AN IMPROVED APPROXIMATION TO CONSTRAINED HARTREE–FOCK CALCULATIONS★

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A previously proposed microscopical method to calculate deformation energies of heavy nuclei, using Skyrme type effective interactions, is reinvestigated. It is shown that if the effective mass is included in the phenomenological one body Hamiltonian, whose eigenfunctions are used to calculate the expectation value of the total Skyrme Hamiltonian, one can obtain deformation energies very close to the ones obtained in constrained Hartree–Fock calculations.

Since the re-discovery [1] of the effective nucleon–nucleon force of Skyrme [2], constrained Hartree–Fock (CHF) calculations for heavy nuclei have become technically possible [3, 4]. However, such calculations require large amounts of computer time, so that it would be far too time consuming to include nonaxial and left-right asymmetric deformations in a systematical investigation of fission barriers using the CHF method.

A purely microscopical, but less time consuming approximation to the CHF method was proposed some years ago by Ko et al. [5]. The main idea of this approach is to utilize the single particle wave functions of the deformed Woods–Saxon (WS) potential, determined in Strutinsky type fission barrier calculations [6, 7], to calculate the expectation value of the total Skyrme Hamiltonian:

$$E_{\mathrm{EVM}} = \langle \Phi_{\mathrm{WS}}(\beta_i) | T + v_{\mathrm{Sky}} | \Phi_{\mathrm{WS}}(\beta_i) \rangle \,. \qquad (1)$$

Here v_{Sky} is the Skyrme interaction and $\Phi_{\mathrm{WS}}(\beta_i)$ a Slater determinant built of the WS single particle wave functions $\varphi_\nu(\boldsymbol{r}, \beta_i)$ which depend on one or more deformation parameters β_i. The quadrupole moment Q_2 and higher moments can easily be calculated from the φ_ν, too. Thus, eq. (1) gives directly the total energy of a nucleus as a function of deformation $E(\beta_i)$ or $E(Q_2; ...)$, and the parameters β_i play the role of the constraint in the CHF method ‡.

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‡ For simplicity, we omit the indices for protons and neutrons.

The results found with this expectation value method (EVM) were only partially successful [5]. Whereas the shell structure in the deformation energies was reasonably well reproduced, their average part increased too much at large deformations. In ^{240}Pu, e.g., the second fission barrier was found more than twice as large as the one obtained in a CHF calculation with the same force.

We have reinvestigated the EVM with essentially three alterations:

(1) The effective masses $m^*(\boldsymbol{r})$ which for Skyrme forces differ from the free nucleon masses in the interior of the nucleus, have been included in the one body Hamiltonian.

We thus solve the equations

$$\hat{H}\varphi_\nu(\boldsymbol{r}) = \left\{ -\boldsymbol{\nabla}\cdot\frac{\hbar^2}{2m^*(\boldsymbol{r})}\boldsymbol{\nabla} + V(\boldsymbol{r}) - \mathrm{i}\boldsymbol{\nabla}S(\boldsymbol{r})\cdot[\boldsymbol{\nabla}\times\boldsymbol{\sigma}] \right\}\varphi_\nu(\boldsymbol{r}) = \epsilon_\nu\varphi_\nu(\boldsymbol{r}) \,, \qquad (2)$$

by diagonalization of $\hat{H}$ in a deformed harmonic oscillator basis [6–8]. For each kind of nucleons the effective mass $m^*(\boldsymbol{r})$, the local nuclear potential $V(\boldsymbol{r})$ and the spin-orbit form factor $S(\boldsymbol{r})$ are chosen to have a generalized Woods–Saxon form:

$$V(\boldsymbol{r}) = V_0\{1 + \exp[l(\boldsymbol{r}, R_{\mathrm{v}})/a_{\mathrm{v}}]\}^{-1} \,, \qquad (3)$$

$$m^*(\boldsymbol{r})/m = 1 - (1-\mu)\{1 + \exp[l(\boldsymbol{r}, R_{\mathrm{s}})/a_{\mathrm{s}}]\}^{-1} \,, \qquad (4)$$

$$S(\boldsymbol{r}) = \chi\{1 + \exp[l(\boldsymbol{r}, R_{\mathrm{s}})/a_{\mathrm{s}}]\}^{-1} \,. \qquad (5)$$

The variable $l(\boldsymbol{r}, R_0)$ is defined such that $l(\boldsymbol{r}_{\mathrm{s}}, R_0) = 0$

along the surface r_s of the nucleus in a given shape parametrization. It is normalized to give a constant gradient along the surface (i.e. a constant surface thickness) and to be $l = r - R_0$ for a spherical nucleus. (For more details of this way of deforming a WS potential, see refs. [6–8].)

(2) In diagonalizing the Hamiltonian (2), the size $\hbar\omega_0$ and the deformation $q = \omega_\perp/\omega_z$ of the axial harmonic oscillator basis are optimized for each nucleus at each deformation. Since $E_{\mathrm{EVM}}(1)$ depends in a simple analytical way on $\hbar\omega_0$ [9], it can easily be minimized with respect to $\hbar\omega_0$. (This has, in fact, already been done in ref. [5].) For each deformation, characterized by the shape parameters β_i and the corresponding quadrupole moment $Q_2(\beta_i)$, we define the axis ratio q of the basis to be that of a rotationally symmetric ellipsoid with the same quadrupole moment. The latter is given by

$$Q_2(q) = \frac{8\pi}{15} R_0^5 (q^{4/3} - q^{-2/3}) \tag{6}$$

for a constant volume $V = (4\pi/3)R_0^3$. By equating $Q_2(q)$ in eq. (6) with $Q_2(\beta_i)$ we thus determine uniquely q as a function of the β_i. This procedure is justified by the results of CHF calculations [3] where it was observed that the optimal values of q for each (constrained) quadrupole moment are closely fulfilling eq. (6). For the (c, h) parametrization of ref. [6] which we used in our calculations, the relation is

$$q = c^{3/2}\,[1 + 6x - 6x^2 + \mathrm{O}(x^3) + \ldots]\ , \qquad x = \tfrac{1}{35}\, c^3\,[2h + \tfrac{1}{2}(c-1)]\ . \tag{7}$$

Taking the terms up to order x in eq. (7) appears to be sufficient for deformations up to the second fission barrier in the actinide region ($c \approx 1.6, h \approx 0$). (In the calculations of ref. [5] the prescription of Damgaard et al. [8] was used for q which yields a coefficient 1 instead of 6 in the term linear in x in eq. (7), and thus leads to appreciably smaller values of q at large deformations.)

(3) The parameters of the WS functions (3)–(5) are chosen to reproduce approximately the results of a HF calculation for a given nucleus in its spherical configuration. The spherical HF code of Beiner et al. [10] is used, which is not very time consuming, and the selfconsistent solutions for $V(r)$, $S(r)$ and $m^*(r)$ are fitted by the functions (3)–(5) separately for neutrons and protons. (For $S(r)$ and $m^*(r)$ which both are proportional to the nuclear densities [1], the same radii R_s and surface thicknesses a_s can be used.) The parameters R_v, a_v, R_s and a_s are easily adjusted to reproduce the correct fall-off in the surface region, and the constants V_0, μ, χ are chosen to fit the average values of the selfconsistent results in the interior region of the nucleus. This procedure allows one to get rid of the shell model parameters used in ref. [5], so that the only free parameters are those of the effective force. For the latter, we used here the set SIII of Skyrme parameters [10].

In figs. 1 to 3 we present the deformation energy curves obtained in this improved EVM for three different nuclei and compare them to results of CHF calculations. In all cases a deformation dependent cut-off (see, e.g., refs. [6, 7]) was used corresponding to the inclusion of 11 (^{168}Yb) and 13 (^{240}Pu, ^{354}SH) major spherical shells in the basis. Such a basis is certainly not big enough for large deformations in the very heavy nuclei; but for the present comparison of the two curves E_{EVM} and E_{HF} the truncation error does not matter. Pairing correlations are included consistently in all curves using the BCS method with a constant average pairing gap $\tilde{\Delta} = (12A^{-1/2})$ MeV [6].

For the deformation parameters β_i we used the $\{c, h(\alpha = 0)\}$ shape parametrization of ref. [6]. In the actinide region, $h = 0$ corresponds to the fission path in the pure liquid drop model ("LDM valley"). Even including the shell effects, $h = 0$ gives a reasonable estimate of the fission barriers in a 1-dimensional

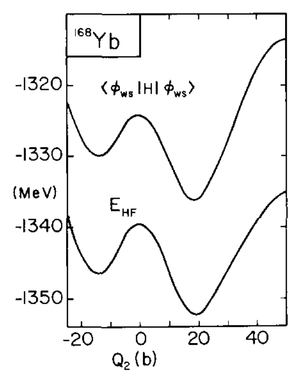

Fig. 1. Deformation energy of ^{168}Yb as a function of the total mass quadrupole moment. Upper curve: present method (EVM), calculated for (c, h) shapes along $h = 0$. Lower curve: result of CHF calculation.

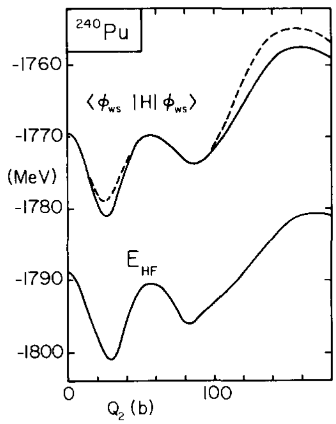

Fig. 2. Same as fig. 1 for ^{240}Pu. Dashed portions of upper curves are obtained with h = 0, the solid upper curve by minimizing the energy in the (c, h) plane for each fixed value of Q_2.

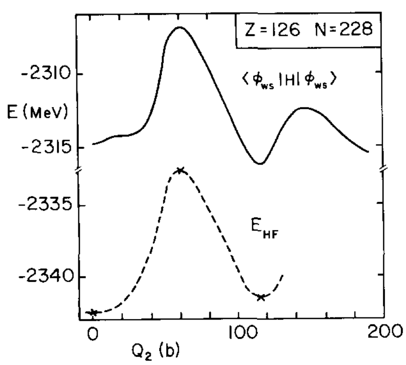

Fig. 3. Same as fig. 2 for a hypothetical superheavy element with Z = 126, N = 228. In the lower curve (E_{HF}) only the three points marked by crosses were calculated selfconsistently.

representation as function of c. For the nucleus ^{168}Yb (fig. 1), the path of minimal energy deviates from h = 0 only for $Q_2 \gtrsim 30$ barns, as noted earlier [11]. For ^{240}Pu (fig. 2), the regions around the ground-state minimum and the second saddle point turn out to have lower energies for $h \approx -0.1$ to -0.2, which is in agreement with Strutinsky calculations [6]. In the upper curve of fig. 2, the dashed parts correspond to h = 0, whereas the solid curve is obtained by minimizing the energy in the (c, h) plane for each fixed Q_2.

The lower curves in figs. 1 and 2 are the results of earlier CHF calculations [4, 11], reproduced under the same numerical conditions as the present EVM calculations. (Hereby the quadrupole moment Q_2 was constrained quadratically [4].) We see that, apart from a constant shift of ~15–20 MeV of the total energy, the deformation behaviour of the EVM curves closely reproduces that of the selfconsistent calculations. In particular, the stationary points (and thus the barrier heights) agree within ~2 MeV. For ^{240}Pu, this is a considerable improvement compared to the earlier EVM calculations (see especially fig. 12 of the second paper in ref. [5]), which is essentially due to the inclusion of the effective mass. (The better optimization of the basis parameter q mainly reduces the second barrier region by some MeV).

We did a similar test for a hypothetical superheavy element ^{354}SH with Z = 126 and N = 228. For reasons of computer time, we calculated only three stationary points selfconsistently, corresponding to the (spherical) ground state, the first saddle point and the secondary minimum. These three points are shown by crosses in the lower part of fig. 3. The rest of the dashed curve E_{HF} is interpolated by hand in order to guide the eye. The upper curve is the EVM result, minimized in the (c, h) plane for Q_2 up to 120 barns. In this case again, the relative positions of the first three stationary points agree within ~2 MeV, although the energy difference between the two minima (~1 MeV) has opposite signs in the two cases. The quadrupole moment of the second minimum, however, is very accurately reproduced in the EVM calculation, as it is the case also in the other results presented in figs. 1 and 2.

We do not want here to draw any definite conclusions about the fission barrier of this superheavy nucleus ^{354}SH. Before quantitative statements about the barrier height can be made, the numerical convergence of the results (both with respect to the basis size and the accuracy of integration) has to be tested and the influence of nonaxial and left-right asymmetric shapes must be investigated as well as the dependence on the Skyrme parameters. Such an investigation is presently under way [12]. (For those interested in superheaviology, we note that almost all of the spherical shell effect comes from the neutrons which have a very strong magicity at N = 228, as already pointed out by Vautherin et al. [13].)

Summary and conclusions. We have shown that the expectation value method is a powerful and time saving tool to obtain approximately selfconsistent deformation energy curves, if the effective mass is included in the one body Hamiltonian and the basis carefully optimized. The time saved in comparison to a CHF calculation is a factor of 5–10 or more, depending on how carefully one wants to optimize the basis in the CHF method. This pays out especially for very heavy nuclei, and it will be indispensible when nonaxial deformations are included.

The accuracy of the barrier heights obtained with the EVM as compared to the selfconsistently calculated ones can, on the basis of the present investigation, be estimated to be ~1–2.5 MeV. This may not seem sufficient for the comparison with experiment. But one should bare in mind that the overall accuracy of fission barriers obtained with the Skyrme-CHF method is not better than a few MeV, taking into account truncation errors, uncertainties in the amount of spurious centre of mass and rotational energies included and, last but not least, the possible variation of the Skyrme parameters [10] and especially the spin-orbit force. Still, for extrapolations far away from known stable nuclei, this method should be more reliable than the Strutinsky method which depends on the phenomenologically fitted shell-model and liquid drop model parameters.

Our way of fitting the functions (3)–(5) to the results of spherical HF calculations may be regarded as a preliminary step only. In the context of Skyrme-HF theory, all these functions are determined by the nucleon densities $\rho(\boldsymbol{r})$ and the kinetic energy and spin-orbit densities $\tau(\boldsymbol{r})$ and $\boldsymbol{J}(\boldsymbol{r})$ [1]. Recent investigations [14–16] have shown that the densities τ and $\boldsymbol{J}$ may be expressed as functionals of ρ in a semiclassical expansion, and with this the average binding energies may be calculated variationally in a very good approximation without using single particle wavefunctions. In particular, it was demonstrated in ref. [15, 16] that the expectation values E_{EVM} obtained with the potentials derived from the semiclassical variational densities are within less than 10 MeV of the exact HF energies for spherical nuclei (even for A = 354).

In further applications of the EVM we thus intend to use the functions $V(\boldsymbol{r})$, $S(\boldsymbol{r})$ and $m^*(\boldsymbol{r})$ derived from the semiclassical densities of refs. [15, 16]. For the deformed cases this may be done (1) by using the same scaling procedure as described above or (2) by extending the method of Chu et al. [16] to include deformations with a constraint. In the latter case one will be independent of a shape parametrization, and all quantities will be consistently derived from the effective nuclear interaction.

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