Semiclassical Approximation in a One-Body Potential

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For a system of noninteracting fermions in a local potential with no discontinuous edges, an explicit series in the expansion parameter $\hbar^2$ is derived for the "smooth" part of the energy. The method is based on the semiclassical partition function developed by Wigner and Kirkwood. Numerical calculations are done for spherical and deformed Woods-Saxon potentials. Comparisons are made with other methods, and in particular the numerical accuracy of the Strutinsky smoothing is tested.

It is well known[1,2] that one can extract the dominant contribution of shell effects to nuclear masses by considering the nucleons to be moving in a realistic one-body shell-model–type potential. One calculates in this potential the sum of the occupied single-particle energies, and substracts from it the part that varies smoothly with particle number and deformation. In the widely used Strutinsky method,[2] this smooth part is obtained by smearing the eigenenergies in the energy space, and in finite potentials this involves smearing over a set of suitably chosen artificial unbound states in the continuum.[3,4] In another approach, advocated by Bohr and Mottelson,[5] one examines the asymptotic form of the energy for large spatial dimension of the potential, and writes the smooth energy as a sum of terms proportional to the volume, surface area, etc. Siemens and Sobiczewski[6] have calculated the first two terms of this series for a spherical Woods-Saxon potential. In this note we shall develop an alternative method which emphasizes the semiclassical nature of this so-called smooth energy.

For a one-body potential that has no discontinuous edges, we shall derive an accurate and readily calculable expression for this energy in a power series of $\hbar^2$, involving the potential and its derivatives. In this note we shall only consider a local attractive potential which may be spherical or deformed, and omit the spin-orbit and Coulomb potentials. The Coulomb potential is excluded only for the sake of simplicity, but nontrivial modifications are necessary to take account of the spin-orbit part. These are feasible, and detailed practical calculations will be published elsewhere.

We use the partition-function[7-9] approach to arrive at the semiclassical series for the energy. The semiclassical partition function was written down by Wigner[10] and Kirkwood[11] more than forty years ago, and has been used, amongst other applications, in obtaining higher-order corrections to the classical second virial coefficient.[12] For a given potential $U(\vec{r})$, the one-body semiclassical partition function is expressed[11] as (with a spin degeneracy of 2),

$$Z_{sc}(\beta)=\frac{2}{h^3}\int[1+\hbar^2 w_2(\beta)+\hbar^4 w_4(\beta)+\ldots]\exp\left[-\left(\frac{p^2}{2M}+U\right)\beta\right]d^3r\,d^3p, \tag{1}$$

where we have omitted the terms with odd powers of $\hbar$ since they vanish on p integration. Here M is the nucleon mass and β an inverse temperature; the latter will not appear in our final result. The expressions for w_2 and w_4, which may be found in Uhlenbeck and Beth,[12] contain scalar combinations of the gradients and higher derivatives of $U(\vec{r})$ and the momentum $\vec{p}$. The p integrations in these expressions are done analytically. For a given number of fermions (say neutrons) N in the potential well, the Fermi energy $\tilde{\lambda}$ and the semiclassical energy $\tilde{E}$ may be directly worked out using the fact that the density of states is the inverse Laplace transform of the partition function. We obtain

$$N=L_{\tilde{\lambda}}^{-1}[Z_{sc}(\beta)/\beta],\quad \tilde{E}=\tilde{\lambda}N-L_{\tilde{\lambda}}^{-1}[Z_{sc}(\beta)/\beta^2], \tag{2}$$

where $L_{\tilde{\lambda}}^{-1}$ denotes the Laplace inverse with respect to $\tilde{\lambda}$. Note that although the classical partition

function given by the first term in the series (1) diverges for finite potentials, N and $\tilde{E}$, given by (2), are perfectly well defined.[9] In fact, the classical term alone yields the usual Thomas-Fermi (TF) result. After having done the p integrations in $Z_{sc}(\beta)$, Eq. (2) may be used to obtain N and $\tilde{E}$ which, up to order $\hbar^2$, are [13]

$$N=\frac{1}{(3\pi^2)}\left(\frac{2M}{\hbar^2}\right)^{3/2}\int^{\vec{r}_{\tilde{\lambda}}} d^3r\left[(\tilde{\lambda}-U)^{3/2}-\frac{1}{16}\frac{\hbar^2}{2M}(\tilde{\lambda}-U)^{-1/2}\nabla^2 U\right], \tag{3}$$

$$\tilde{E}=\frac{1}{(3\pi^2)}\left(\frac{2M}{\hbar^2}\right)^{3/2}\int^{\vec{r}_{\tilde{\lambda}}} d^3r\left(\left[\tfrac{3}{5}(\tilde{\lambda}-U)^{5/2}+U(\tilde{\lambda}-U)^{3/2}\right]+\frac{1}{16}\frac{\hbar^2}{2M}\left[(\tilde{\lambda}-U)^{1/2}\nabla^2 U-U(\tilde{\lambda}-U)^{-1/2}\nabla^2 U\right]\right). \tag{4}$$

Here the integrals are cut off at the classical turning point $\vec{r}_{\tilde{\lambda}}$ such that $U(\vec{r}_{\tilde{\lambda}})=\tilde{\lambda}$. We emphasize that we have also worked out the next term of order $\hbar^4$ for central potentials, which is straightforward, and have evaluated it numerically. We do not give its expression here since it is somewhat lengthy, and its contribution to $\tilde{E}$ is small (see Table I). For a given number of neutrons N, $\tilde{\lambda}$ may be calculated from Eq. (3), and $\tilde{E}$ from Eq. (4). Note that in these equations, the terms of order $\hbar^2$ are the corrections to the standard TF results.

Numerical calculations have been done for spherical Woods-Saxon potentials and also for the deformed potentials as parametrized by Eqs. (VII, 5) and (VII, 21) of Brack *et al.*,[14] taking $N=Z=A/2$. For the spherical case, $U=V_0[1+\exp(r-R)/a]^{-1}$, and we chose $V_0=-44$ MeV, $a=0.67$ fm, and $R=1.27A^{1/3}$ fm. The calculations were done for about twenty "nuclei" in the range $A=40$ to 500, and a few typical results are displayed in Table I, with the layout explained in the caption. It will be seen that for such potentials the numerical convergence of our series is excellent, and we can claim to have found $\tilde{E}$ for the spherical case within an absolute accuracy of 0.1 MeV.

Our results are also compared with the smooth energies $\tilde{E}_S$ obtained from Strutinsky calculations. In such calculations, the single-particle energies were obtained by diagonalizing the Hamiltonian in a harmonic-oscillator basis of optimum size (8 to 14 shells), and quasibound states in the continuum were included.[3,4] The stationary condition[4] for $\tilde{E}_S$ was carefully applied to minimize the ambiguity with respect to the smearing parameter γ and the curvature correction order which was varied from 4 to 16. This ambiguity increases for lighter nuclei for the potentials considered here, and we therefore limit the comparison to $A\geq 70$. Note that in such comparisons we have included the estimate of the truncation error in $\tilde{E}_S$, which is larger than 10 MeV for the heavier nuclei. A detailed discussion of the Strutinsky calculations will be found in Sobiczewski *et al.*[15] In Table II we display the results of a calculation $A=164$ for the axially symmetric deformed potential of Brack *et al.*[14] mentioned earlier. In this case we have neglected in the semiclassical $\tilde{E}$ the contribution of the $\hbar^4$ term, which is positive and of the order of 1 MeV and should improve the agreement further.

TABLE I. Smooth energy in spherical Woods-Saxon well. All energies are in MeV. The parameters of the potential are given in the text. The first column gives the nucleon number in a hypothetical nucleus with $N=Z=A/2$. The second, third, and fourth columns give $\tilde{E}^{(0)}$, $\tilde{E}^{(2)}$, and $\tilde{E}^{(4)}$, which are the contributions of the leading TF term, the term of order $\hbar^2$, and the term of order $\hbar^4$, respectively, in the semiclassical series. The fifth column is the sum of these to give the semiclassical energy to order $\hbar^4$. The last column gives the result of the Strutinsky calculation, with the associated numerical uncertainty in parentheses.

A	$\tilde{E}^{(0)}$	$\tilde{E}^{(2)}$	$\tilde{E}^{(4)}$	$\tilde{E}$	$\tilde{E}_S$
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 II. Smooth energy in deformed potential ($A=164$). All energies are in MeV. The deformed potential is axially symmetric, and is defined in Ref. 14 (see text). Here the parameter C is varied while the parameter $h=0$. The second column gives the semiclassical result from Eq. (4), while the last column is the Strutinsky result with the associated uncertainty in parentheses.

C	$\tilde{E}$	$\tilde{E}_S$
1.0	−3348.0	−3347.4 (0.4)
1.2	−3343.2	−3343.1 (1.2)
1.4	−3321.1	−3320.3 (0.9)
1.6	−3280.7	−3279.6 (0.8)

We see that for both spherical and deformed potentials, the Strutinsky smoothing yields results in agreement with our values. The difference of about an MeV is within the numerical uncertainties of the Strutinsky calculation, shown within parentheses in the tables.

Finally, for the spherical case, we find that the smooth energy $\tilde{E}$ in the range $A=40$ to 500 may be accurately fitted by a series of the form

$$\tilde{E} = C_1 A + C_2 A^{2/3} + C_3 A^{1/3} + C_4 + C_5 A^{-1/3}. \quad (5)$$

The leading (TF) term in the series (4) yields the coefficients (in MeV) $C_1 = -26.10$, $C_2 = 34.81$, $C_3 = -7.83$, $C_4 = -81.75$, and $C_5 = 94.85$, while the inclusion of the $\hbar^2$ and $\hbar^4$ correction terms alters these values to $C_1 = -26.10$, $C_2 = 37.65$, $C_3 = -7.13$, $C_4 = -80.48$, and $C_5 = 95.46$. Note that the TF contribution to $\tilde{E}$ not only contains all the volume term but also the bulk of the surface and curvature terms for the case of a Woods-Saxon potential with realistic surface thickness. Our volume and surface terms are in excellent agreement with those found by Sobiczewski *et al.*[15] using the same potential. Note that our expansion of $\tilde{E}$ in powers of $\hbar^2$ not only emphasizes the semiclassical nature of this quantity, but it also demonstrates that the convergence of this series is much faster than an expansion in powers of $A^{1/3}$ for the Woods-Saxon potential considered here. Our method, which adds correction terms to the TF result in a systematic manner, has no free parameters, makes no reference to the states in the continuum, and involves integrals that are easily and accurately calculable using a computer.

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[1]W. D. Myers and W. J. Swiatecki, Nucl. Phys. 81, 1 (1966).

[2]V. M. Strutinsky, Nucl. Phys. A95, 420 (1967), and A122, 1 (1968).

[3]M. Bolsterli, E. O. Fiset, J. R. Nix, and J. L. Norton, Phys. Rev. C 5, 1050 (1972).

[4]M. Brack and H. C. Pauli, Nucl. Phys. A207, 401 (1973).

[5]A. Bohr and B. R. Mottelson, "Nuclear Structure" (Addison-Wesley, Reading, Mass., to be published), Vol. 2.

[6]P. J. Siemens and A. Sobiczewski, Phys. Lett. 41B, 16 (1972).

[7]R. K. Bhaduri and C. K. Ross, Phys. Rev. Lett. 27, 606 (1971).

[8]B. K. Jennings, Ann. Phys. (New York) 84, 1 (1974).

[9]B. K. Jennings and R. K. Bhaduri, to be published.

[10]E. Wigner, Phys. Rev. 40, 749 (1932).

[11]J. G. Kirkwood, Phys. Rev. 44, 31 (1933).

[12]G. E. Uhlenbeck and E. Beth, Physica (Utrecht) 3, 729 (1936).

[13]These results can also be derived using the method developed by R. Balian and C. Bloch, Ann. Phys. (New York) 63, 592 (1971).

[14]M. Brack, J. Damgaard, A. S. Jensen, H. C. Pauli, V. M. Strutinsky, and C. Y. Wong, Rev. Mod. Phys. 44, 320 (1972).

[15]A. Sobiczewski *et al.*, to be published.