplify the presentation, we will show results for only two kinds of quantities : a) single particle and total energies, and b) expectation values for operators of the simple form $F = |x|^m$. The discussion of the properties of the level density, $g(\varepsilon)$, and of other expectation values is left for a future publication. We shall also discuss the convergence of the $\hbar^2$ expansion in detail for the energies , and for the expectation values we shall illustrate it only for the case of the one dimensional harmonic oscillator. Again , other cases will be dealt with in a future publication.

5.1 *One dimensional examples*

5.1.1 *The harmonic oscillator* : The potential is written as :

$$U(x) = \frac{1}{2} m \Omega^2 x^2$$

which, following the conventions introduced in Sec. 2, becomes :

$$V(x) = \frac{1}{4} \omega^2 x^2$$

where $\omega = 2m\Omega$.

Energies: This is the only case among those considered here where quantal and semiclassical results for the energies agree. As is well known the WKB method in lowest order gives already the exact result for the single particle energies, and the higher order terms in (2.37) vanish identically. Therefore in this case the total WKB energies coincide also with the quantal ones. The same is true for the Wigner Kirkwood expansion : its lowest order term (Thomas Fermi) already agrees with the quantal result, and the higher order contributions vanish. We give further details in Appendix B.

Expectation values For the expectation values of $|x|^m$ (m=1,2,3 and 4), the results both quantal and WKB are analytic and their ratio :

$$< |x|^m >_{WKB} \; / \; < |x|^m >_Q$$

is independent of the harmonic oscillator parameter (see eq.(B.9)). In Table 1.a we present these ratios for the lowest five levels : We use the notation WKB0 for the results of lowest order in the $\hbar^2$ expansion, and WKB2 for those with the contribution of the terms of $O(\hbar^2)$ included. For the $m = 2$ case the WKB results are exact, an immediate consequence of the same property for the energies. For the other values of m one finds the usual behaviour for potentials that go to infinity when $|x| \to \infty$, i.e.: as n increases the accuracy of the semiclassical approximation improves: the lowest level is poorly reproduced, but for the others the agreement is very good, improving as n rises and degrading when m increases. In all cases the $\hbar^2$ correction leads to better agreeement with the quantal values. So that although , as stressed, the convergence of the series is only asymptotic, these terms still improve on the accuracy of the expectation values and therefore should be included.

It is also clear that the remaining , $O(\hbar^4)$, discrepancies are only sizeable for the lowest n, so that for total expectation values for N fermion systems the relative accuracy of the semiclassical results will increase with N . For a N=5 system this is shown explicitly for the total expectation values again in Table 1.a. The comparison of the WKB expectation values with the quantal ones shows the very good accuracy of the semiclassical approximation

when terms up to O($\hbar 2$) are included. We shall later see that a similar agreement is also found for the Woods Saxon well, showing that for realistic examples this convergence property is little dependent on the shape of the potential. We also show the Thomas Fermi (TF) and the Wigner Kirkwood up to $O(\hbar^2)$ (WK2) predictions : as can be seen they follow closely the WKB0 and WKB2 results, but surprisingly , in this particular example, they agree even better with the quantal results than with the WKB values of which they are approximations.

5.1.2 *The Woods Saxon well :* We have chosen the standard form:

$$U_{WS}(x) = U_0(1 + \exp((x - x_0)/a))^{-1} \quad \text{for} \quad x > 0 \tag{5.1}$$

and

$$U_{WS}(-x) = U_{WS}(x)$$

To avoid any discontinuous behaviour at the origin that would make inapplicable the results of previous sections ,we have symmetrized the potential defining:

$$U_S(x) = U_{WS}(x) + U_{WS}(-x) - U_0 \tag{5.2}$$

In practice however there is no difference in the numerical results obtained by either of the above two forms and therefore in the Appendix we only quote equations for the simpler form (5.1). We have chosen the parameters so that some of the features of the results ressemble at least qualitatively those of the three dimensional case later to be discussed. Thus we have fixed U_0 = -50. MeV., a = 0.6 fm. and R_0 = 5.65 fm. (This value for the radius has been chosen to have a Fermi energy of approximately - 10. MeV. for the case of N=5 levels.)

Energies We discuss first the results for the semiclassical single particle energies $e_{\alpha,WKB}$, which now do not coincide any more with the quantal values $e_{\alpha,Q}$. The WKB energies are determined from eqs. (B.10) and (B.11) . We present in Table 2 the comparison with the quantal values obtained solving numerically the Schrodinger equation. Several remarks are in order:

a) Already at zeroth order the quantal and WKB values are very close , the second order correction being always less or at most of the order of 0.5 MeV. Again this hints at a very good convergence of the first two terms of the asymptotic series towards the quantal value. To give a more quantitative measure of the quality of these results for a N fermion system, we have introduced a "mean square deviation" defined as :

$$\sigma = \left[\sum_{\alpha=1}^{N} [e_{\alpha,Q} - e_{\alpha,WKB}]^2/N\right]^{1/2} \tag{5.3}$$

whose values , for the N=5 case as before, are also given in Table 2. They show the clear improvement in the semiclassical energies when terms of order $\hbar^2$ are included. As a further illustration of the usefulness of these quantities to determine the domains of validity of the semiclassical approximation ,we show in fig. 2a their changes when the diffuseness of the well ,a, is varied with all the remaining parameters being kept fixed (notice that a increases to the left). As expected, the more the potential ressembles a square well, the worse the semiclassical expansion becomes [17]. For values of $a \leq 0.3$ fm. the convergence of the series is very doubtful since σ_0 and σ_2 are of comparable magnitude. At $a \approx 0.2fm.$ the two curves cross , a clear indication of the asymptotic nature of the $\hbar^2$ expansion . Similar analysis can be performed varying the other parameters of the potential.

b) Going back to the values in Table 2, it is interesting to remark that , as expected, the second order contribution to the energy is large for the lowest levels, decreases up to energies of $\approx 3/4U_0$ and then changes sign and increases again in absolute value. This is apparently in contradiction with the usual "prejudice" that the lowest order semiclassical approximation improves when the energy rises, as seen e.g. in the previous example (h.o.). Mathematically this behaviour can be understood by looking at eq. (B.11) for the second order correction: since $f(0) \approx 1$ the change in sign of ε_1 happens when ε_0 is such that the numerator vanishes, i.e. when : $\varepsilon_0 \approx 3/4V_0$ in agreement with what is shown in Table 2. It is therefore the dependence on S_1 that is

responsible for that change and by looking at (2.14b) it can be seen that the value of S_1 is determined by the second derivative of the potential, V", particularly its value near the turning points, where the denominator gets larger. Since as ε_0 increases the turning points get shifted outwards and V" changes sign (it has to for potentials that tend to zero , rather than to infinity ,when $|x|$ gets large) this explains the behaviour of ε_1.

c) Due to the variation with energy of the second order correction that we just discussed, in the total energies also shown in Table 2 there is a compensation between the second order contributions from each level. Therefore the excellent agreement between quantal and WKB0 results for the total energy is in part " an accident " due to this fact (notice that the WKB0 value is closer to the quantal energy than the WKB2) . Again for different values of a the differences are plotted in Fig. 2b. Comparison with the behaviour of the σ's plotted in the same figure shows that the closeness of quantal and WKB0 energies for $a \approx 0.5$ fm. is somewhat misleading, and does not imply that the same should be true for other quantities like expectation values.

The second approximation involved in the semiclassical developments for N-fermion systems, i.e.: the replacement of the sum over discrete states by an integration over continuously varying energies (Section 3) can be checked in the same Table 2, now comparing the WKB0 values with the Thomas Fermi ones and the WKB2 with the Wigner Kirkwood up to second order prediction, WK2. This is again also done in Fig.2.c : it can be seen that this approximation implies a loss of about 0.4 to 0.5 MeV. total binding energy for all values of a. Compared to the error in the $\hbar^2$ expansion for the single particle energies this is about twice as large and of opposite sign, so that again in the WK2 estimate there is a compensation between the two errors. It is also clear that there is no point in including more terms in the Wigner Kirkwood expansion to improve on the accuracy of the results if simultaneously the effect of the oscillating terms neglected in the smoothed level density is not taken into account.

For an N fermion system expression 3.1 , with $\kappa = 0$ allows to obt

Expectation values : In Table 1.b. we present the same comparison for the expectation values as done in 1.a. for the harmonic oscillator potential. Clearly the semiclassical results are not as good as in the previous case ; as before the agreement is poorer for the lowest levels and the higher m's , but now it worsens again for the least bound levels, as already found for the single particle energies. The same discussion made for the second order correction to the energy applies here. For the total expectation values of the N=5 system we again find a much better agreement with the quantal values due to the cancellation of the level by level discrepancies of opposite signs. The $\hbar^2$ correction improves remarkably the agreement with the quantal results, as can be seen comparing the TF and WK2 total values with the latter. It is remarkable that the error introduced by the smoothing of the level density appears to be quite small: comparing the WKB0 and TF values it is seen that it amounts to $1 - 2\%$.

We conclude this analysis for the one dimensional case stressing that in both examples, for the standard choices of parameters, the $\hbar^2$ expansion converges very well, and that for these potentials the accuracy of the WKB method is excellent, particularly so for the total quantities, where the discrepancies found for the single particle levels tend to compensate. The further simplification due to the smoothing over energies reduces very little the good agreement found with the exact quantal results.

5.2 *Three dimensional examples*

5.2.1 *Harmonic oscillator :*

Energies: As for the Coulomb case, for this potential the WKB method to lowest order gives the correct single particle energies provided that the Langer correction is included. Consequently, also the total WKB energies agree with the quantal ones. Here the integration over r can be explicitly made before summing over ℓ ; therefore a direct calculation of the action for each separate ℓ can be done starting from eqs. (A.10) and (A.12). We give the results as an illustration of the Sec. 4. We have :

Expectation values : From the ex ressions for the de

$$S_0^\ell = \pi\hbar(\tfrac{\varepsilon}{\hbar\omega} - (\ell+1/2))\theta(\varepsilon - (\ell+1/2)\hbar\omega)$$
$$S_1^\ell(\varepsilon) = \tfrac{1}{6}\pi\omega\delta(\varepsilon - (\ell+1/2)\hbar\omega) \tag{5.4}$$

(in this direct calculation the S_p^ℓ contain still the θ or δ distributions , in contrast to the $S_{p,\ell}$ which are necessarily regular functions; here for instance $S_{p,\ell} = 0$ for $p \geq 1$.), and therefore from (2.13) to lowest order

$$\varepsilon_{0;n\ell} = (2n + \ell + 3/2)\hbar\omega \tag{5.5}$$

as it should. S_1^ℓ vanishes for those values, so that the $\varepsilon_{1,n\ell}$ also vanish. However if the total $S_1(\varepsilon)$ is computed replacing the sum over ℓ by an integral, then the summation over the δ terms in (5.4) gives a contribution

$$\tilde{S}_1 = \nu\frac{\pi}{3}\frac{\varepsilon}{\hbar^2\omega} \tag{5.6}$$

In addition there is a contribution of the same order in $\hbar$ coming from the Euler McLaurin correction in the summation over ℓ in S_0 , eq.(4.23). Fig. 3 illustrates the improvement on the Thomas Fermi approach due to this term (for comparison we show also the same effect in the case of the Woods Saxon potential). When these contributions are added, there is a total non vanishing contribution of $O(\hbar^2)$ to the level density. Taking that into account $g_{sc}(\varepsilon)$ is found to be

$$g_{sc}(\varepsilon) = \frac{\nu}{\hbar\omega}\left[\left(\frac{\varepsilon}{\hbar\omega}\right)^2 - \frac{1}{4}\right] \tag{5.7}$$

This $O(\hbar^2)$ contribution does not come from the improvement on the energy spectrum, but only from the summation over ℓ. As we will see in Sec. 5.2.2. this property remains almost true also when the potential is not too anharmonic.

In addition we show the total Thomas Fermi and WK2 energies, these read:

$$E_{TF} = A(\frac{6A}{\nu})^{1/3}\frac{3}{4}\hbar\Omega \tag{5.8}$$

and

$$E_{WK2} = E_{TF} + A(\frac{6A}{\nu})^{-1/3}\frac{3}{8}\hbar\Omega\ , \tag{5.9}$$

References

which do not coincide with the total quantal energy contrarily to what happens in the WKB approach. For a closed shell $N = Z$ nucleus and for large A it can be expanded in powers of $A^{-1/3}$, giving :

$$E_Q = E_{TF} + A(\frac{6A}{\nu})^{-1/3}\frac{1}{4}\hbar\Omega + \dots \quad . \tag{5.10}$$

Showing that the $O(\hbar^2)$ correction term is different for closed shell nuclei , where the shell effect is maximal , from that given by WK2, where the shell effect contribution has been smoothed. These expressions show that for this potential the genuine shell correction amounts to 1/3 of the WK2 contribution and has opposite sign.

Expectation values

Quantal and WKB0 results agree not only for $m = 2$ but also for $m = 1$. The reason for this is the following: to apply the method described in Section 2.3, see eq.(2.31), we must look for eigenvalues of the potential $V_\lambda = V + \lambda F$. When $F = r$ and $V = \frac{1}{4}\omega^2 r^2$ it is immediate that V_λ can be rewritten as:

$$V_\lambda = \frac{1}{4}\omega^2(r - r_0)^2 - \frac{1}{4}\omega^2 r_0^2$$

with $r_0 = -2\lambda/\omega^2$, so that it is again a harmonic oscillator and therefore the WKB0 eigenvalues coincide with the quantal ones. Thus from (2.31), already at lowest order, one recovers the exact expectation values.

Results for a N=Z pseudonucleus of $A = 224$ particles are shown in Table 3 for $m = 3, 4$. We find the same tendency as for the one dimensional case: the accuracy decreases with increasing m, but quantitatively it is always much better here than in the one dimensional case. The agreeement for the total WKB0 expectation values is very good, and the same is true for the TF values. Comparison with the WK2 result shows that again the $\hbar^2$ terms are relevant in improving the already very good agreement with the quantal results. We observe also that , as found in the one dimensional case, the smoothing does not modify the results by more than 1% .

5.2.2 *Woods Saxon potential :*

[14] M. Abramowitz and I. A. Ste un "Handbook of Mathematica "

The analytic form is the same already given in (5.1) but now for the three dimensional case. The parameters were taken from Ref.[5] : U_0 = -44 MeV., $x_0 = R_0 = 1.27\ A^{1/3}$fm. and a = 0.67 fm. We have checked that varying these values within reasonable limits does not change qualitatively our conclusions.

Single level energies:

To present our results we have chosen the same pseudonucleus of $A = 224$ particles as before. In Table 4 are given the single particle energies for its 12 levels. Their behaviour is very similar to the one dimensional case :

a) The WKB0 results are again very close to the quantal ones, with differences of at most 0.5 MeV, so that the value of σ (WKB0) is of the same order as that for the one dimensional case.

b) The second order correction is also largest for the lowest levels and changes sign again at about 3/4 U_0, even though now the contribution of the centrifugal term makes a little more involved the study of this behaviour. The energy dependence of the correction is shown in Fig. 4, where values with the same n but different ℓ have been joined by continuous lines : it can be seen that these are practically straight, and that their slope decreases slightly with ℓ.

Total energies :

a) Now the WKB2 estimate for the total energies is better than the WKB0 value . The compensation between contributions of opposite sign found in the one dimensional case here applies only to the levels with the lowest ℓ, whereas those that give the most important contribution to the total energy , the ones with larger ℓ since they contain the largest number of particles, have all corrections of the same sign.

b) Another striking difference with the one dimensional case is that while the WKB0 and WKB2 single particle spectra are very close to the quantal , the relative differences between the two WKB total energies and the quantal are - 0.91% and 0.14%

Figure Captions

respectively, the same relative differences are 2.57% and 0.09% for the Wigner Kirkwood at zeroth and second order v.s. the quantal value. Obviously the smoothing of the summation over the discrete quantum numbers is responsible for the differences between these pairs of values, but why the role of the smoothing is so important at the Thomas Fermi order ? Or more precisely : i) why is WKB0 so good and Thomas Fermi so bad ? ii) how is it that WKB2 and WK2 are so similar ? To understand that we have to go back to Sec. 4 where $g(\varepsilon)$ was calculated. If we add to $g_{TF}(\varepsilon)$ that part of $g^{(2)}(\varepsilon)$ due to the S_0 terms

$$\Delta g^{(2)}(\varepsilon) = g_b^{(2)}(\varepsilon) + g_c^{(2)}(\varepsilon),$$

eqs. (4.23), (4.25),i.e. if we consider only the WKB0 spectrum but include properly the $\hbar^2$ Euler Mc Laurin correction coming from the smoothing on the quantum numbers, we can construct a level density : $g_{TF}(\varepsilon) + \Delta g^{(2)}(\varepsilon)$ which leads , after integration, to an energy $E_{TF} + \Delta E_o^{(2)}$ given at the bottom of Table 4. The relative difference between this new energy and the quantal is -0.85% . This improvement, from 2.57% to -0.85%,is not at all due to a change in the spectrum (the same WKB0 is used in the two cases), but to a more careful estimate of the sum over the level energies that includes the $\hbar^2$ Euler McLaurin correction. In this respect the harmonic oscillator is an extreme case : the WKB0 spectrum is already exact but $g_{sc}(\varepsilon)$ has to incorporate an $\hbar^2$ correction of the type $\Delta g^{(2)}$ discussed above. *This shows that there is no term to term correspondence between the WKB and WK $\hbar^2$ expansions.*

Thirty years ago, March and Plaskett [16] performed a similar analysis, finding all the contributions due to the lowest WKB0 terms (those given by our $\Delta g^{(2)}(\varepsilon)$) . They were however unable to include the anharmonic contribution , $g_a^{(2)}$, and therefore missed the connection between WKB and the Wigner Kirkwood expansion (in this respect it is illustrative to read the last paragraph in their Sec. 7).

Expectation values :

Table Ca ti

The overall agreement between quantal and WKB0 results is very good, and again it is best for the lowest m. Thus, e.g. the r.m.s. radius is predicted with only a 4% error using WKB0. The agreement for the lowest m does not show any significant dependence on n or ℓ, for $m = 4$ however the WKB0 results are slightly worse for the highest n, probably due to the same reasons already given for the energies of the least bound levels. Whereas the results for the lowest m are of comparable accuracy to those for the harmonic oscillator potential, for the largest m they are somewhat less accurate, a trend also found in the one dimensional case.

Table 1.a

6 Summary and conclusions

We have presented a new derivation of the semiclassical expansions for the observables of a N-fermion system starting from the well known WKB expansion for the energy of a single level and the somewhat less familiar expressions for the expectation values. We have shown how in the semiclassical approach the "smallness" of $\hbar$ is exploited twice: i) to make the level density distribution continuous, ii) to obtain it explicitly as an $\hbar^2$ expansion. In the first step use was made alternatively of the Poisson formula or of the Euler McLaurin expansion. For the second step the elegant WKB formalism of Dunham has been shown to be the most appropriate.

In the derivation of the Wigner Kirkwood method where truncated expansions of Laplace transforms are used , both of the above steps are done simultaneously. Their advantage is that the derivation holds even for non spherically symmetrical three dimensional systems. But apart from adding more terms in the $\hbar^2$ expansion, which becomes cumbersome (and perhaps is not desirable because of the asymptotic nature of the expansion), this method cannot be improved upon. Furthermore the usual derivation leads to diverging quantities (at the turning points) whose meaning is not clear. Our work gives a well defined prescription to deal with these terms. In particular we have shown that the price to pay for having changed the level density from a distribution to a continuous function is that the matter density is conversely changed from a regular function to a distribution. To deal with the difficulties in the computation of expectation values using this matter density, the method due to Dagens has been developped and in this way the problems with turning points have been avoided.

We have discussed separately the one dimensional and the three dimensional cases, the latter only when there is spherical symmetry. Using the Langer prescription we have recovered the Wigner-Kirkwood expansion for the three dimensional case, and have discussed also the appropriate smoothing over the angular momentum quantum numbers. Beyond the lowest order the three dimensional case has been shown to be a non trivial extension of the one dimensional case because of the additional summation over ℓ , which introduces

Table 2

further $\hbar^{(2n)}$ contributions. From all of this emerges a much clearer picture of the role of each of the separate approximations required to recover the standard semiclassical results for confined fermion systems such as atoms and nuclei. The accuracy of each of those can then be tested separately. This has been done in the last Section for selected nuclear potentials. Developping the work of March and Plaskett we have explained why the Thomas Fermi energy is so inaccurate in comparison to the WKB energy to the same order. Indeed the accuracy of the WK expansion truncated at second order is not mainly due to the improvement on the energy spectrum (going from zeroth to second order WKB) but to a better accounting of the error due to the smoothing of the sum over quantum numbers. This implies that in applications accurate results can be already obtained with a zeroth order WKB calculation with a proper treatment of the discrete summations.

Among the extensions suggested by this work on the semiclassical expansion, we intend to focus in the future on systematic ways to improve on it, and particularly in the two following lines :

i) introduction of semiclassical "quantum oscillations" by including additional terms in the Poisson formula. For the matter density this inclusion has already proved its interest in a model calculation [12].

ii) extension of our work to the WKB-like method of Comtet [18]. Although not fully understood at the theoretical level, this method turns out to be closer to the quantum results than the standard WKB, in particular it is exact for the Morse potential ($V = V_o/cosh(\alpha x^2)$). This gives hope that it will give a good approximation for the level density near the continuum.

Table 3

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Table 4

A The semiclassical level density in three dimensions :

When the sum over ℓ in (4.18) is approximated using the Euler McLaurin summation formula of eq. (2.20) the second non-vanishing term in this expansion for an arbitrary function $F(\ell)$ is :

$$-\frac{1}{24}[F'(\ell)]_{\ell=-1/2}^{\ell=\infty}$$

which in our case gives :

$$g_c^{(2)}(\varepsilon) = -\frac{1}{24\hbar^2}\left[\frac{\partial}{\partial \ell}\left((2\ell+1)\frac{1}{h}\frac{\partial S_{0,\ell}}{\partial \varepsilon}\theta(\varepsilon-\varepsilon^0_{m,l})\right)\right]_{\ell=-1/2}^{\ell=\infty} \qquad (A.1)$$

where we have only included the $g_{0,\ell}(\varepsilon)$ because we only need the $O(\hbar^2)$ contribution. Due to the $\theta(\varepsilon-\varepsilon^0_{m,\ell})$ factor, the contribution of the $\ell=\infty$ term is nil and the lower limit gives :

$$g_c^{(2)}(\varepsilon) = \frac{1}{24\pi\hbar^3}\left(\frac{\partial S_{0,\ell}}{\partial \varepsilon}\right)_{\ell=-1/2} \qquad (A.2)$$

which using (4.11) becomes (4.23).

The other two contributions of $O(\hbar^2)$, eqs. (4.20) and (4.21), can be straighfordwardly computed once the sums over ℓ are replaced by integrals.

We first compute $g_b^{(2)}$. For that purpose one has to evaluate

$$\frac{\partial S_{0,\ell}}{\partial \varepsilon} = \frac{1}{2}\oint(\varepsilon-\overline{V})^{-1/2}dz \qquad (A.3)$$

at the limit $\varepsilon = \varepsilon^o_{m,\ell}$, where

$$\varepsilon^0_{m,\ell} = \overline{V}(r_m) = V(r_m) + \hbar^2\frac{t}{r_m^2} \qquad (A.4)$$

and r_m is such that

$$V'(r_m) - 2\hbar^2\frac{t}{r_m^3} = 0 \qquad (A.5)$$

where $t = (\ell+1/2)^2$.

Table 5

For ε sufficiently close to $\varepsilon^0_{m,\ell}$ the integration contour can be chosen very close to the minimum and $\overline{V}$ can be replaced by a Taylor expansion around r_m so that

$$(\varepsilon - \overline{V}(z))^{1/2} = i\sqrt{\frac{\overline{V}''(r_m)}{2}}(z - r_m) \tag{A.6}$$

and the integral becomes :

$$\left(\frac{\partial S_{0,\ell}}{\partial \varepsilon}\right)_{\varepsilon=\varepsilon^0_{m,\ell}} = \pi\sqrt{\frac{2}{\overline{V}''}} \tag{A.7}$$

Using this result $g_b^{(2)}(\varepsilon)$ can be written as :

$$g_b^{(2)}(\varepsilon) = -\frac{1}{24\hbar}\int_{t=0}^{\infty} dt\ \sqrt{2\overline{V}''(r_m)}\ \delta'(\varepsilon - \varepsilon^0_{m,\ell}) \tag{A.8}$$

From eq.(A.4) we get the t dependence of $\varepsilon^0_{m,\ell}$ and r_m ;introducing the appropriate change of variables the integration is easily performed and one finds

$$g_b^{(2)}(\varepsilon) = -\frac{\sqrt{2}}{24\hbar^3}\frac{\partial}{\partial\varepsilon}\left(r_m^2(\varepsilon)\ \sqrt{\overline{V}''(r_m(\varepsilon))}\right) \tag{A.9}$$

where $r_m^2(\varepsilon)$ is determined solving eqs. (A.3) and (A.4) when $\varepsilon^0_{m,\ell} = \varepsilon$.

For the evaluation of $g_a^{(2)}(\varepsilon)$, eq. (4.20), in analogy with what was done for the Thomas Fermi expressions, from eqs. (4.11) to (4.15), we first compute the total action integral S_1 : We start considering the second order WKB term and sum over ℓ. Eqs (2.8) and (2.12) then lead to

$$S_{1,\ell} = \oint \tilde{\chi}_2 dz = \frac{1}{2}\oint \frac{\tilde{\chi}_1^2}{\tilde{\chi}_0} dx\ . \tag{A.10}$$

Combining with eq.(4.10) one gets

$$S_{1,\ell} = \frac{1}{8}\oint \frac{[1 - \frac{r\bar{V}'}{2[\varepsilon-\bar{V}]}]^2}{r^2(\varepsilon - \bar{V})^{1/2}}\, dr \tag{A.11}$$

which gives, after integration by parts, the formula already derived by Dagens [8]

$$S_{1,\ell} = -\frac{1}{2}\oint \frac{dr}{(\varepsilon - \bar{V})^{1/2}}\frac{1}{4r^2} + \frac{1}{24}\frac{d}{d\varepsilon}\oint \frac{\bar{V}''}{(\varepsilon - \bar{V})^{1/2}} dr \tag{A.12}$$

Replacing the discrete summation over ℓ by an integral one obtains

$$\tilde{S}_1 = \frac{1}{48\pi\hbar^2}\int \frac{\Delta V}{\sqrt{\varepsilon - V}}\theta(\varepsilon - V)d\vec{r} + \frac{1}{6\hbar^2}\int \sqrt{\varepsilon - V}\,\theta(\varepsilon - V)dr \tag{A.13}$$

$$-\frac{\sqrt{2}\pi}{12\hbar^2}r_m^2(\varepsilon)\sqrt{\overline{V}''(r_m(\varepsilon))}.$$

whose last term is again due to the pole in $(\varepsilon - \overline{V})^{-1/2}$ but now when $\ell \to \ell_m$ for a fixed energy. From this result, differentiation with respect to ε leads immediately to the expression for $g_a^{(2)}(\varepsilon)$, eq. (4.24).

B One dimensional potentials :

B.1.1.*Harmonic oscillator :*

The expressions for $S_0(\varepsilon, V)$ and $S_1(\varepsilon, V)$ can be easily derived from eqs. (2.14). Writing

$$V(x) = \frac{1}{4}\omega^2 x^2 \tag{B.1}$$

it is immediate that :

$$S_0(\varepsilon, V) = \frac{2\pi\varepsilon}{\omega} , \tag{B.2}$$

in addition, S_1 can be written as

$$S_1(\varepsilon, V) = \frac{1}{24}\omega^2 \frac{d^2}{d\varepsilon^2} S_0(\varepsilon, V) \tag{B.3}$$

and is therefore nil. From (2.29) one then gets

$$g_{sc}(\varepsilon) = (\hbar\omega)^{-1} \tag{B.4}$$

and therefore, using (3.1),

$$\varepsilon_F = N\hbar\omega \tag{B.5}$$

and

$$\varepsilon_{TF} = \varepsilon_{WK2} = \frac{1}{2}N^2\hbar\omega . \tag{B.6}$$

This is identical to the quantal result, since :

$$\varepsilon_Q = \sum_{n=0}^{N-1}(n + \frac{1}{2})\hbar\omega = \frac{1}{2}N^2\hbar\omega . \tag{B.7}$$

We now compute the expectation values of $< |x|_m >$. The WKB quantities are found using eq. (2.44). All these expressions are analytic, so that the ratios

$$R =< |x|^m >_{WKB} / < |x|^m >_Q \tag{B.8}$$

can be written explicitly. For simplicity we give only these for the first three levels and to lowest order in $\hbar^2$ (it is interesting to remark however that for m=1 the second order contribution is always nil):

$$\begin{aligned} R_{n=0} &= 1/\Gamma(\frac{m+2}{2}) \\ R_{n=1} &= \frac{1}{\Gamma(\frac{m+2}{2})}\frac{3^{m/2}}{m+1} \\ R_{n=2} &= \frac{5^{m/2}}{\Gamma(\frac{m+2}{2})(\frac{m^2+2m+2}{2})} \end{aligned} \tag{B.9}$$

Using eq. (3.4) the Thomas Fermi expectation values are easily computed. It is immediate to check that again $< x^2 >_{TF} =< x^2 >_Q$ and the expressions for the other m are very simple, thus e.g. $< x^4 >_{TF} = 2/N < x^2 >^2_{TF}$.

B.1.2. *Woods Saxon potential :*

It is possible to obtain analytical expressions for $S_0(\varepsilon, V)$ and $S_1(\varepsilon, V)$:

$$\begin{aligned} S_0(\varepsilon, V) &= 4a\left\{\frac{2\varepsilon}{\sqrt{-\varepsilon}}\tan^{-1}\left(\sqrt{\frac{\varepsilon - V_0 f(0)}{-\varepsilon}}\right) - \sqrt{\varepsilon - V_0}\ln\left|\frac{\sqrt{\varepsilon - V_0 f(0)} - \sqrt{\varepsilon - V_0}}{\sqrt{\varepsilon - V_0 f(0)} + \sqrt{\varepsilon - V_0}}\right|\right\} \\ S_1(\varepsilon, V) &= \frac{1}{6a}\left\{(\varepsilon - V_0 f(0))^{1/2}\frac{16}{5V_0} + (\varepsilon - V_0 f(0))^{-1/2}(-1 + \frac{6f(0)}{5} + \frac{4\varepsilon}{5V_0})\right\} \end{aligned} \tag{B.10}$$

where $f(0) = [1 + e^{-r_0/a}]^{-1}$. Then the energy in lowest order is given implicitly by (2.13) with S replaced by S_0:

$$S_0(\varepsilon, V) = (n + 1/2)h$$

This equation is solved using the Raphson Newton method. The $O(\hbar^2)$ correction, $\hbar^2\varepsilon_1$, is given by (2.38) and reads:

$$\varepsilon_1 = \frac{1}{24a^2}\frac{(4\varepsilon_0/V_0 - 2f(0) - 1)/(\varepsilon_0 - V_0 f(0))^{1/2}}{\frac{1}{\sqrt{-\varepsilon_0}}\tan^{-1}\sqrt{\frac{\varepsilon_0 - V_0 f(0)}{-\varepsilon_0}} - \frac{1}{\sqrt{\varepsilon_0 - V_0}}\ln\left|\frac{\sqrt{\varepsilon_0 - V_0 f(0)} - \sqrt{\varepsilon_0 - V_0}}{\sqrt{\varepsilon_0 - V_0 f(0)} + \sqrt{\varepsilon_0 - V_0}}\right|} \tag{B.11}$$

For an N fermion system expression (3.1), with $\kappa = 0$ allows to obtain the Fermi energy, ε_F^0, solving again an equation analogous to the one above for the ε_0 energies. The correction of order $\hbar^2$ is also given by an expression similar to (B.11). The same equation (3.1) gives the total energy when κ =1. To lowest order , Thomas Fermi, we find

$$\begin{aligned}\varepsilon_{TF} &= N\varepsilon_F^0 - \frac{8a}{3\pi\hbar}\left[V_0(\varepsilon_F^0 - V_0 f(0))^{1/2} + (-\varepsilon_F^0)^{3/2}\tan^{-1}\left(\sqrt{\frac{\varepsilon_F^0 - V_0 f(0)}{-\varepsilon_F^0}}\right)\right. \\ &\left. -\frac{1}{2}(\varepsilon_F^0 - V_0)^{3/2}\ln\left|\frac{\sqrt{\varepsilon_F^0 - V_0} - \sqrt{\varepsilon_F^0 - V_0 f(0)}}{\sqrt{\varepsilon_F^0 - V_0} + \sqrt{\varepsilon_F^0 - V_0 f(0)}}\right|\right] \qquad (B.12)\end{aligned}$$

and, using the first two terms of the semiclassical expansion of $g(\varepsilon)$,we obtain the Wigner Kirkwood energy to order $\hbar^2$:

$$\begin{aligned}\varepsilon_{WK2} &= \varepsilon_{TF} + \frac{\hbar}{2\pi}\left[\frac{8}{45aV_0}(\varepsilon_F^0 - V_0 f(0))^{3/2} + \right. \\ &+\frac{1}{3a}(\varepsilon_F^0 - V_0 f(0))^{1/2}(-1 + \frac{6f(0)}{5} - \frac{4\varepsilon_F^0}{5V_0}) + (\varepsilon_F^0 - V_0 f(0))^{-1/2}.\frac{\varepsilon_F^0}{6a}\cdot \\ &\left.(1 - \frac{6f(0)}{5} - \frac{4\varepsilon_F^0}{5V_0})\right] + \frac{\hbar}{\pi}\varepsilon_F^1\varepsilon_F^0.2a\left[\frac{1}{\sqrt{-\varepsilon_F^0}}\tan^{-1}(\sqrt{\frac{\varepsilon_F^0 - V_0 f(0)}{-\varepsilon_F^0}})\right] \qquad (B.13) \\ &-\frac{1}{2\sqrt{\varepsilon_F^0 - V_0}}\ln\left|\frac{\sqrt{\varepsilon_F^0 - V_0} - \sqrt{\varepsilon_F^0 - V_0 f(0)}}{\sqrt{\varepsilon_F^0 - V_0} + \sqrt{\varepsilon_F^0 - V_0 f(0)}}\right|\end{aligned}$$

B.2 Three dimensional potentials :

The expression for the TF density is given in (4.17), that for WK2 can be easily derived from the expressions (4.28) for $S_{1,sc}$, and has been given many times in the literature [3,5]. The same is true for the energies. We only summarize the most useful expressions.

B.2.1. *Harmonic oscillator potential :*

We only discuss the expectation values, since the expressions for the energies are well known.

Expectation values : From the expressions for the densities one easily gets:

$$< r^m >_{TF} = \frac{\nu}{4\sqrt{\pi}} (\frac{\varepsilon_F}{\hbar^2})^{3/2} r_t^{m+3} \frac{\Gamma(\frac{m+3}{2})}{\Gamma(\frac{m+8}{2})} \qquad (B.14)$$

where the value of r_t, the turning point , is given by:

$$r_t = 2\frac{\sqrt{\varepsilon_F}}{\omega} \qquad (B.15)$$

For the contribution of the $\hbar^2$ term we find:

$$\delta < r^m >= \frac{\nu(m-3)}{3\sqrt{\pi}} 2^{\frac{m}{2}-2} (\frac{6A}{\nu})^{\frac{m}{6}+\frac{1}{3}} \frac{\Gamma(\frac{m+3}{2})}{\Gamma(\frac{m+4}{2})} (\frac{2\hbar}{\omega})^{m/2} , \qquad (B.16)$$

and care should be taken when evaluating the WK2 expectation values to compute the TF contribution with a Fermi energy that includes the second order correction:

$$\delta\varepsilon_F = \frac{(\hbar\omega)^2}{4\varepsilon_F^o} \qquad (B.17)$$

Woods Saxon potential :

Here all results have to be obtained numerically. We only comment on the computation of the second order correction to the single particle energies. Using the expression analogous to (2.38) for the three dimensional case, we find:

$$\varepsilon_1 = \frac{1}{8} \frac{\oint \frac{[\varepsilon - V - \frac{1}{2}rV']^2}{[\varepsilon - V - \frac{\hbar^2(\ell+1/2)^2}{r^2}]^{5/2}} \frac{dr}{r^2}}{\frac{\partial}{\partial\varepsilon} \oint [\varepsilon - V - \frac{\hbar^2(\ell+1/2)^2}{r^2}]^{1/2} dr} \qquad (B.18)$$

The contour integral in the numerator cannot be replaced directly by one along the real axis due to the divergences at the turning points. If we rewrite it in a way similar to that in the denominator or to (2.44) taking out derivatives with respect to the energy, we end up having to compute numerically third derivatives, and that is very inaccurate. Thus we have performed the integration directly in the complex plane following for instance the method of ref. [19].

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Figure Captions

Fig. 1 Particle number as a function of ϵ for the quartic oscillator. The step function corresponds to the quantal result , the continuous line to the Poisson formula respectively up to the 1^{st} and 6^{th} terms.

Fig. 2 One dimensional Woods Saxon potential. a) Variation of the mean square deviations of the single level energies, eq. (5.3), with the diffuseness of the well. b) Same but for the differences between total WKB and quantal energies. c) Same for the differences between Thomas Fermi or Wigner Kirkwood and corresponding WKB total energies.

Fig. 3 Values of $\sum(2\ell+1)S_0^\ell/S_{TF}$ as a function of ϵ. Full line : discrete summation, dash-dotted line : Euler McLaurin correction.

a) Case of the harmonic potential

b) Case of the Woods-Saxon potential

Fig. 4 Second order correction to the single particle energy versus the WKB0 energy for the levels of the A=224 pseudonucleus in a three dimensional Woods Saxon potential (the values of the parameters are given in the text) . Circles : n=1 levels, squares : n=2 levels and stars n=3 levels. The lines are drawn only to guide the eye.

Table Captions

Table 1 One dimensional potentials: a) harmonic oscillator, b) Woods Saxon. Ratios of WKB to quantal expectation values of $|x^m|$ for each single particle level (upper part), and for the N=5 system (lower part). The results for the Thomas Fermi and Wigner Kirkwood $O(\hbar^2)$) approximations are given in the lowest row. In Table 1.b only the WKB0 results for the single particle levels are shown.

Table 2 Single particle (upper part) and total binding energies (lower part) , in MeV. , for the one dimensional Woods Saxon potential (the values of the parameters are given in the text). Also shown are the values of σ, eq.(5.3), and in the last row the Thomas Fermi and Wigner Kirkwood $O(\hbar^2)$ total binding energies.

Table 3 Three dimensional harmonic oscillator potential. Upper rows: ratios of WKB0 to quantal expectation values of $|r^m|$ for each single particle level. Lower rows : ratios of total expectation values for the A=224 pseudonucleus in the three semiclassical approximations, WKB0, Thomas Fermi and Wigner Kirkwood $O(\hbar^2)$, to the quantal values.

Table 4 Same as in Table 2 but now for the three dimensional Woods Saxon potential. In the last two rows the Thomas Fermi, Thomas Fermi + $\Delta E_o^{(2)}$ and WK2 total binding energies are shown. The values of the parameters are given in the text.

Table 5 Same as in Table 3 but for the three dimensional Woods Saxon potential.

Table 1.a

m =	1		2		3		4	
	WKB0	WKB2	WKB0	WKB2	WKB0	WKB2	WKB0	WKB2
n								
0	1.13	1.13	1.	1.	0.75	0.85	0.50	0.75
1	0.98	0.98	1.	1.	0.98	0.99	0.90	0.95
2	1.01	1.01	1.	1.	0.99	0.99	0.96	0.98
3	1.00	1.00	1.	1.	1.00	1.00	0.98	0.99
4	1.00	1.00	1.	1.	1.00	1.00	0.99	1.00
Totals								
	1.01	1.01	1.	1.	0.99	0.99	0.97	0.99
	TF	WK2	TF	WK2	TF	WK2	TF	WK2
	1.00	1.00	1.	1.	0.99	1.01	0.98	1.01

Table 1.b

	m =	1	2	3	4
	n				
	0	1.03	0.89	0.69	0.49
	1	0.86	0.83	0.80	0.74
	2	0.98	0.92	0.88	0.84
	3	0.99	0.99	0.97	0.94
	4	1.04	1.05	1.05	1.03
Totals					
	WKB0	0.98	0.96	0.95	0.93
	T-F	0.99	0.97	0.95	0.91
	WK2	1.00	1.01	1.01	1.01

Table 2

		Quantal	WKB0	WKB2
e_n	n			
	0	48.13	48.68	48.09
	1	42.99	43.28	43.04
	2	35.43	35.41	35.48
	3	26.19	25.86	26.25
	4	16.05	15.46	16.09
σ			0.41	0.05
E_T		168.79	168.69	168.95
			TF	WK2
			168.33	168.48

Table 3

	m =	3	4
	1 s	0.95	0.86
	1 p	0.97	0.94
	1 d	0.99	0.97
	1 f	0.99	0.98
	1 g	0.99	0.98
	1 h	1.00	0.99
	2 s	0.98	0.96
	2 p	0.99	0.97
	2 d	0.98	0.97
	2 f	0.98	0.97
	3 s	0.99	0.98
	3 p	0.99	0.98
Totals			
	WKB0	0.99	0.97
	TF	0.98	0.97
	WK2	1.00	1.01

Table 4

	Quantal	WKB0	WKB2
1 s	40.13	40.50	40.12
1 p	36.34	36.61	36.34
1 d	31.76	31.90	31.78
1 f	26.50	26.49	26.53
1 g	20.62	20.45	20.66
1 h	14.20	13.85	14.26
2 s	30.07	30.09	30.08
2 p	23.91	23.77	23.93
2 d	17.35	17.06	17.37
2 f	10.54	10.09	10.56
3 s	16.19	15.86	16.19
3 p	9.01	8.55	9.01
σ		0.29	0.03
E_T	4563.5	4521.9	4569.7
		TF	
		4680.6	
		TF + $\Delta E_o^{(2)}$	WK2
		4524.8	4567.4

Table 5

Expectation values : Ratios R_n (Woods Saxon potential)

	m =	1	2	3	4
	1 s	0.97	0.98	1.00	1.01
	1 p	0.97	0.96	0.96	0.95
	1 d	0.98	0.96	0.95	0.94
	1 f	0.98	0.96	0.95	0.93
	1 g	0.98	0.96	0.94	0.92
	1 h	0.98	0.96	0.94	0.92
	2 s	0.98	0.96	0.94	0.92
	2 p	0.98	0.96	0.94	0.92
	2 d	0.98	0.96	0.93	0.90
	2 f	0.98	0.96	0.93	0.90
	3 s	0.98	0.95	0.92	0.89
	3 p	0.98	0.96	0.92	0.88
Totals					
	WKB0	0.98	0.96	0.94	0.91
	T-F	1.00	0.98	0.95	0.91

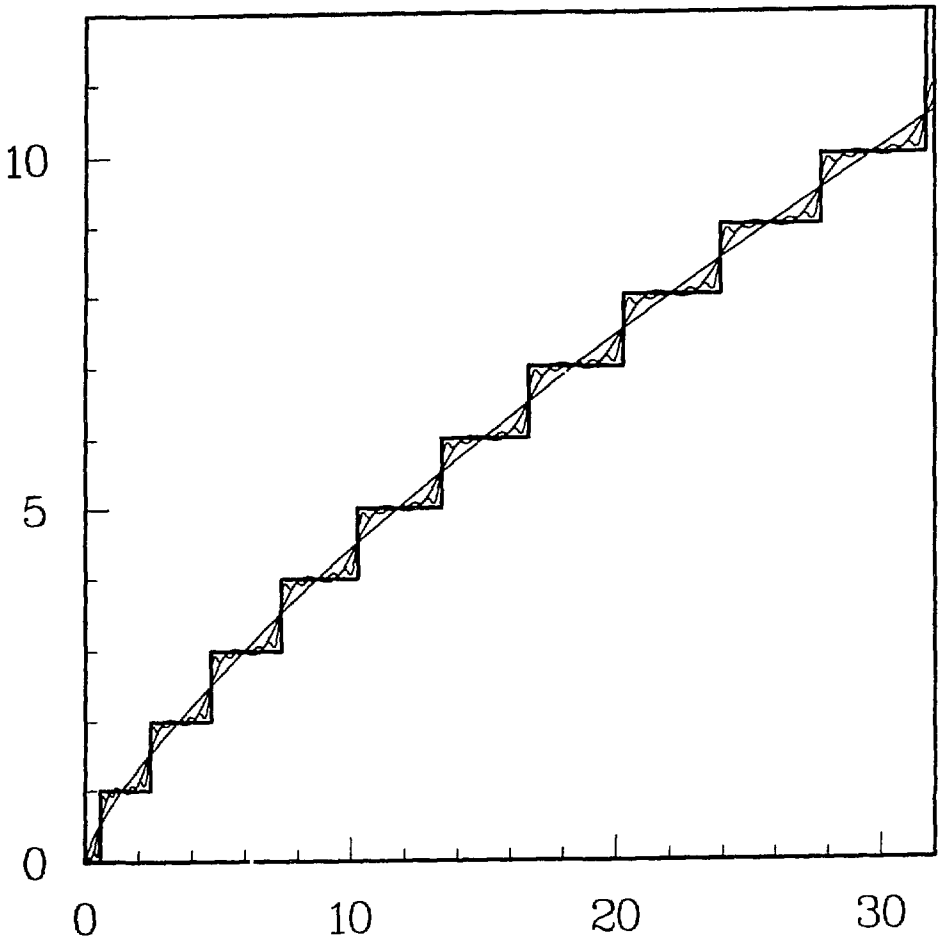


FIG.1

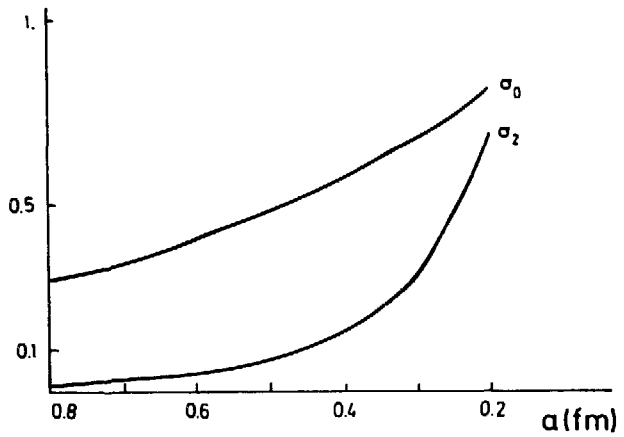
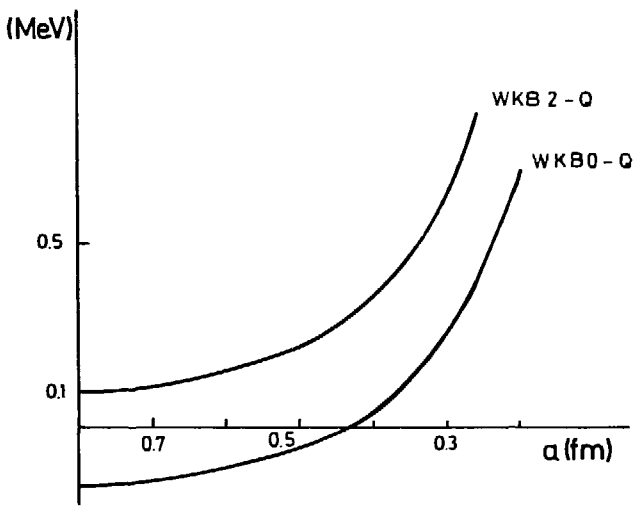


Fig. 2a



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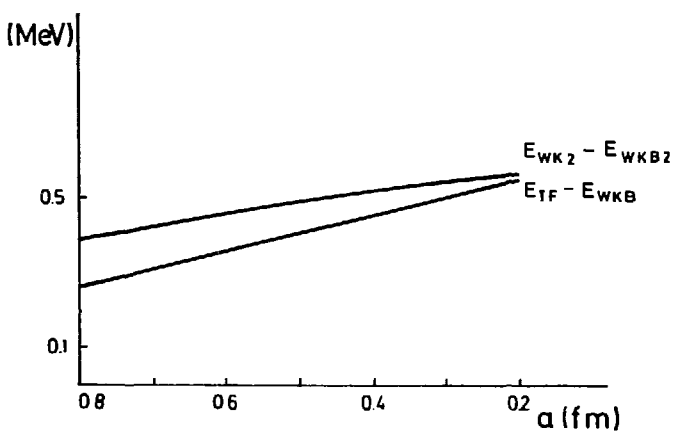

Fig. 2c

Harmonic Oscillator

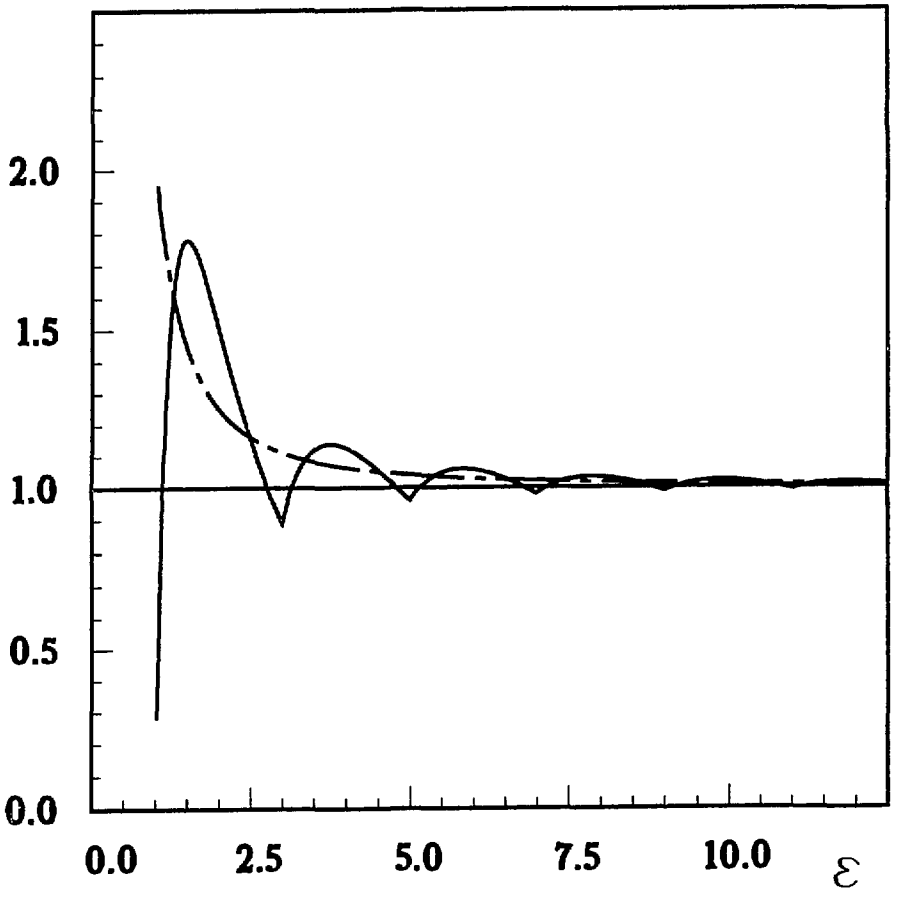

Fig. 3a

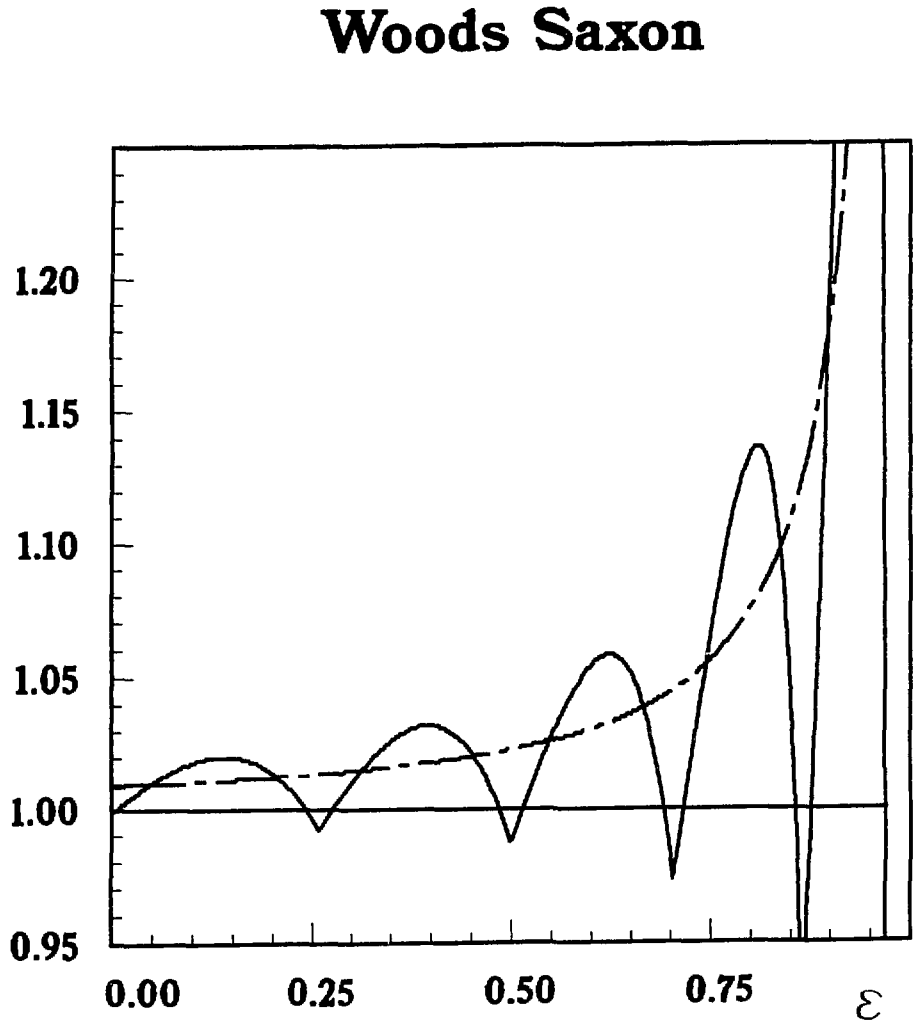

Fig. 3b

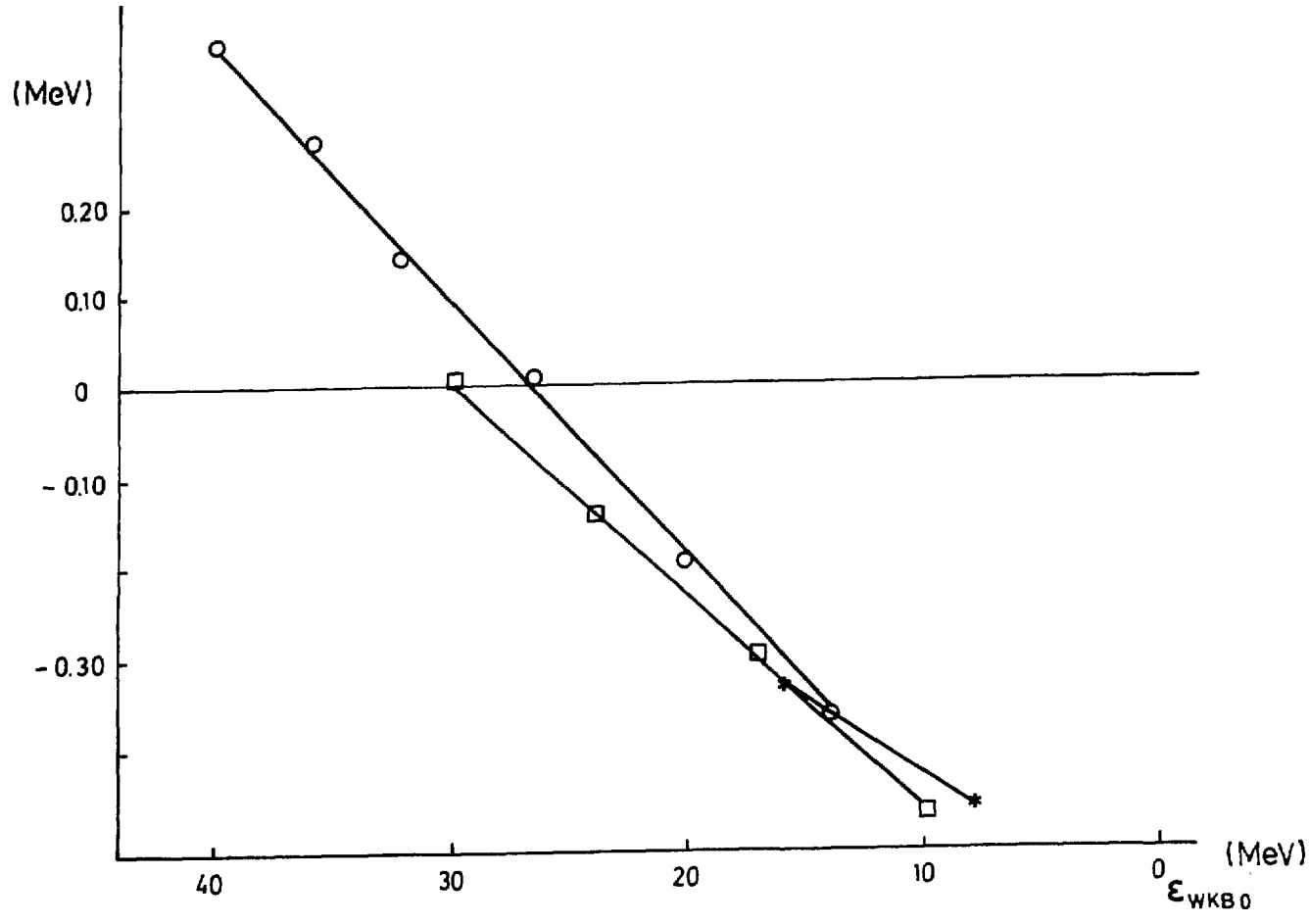

FIG.4