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# Semi-classical smoothing in a non-monotonic field

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**Abstract.** It is pointed out that the semi-classical method of Jennings, Bhaduri and Brack for smoothing the total energy of a system of non-interacting fermions in a potential well $V(\mathbf{r})$ breaks down in the fourth-order term if this potential is non-monotonic. This means that the method as it stands can only be used by neglecting the Coulomb force on protons. We propose a modified treatment for the fourth-order term which appears to be entirely satisfactory.

**Keywords.** Nuclear binding energy; Strutinsky theorem; semiclassical smoothing.

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## 1. Introduction

It is well known from the Strutinsky theorem (Brack and Quentin 1975) that the Hartree-Fock (HF) energy of a nucleus can be written approximately as the sum of two contributions,

$$E_{\mathrm{HF}} = E_{\mathrm{mac}} + \delta E. \tag{1}$$

The first term here, the so-called macroscopic energy, varies smoothly from nucleus to nucleus, while the second term, the shell correction, fluctuates about these smooth values. According to the Strutinsky theorem, the shell correction is given by

$$\delta E = E_{\mathrm{sh}} - \tilde{E}_{\mathrm{sh}}, \tag{2}$$

where $E_{\mathrm{sh}}$ is the sum of single-particle (s.p.) energies,

$$E_{\mathrm{sh}} = \sum_i \varepsilon_i n_i, \tag{3}$$

$\varepsilon_i$ denoting the single-particle eigen-energy of the level $i$ in the self-consistent field, and $n_i$ the occupancy of this level. As for $\tilde{E}_{\mathrm{sh}}$, this represents some smoothed value of $E_{\mathrm{sh}}$; see below for the actual way in which the smoothing is performed.

These results are basic to the macroscopic-microscopic approach to the calculation of nuclear binding energies. In this approach the term $E_{\mathrm{mac}}$ in (1) is replaced by some model such as that of the liquid droplet, while the s.p. energies are calculated in some phenomenological shell-model potential, rather than in the self-consistent field (Brack and Quentin 1975).

Strutinsky's original procedure for performing the smoothing implicit in $\tilde{E}_{\mathrm{sh}}$

amounts simply to smearing out the discrete s.p. levels in some suitable manner. However, in adopting this prescription to the real situation of finite potential wells, it is well known that some serious ambiguities arise, because of the continuum (Brack and Pauli 1973; Sobiczewski *et al* 1977).

All these ambiguities associated with the so-called plateau condition are avoided in the alternative smoothing procedure developed by Jennings *et al* 1975 (JBB). We give now a brief account of this essentially semi-classical method, which amounts to doing an Extended Thomas-Fermi (ETF) calculation of the total energy $E_{sh}$ of a system of non-interacting fermions in a potential well $V(\mathbf{r})$ (JBB considered also a spin-orbit term in the field, but we are not concerned with this in the present note).

Considering for simplicity just one kind of nucleon, let there be $N$ of them. Then (3) can be written exactly as

$$E_{sh} = \lambda N - \mathscr{L}_{\lambda}^{-1} \frac{Z(\beta)}{\beta^2}, \tag{4}$$

where $\lambda$ is the exact chemical potential and $Z(\beta)$ the exact single-particle partition function for inverse temperature $\beta$; we have introduced the inverse Laplace transform

$$\mathscr{L}_{\lambda}^{-1} f(\beta) \equiv \frac{1}{2\pi i} \int_{\beta_0 - i\infty}^{\beta_0 + i\infty} e^{\lambda\beta} f(\beta) \mathrm{d}\beta, \tag{5}$$

where $\beta_0$ takes any positive value. (We see that temperature is involved only in a formal way, and is eliminated from the final expression (4) for $E_{sh}$). The chemical potential $\lambda$ is determined by the normalization condition

$$N = \mathscr{L}_{\lambda}^{-1} \left[ \frac{1}{\beta} Z(\beta) \right]. \tag{6}$$

The smoothing of $E_{sh}$ is then effected by replacing $Z$ with its expansion in powers of $\hbar^2$; up to terms in $\hbar^4$ we have

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

It follows that

$$\tilde{E}_{sh} = \lambda_{sc} N - \mathscr{L}_{\lambda_{sc}}^{-1} \frac{Z_{sc}(\beta)}{\beta^2}, \tag{8}$$

where the semi-classical chemical potential $\lambda_{sc}$ is determined by

$$N = \mathscr{L}_{\lambda_{sc}}^{-1} \frac{Z_{sc}(\beta)}{\beta}. \tag{9}$$

Substituting (7) in (8), the indicated inverse Laplace transforms for all but the last two terms in $Z_{sc}$ are evaluated by employing the identity

$$\mathscr{L}_{\lambda}^{-1}\frac{e^{-\beta V}}{\beta^n}=\frac{(\lambda-V)^{n-1}}{\Gamma(n)}\theta(\lambda-V), \qquad n>0, \tag{10}$$

where $\Gamma(n)$ is the gamma function and $\theta(\lambda-V)$ the unit step function. But since (10) is not valid for $n\leqslant 0$ it cannot be applied directly to the last two terms of (7), for which $n=-1/2$. JBB handled this problem by using the identity

$$e^{-\beta V}=-\frac{1}{\beta}\frac{\nabla V\cdot\nabla e^{-\beta V}}{(\nabla V)^2}. \tag{11}$$

An integration by parts then permits the use of (10), with $n=1/2$, whence (8) can be written as

$$\tilde{E}_{sh}=\lambda_{sc}N-(E_{-3}+E_{-1}+E_1) \tag{12}$$

where

$$E_{-3}=\frac{2}{15\pi^2}\left(\frac{2M}{\hbar^2}\right)^{3/2}\int d^3\mathbf{r}(\lambda_{sc}-V)^{5/2}, \tag{13a}$$

$$E_{-1}=-\frac{1}{24\pi^2}\left(\frac{2M}{\hbar^2}\right)^{1/2}\int d^3\mathbf{r}(\lambda_{sc}-V)^{1/2}\nabla^2 V, \tag{13b}$$

$$\begin{aligned}E_1=\frac{1}{5760\pi^2}\left(\frac{\hbar^2}{2M}\right)^{1/2}&\int d^3\mathbf{r}\frac{1}{(\lambda_{sc}-V)^{1/2}(\nabla V)^2}\\ &\times[-7(\nabla^4 V)(\nabla V)^2+5(\nabla^2 V)^3+10\nabla^2 V\{\nabla V\cdot\nabla(\nabla^2 V)\}\\ &-\{5(\nabla^2 V)^2+\nabla^2(\nabla V)^2\}\nabla V\cdot\nabla(\nabla V)^2/(\nabla V)^2\\ &+(\nabla^2 V)\nabla^2(\nabla V)^2+\nabla V\cdot\nabla\nabla^2(\nabla V)^2].\end{aligned} \tag{13c}$$

Because of the step function in (10) all the integrals in (13) are cut-off at the classical turning point $\mathbf{r}_c$, given by

$$V(\mathbf{r}_c)=\lambda_{sc}. \tag{14}$$

(Note that in determining $\lambda_{sc}$ by (9) it has been shown by Jennings *et al* (1975) that one can drop the terms in $\hbar^4$ in (7), so that the application of (10) is always direct).

We now point out that singularities arise in (13c) if $\nabla V$ vanishes anywhere within the domain of integration, i.e., inside $\mathbf{r}_c$. Clearly, the problem originates in the fact that (11) will no longer be applicable at such points. JBB did not experience any difficulty on this account, since they limited their numerical calculations to pure Saxon-Woods wells, which are monotonic everywhere. However, when a Coulomb term is added the resultant well for protons goes through a shallow minimum inside the classical turning point, whereupon (13c) for $E_1$ breaks down. (Of course, the same problem could arise for neutrons if the restriction to Saxon-Woods wells was removed).

As an alternative way to evaluate the inverse Laplace transforms arising in $E_1$, one may propose the following identity

$$\mathscr{L}_\lambda^{-1}\frac{z(\beta)}{\beta^m}=\frac{\mathrm{d}}{\mathrm{d}\lambda}\mathscr{L}_\lambda^{-1}\frac{z(\beta)}{\beta^{m+1}}, \tag{15}$$

which follows directly from (5). The purpose of this note is to explore this possibility.

## 2. Method

Using (10) and (15), and writing

$$\phi(\mathbf{r})=\frac{1}{5760\pi^2}(\hbar^2/2M)^{1/2}\{5(\nabla^2V)^2+\nabla^2(\nabla V)^2\}, \tag{16}$$

the contribution of the last two terms of (7) to $E_1$ becomes

$$\begin{aligned}E_1^{(2)}&=\frac{\mathrm{d}}{\mathrm{d}\lambda}\int_0^{r_c}\mathrm{d}^3\mathbf{r}\frac{\phi(\mathbf{r})}{\{\lambda-V(r)\}^{1/2}}\\&=\frac{1}{V'(r_c)}\left[\frac{4\pi r^2\phi(r)}{\{\lambda-V(r)\}^{1/2}}\right]_{r_c}-2\pi\int_0^{r_c}\frac{r^2\phi(r)\mathrm{d}r}{\{\lambda-V(r)\}^{3/2}},\end{aligned} \tag{17}$$

where in the second expression we are limiting ourselves to the case of spherical symmetry. Both terms in the second expression are singular at the turning point, but it is relatively easy to show that the two singularities cancel, so that the indicated derivative does indeed exist. Nevertheless, to evaluate $E_1^{(2)}$ we cannot use the second expression, but rather must calculate the integral in the first expression and differentiate numerically.

Thus in place of (13c) we have

$$E_1=-\frac{7}{5760\pi^2}(\hbar^2/2M)^{1/2}\int\mathrm{d}^3\mathbf{r}\frac{\nabla^4V}{(\lambda_{sc}-V)^{1/2}}+E_1^{(2)}, \tag{18}$$

where $E_1^{(2)}$ is given by (17). When (13c) is applicable, i.e., when the potential $V(\mathbf{r})$ is monotonic, it is numerically equivalent to (18) (see below). As for $E_{-3}$ and $E_{-1}$, the application of the identity (15) to (7), followed by use of (10), leads back once more to (13a) and (13b) respectively.

To test our approach we use the same spherical Woods-Saxon potential as used by Jennings in his thesis (unpublished)

$$V(r)=\frac{V_0}{1+\exp\left(\dfrac{r-R}{a}\right)}, \tag{19}$$

with $V_0=-44$ MeV, $R=1{\cdot}27\times A^{1/3}$ fm and $a=0.67$ fm. Estimates of $E_1$ for a few hypothetical nuclei with $N=Z$ (no Coulomb force and no spin-orbit term) have been made with both (13c) and (18). Comparison of columns (a) and (b) in table 1 show an

**Table 1.** $E_1$ (in MeV) for Saxon-Woods potential with no coulomb force.

| | $E_1$ | |
|---|---|---|
| $A$ | (a) | (b) |
| 40 | −0·61 | −0·59 |
| 72 | −0·72 | −0·70 |
| 164 | −0·85 | −0·82 |
| 204 | −0·87 | −0·83 |
| 260 | −0·89 | −0·84 |
| 292 | −0·89 | −0·85 |
| 416 | −0·87 | −0·82 |

All nuclei shown have $N = Z = A/2$. Columns (a) and (b) refer to calculations based on (13c) and (18), respectively. Parameters of the potential are given in the text.

**Table 2.** Various contributions (in MeV) to smoothed energy of protons in $^{208}$Pb, moving in the realistic potential described in the text.

| | | | |
|---|---|---|---|
| $\lambda_{sc}^{N}$ | −578·63 | $E_1^{LS}$ | −5.77 |
| $E_{-3}$ | 930·93 | $\tilde{E}_{sh}$ | −1446·11 |
| $E_{-1}$ | −72·97 | $E_{sh}$ | −1450·25 |
| $E_1$ | 1·61 | $\delta E$ | −4·14 |
| $E_{-1}^{LS}$ | 13·68 | | |

excellent agreement between the two methods, in this case where both are applicable. (The small residual discrepancies between column (a) of this table and the corresponding results in table 1 of chapter 2 of Jennings's thesis, which in any case do not exceed 0·2 MeV, can be attributed to numerical error in a calculation which involves massive cancellations between the different parts of a rapidly fluctuating integrand. It is to be noted that we obtain complete agreement with Jennings (1976) for all other terms in $\tilde{E}_{sh}$).

With the validity of this approach based on (18) having been checked, it remains simply to show that it can indeed be applied to a situation where (13c) is invalid, i.e., to the case of a non-monotonic potential $V(\mathbf{r})$. We consider the case of protons in $^{208}$Pb, taking for the Saxon-Woods part of the potential the realistic values of the parameters $V_0 = -60{\cdot}6$ MeV, $R = 7{\cdot}40$ fm, and $a = 0{\cdot}577$ fm—see (19). The Coulomb potential is generated by a Fermi charge distribution,

$$\rho_{ch} = \frac{\rho_0}{1 + \exp\left(\dfrac{r - C}{d}\right)}, \tag{20}$$

with $C = 6{\cdot}81$ fm and $d = 0{\cdot}394$ fm. The resultant central potential is shown in figure 1; the shallow minimum inside the classical turning point $r_c$ will be observed.

A spin-orbit term is also included, simply to make the problem realistic: its contributions $E_{-1}^{LS}$ and $E_1^{LS}$ to $\tilde{E}_{sh}$ are calculated as in JBB. We take

$$V_{LS} = \frac{A}{r} \exp\{-(r - B/D)^2\}\, \hat{\sigma} \cdot \hat{\mathbf{l}}, \tag{21}$$

where $A = -5{\cdot}31$ MeV fm, $B = 6{\cdot}84$ fm, and $D = 0{\cdot}968$ fm.

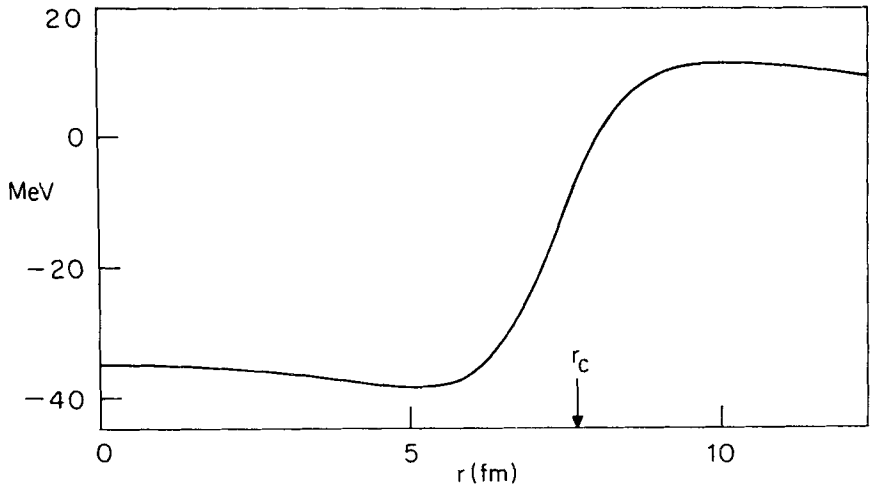


**Figure 1.** Realistic potential well for protons of $^{208}$Pb. Classical turning point is denoted by $r_c$.

We show in table 2 all the various contributions to (12) for the $\tilde{E}_{sh}$ of the protons, along with $E^{LS}_{-1}$ and $E^{LS}_{1}$. The essential point is that $E_1$ could only be calculated with (18).

Note that although $E_1$ is small it is seen, from the last entry of table 2, to constitute a significant component of the shell-model correction $\delta E$ of (2). Thus $E_1$ has to be calculated with some precision; it would not be sufficient to replace the central potential of figure 1 by a similar monotonic one.

## 3. Conclusion

We conclude that with this modification for the protons, the semi-classical smoothing method of JBB constitutes a viable alternative to the usual Strutinsky procedure.

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