Volume Conservation in the Nilsson Model and Effective Many-Body Forces

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It is shown that the Nilsson prescription for calculating equilibrium deformation of nuclei under the constraint of constant volume is equivalent to a Hartree mean-field approximation applied to nucleons interacting via many-body forces. Such an interaction is obtained in closed form, having a Taylor expansion beginning with the familiar quadrupole-quadrupole interaction.

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A very important aspect of the Nilsson model of the atomic nucleus is the determination of equilibrium shapes. In the most pristine version of the model, the equilibrium deformation parameters were obtained by minimizing the sum of the energies of individual nucleons moving independently in a phenomenological deformed potential, subject to the constraint that the volumes enclosed by equipotential surfaces remain constant as the deformation varies.[1,2] This volume-conservation (VC) constraint is intended to simulate the incompressibility of nuclear matter and provides a restoring force. The more modern version of the model, usually called the Nilsson-Strutinskii model,[3] incorporates pairing and Coulomb effects and Strutinskii averaging,[4] but such refinements are peripheral to the discussion at hand. The success of this intuitive prescription over the years has been "disconcertingly spectacular,"[5] especially since it appears at first sight to be rather different from conventional mean-field approximations, such as the Hartree-Fock approximation. In spite of efforts by Moszkowski[6] and later by Bassachis[7] to relate the Nilsson model to the Hartree approximation for small deformations, this model in its full generality poses something of a mystery.

The aim of this note is to at least partially dispel some of the mystery by proving that the equilibrium solutions of the Nilsson model with VC are identical to those of the Hartree approximation applied to a certain effective nucleon-nucleon interaction involving many-body forces. This result is obtained without the limitation of small deformations.

The Nilsson Hamiltonian H_N, excluding for simplicity the hexadecapole term and Coulomb effects, may be written in the form

$$H_N = H_0 + U_D, \tag{1}$$

where H_0 is the spherically symmetric Hamiltonian for A nucleons,

$$H_0 = \sum_{i=1}^{A} \left[p_i^2/2m + \tfrac{1}{2} m \omega_0^{02} r_i^2 + C\vec{1}_i \cdot \vec{s}_i + D(l_i^2 - \langle l^2 \rangle_N)\right] + H_{\text{pair}}\,. \tag{2}$$

The pairing Hamiltonian H_{pair} and the $\vec{1}\cdot\vec{s}$ and the l^2 terms do not play a role in the ensuing arguments, but are included for generality to emphasize the validity of the results even in the presence of these terms. The term U_D is that part of the oscillator potential U_{osc} involving deformation effects:

$$U_D = U_{\text{osc}} - \tfrac{1}{2} m\omega_0^{02} R^2 = \tfrac{1}{2} m \sum_{i=1}^{A} (\omega_x^2 x_i^2 + \omega_y^2 y_i^2 + \omega_z^2 z_i^2 - \omega_0^{02} r_i^2), \tag{3}$$

where R^2 is the monopole operator $R^2 = \sum_{i=1}^{A} r_i^2$.

Let $\langle \cdots \rangle$ denote the expectation value with respect to either an exact ground state of (1) or else a variational approximation, as, for example, a Bardeen-Cooper-Schrieffer state to take care of H_{pair}.[3] In either case, the Hellmann-Feynman theorem is valid, so that the minimization of $\langle H_N \rangle$ with respect to the oscillator frequencies ω_x, ω_y, and ω_z, subject to the constant-volume constraint

$$\omega_x \omega_y \omega_z = \omega_0^{03}, \tag{4}$$

may be written in the form

$$\langle \partial H_N / \partial \omega_k \rangle - \mu\, \partial(\omega_x \omega_y \omega_z)/\partial \omega_k = 0, \quad k = x, y, z, \tag{5}$$

where μ is a Lagrange multiplier whose subsequent elimination yields the condition that the shape of the oscillator potential and that of the density distribution coincide, the justification for which is the short range of nuclear forces,[8] which is equivalent to the following:

$$\langle \sum_{i=1}^{A} x_i^2 \rangle = \frac{\omega_0^{02}}{\omega_x^2}\Lambda, \quad \langle \sum_{i=1}^{A} y_i^2 \rangle = \frac{\omega_0^{02}}{\omega_y^2}\Lambda, \quad \langle \sum_{i=1}^{A} z_i^2 \rangle = \frac{\omega_0^{02}}{\omega_z^2}\Lambda, \quad \Lambda \equiv (\langle \sum_{i=1}^{A} x_i^2 \rangle \langle \sum_{i=1}^{A} y_i^2 \rangle \langle \sum_{i=1}^{A} z_i^2 \rangle)^{1/3}. \tag{6}$$

From Eq. (6), the total energy corresponding to an equilibrium deformation may be written as $E = \langle H_{\rm N} \rangle = \langle H_0 \rangle + \langle U_D \rangle$, where

$$\langle U_D \rangle = \tfrac{3}{2} m\omega_0^{02} (\langle \sum_{i=1}^{A} x_i^2 \rangle \langle \sum_{i=1}^{A} y_i^2 \rangle \langle \sum_{i=1}^{A} z_i^2 \rangle)^{1/3} - \tfrac{1}{2} m\omega_0^{02} \langle R^2 \rangle . \tag{7}$$

It shall now be shown that (7) can be written as the Hartree expectation value of a rotationally invariant many-body interaction. The first step is to express (7) in terms of the expectation values of the monopole operator R^2 and the mass quadrupole operators $Q_{2\mu} = \sum_{i=1}^{A} r_i^2 Y_{2\mu}(\Omega_i)$, $\mu = 0, \pm1, \pm2$. Since $U_{\rm osc}$ is aligned along its principal axes, the conditions $\langle Q_{2\pm1} \rangle = 0$ and $\langle Q_{22} \rangle = \langle Q_{2-2} \rangle$ are fulfilled. Then, $\langle Q_{20} \rangle$, $\langle Q_{22} \rangle$, and $\langle R^2 \rangle$ may be expressed as linear combinations of $\langle \sum_i x_i^2 \rangle$, $\langle \sum_i y_i^2 \rangle$, and $\langle \sum_i z_i^2 \rangle$. These relations may be inverted as follows:

$$\begin{aligned} &\langle \sum_{i=1}^{A} x_i^2 \rangle = \tfrac{1}{3}[\langle R^2 \rangle - (\tfrac{4}{5}\pi)^{1/2} \langle Q_{20} \rangle + (\tfrac{24}{5}\pi)^{1/2} \langle Q_{22} \rangle], \quad \langle \sum_{i=1}^{A} y_i^2 \rangle = \tfrac{1}{3}[\langle R^2 \rangle - (\tfrac{4}{5}\pi)^{1/2} \langle Q_{20} \rangle - (\tfrac{24}{5}\pi)^{1/2} \langle Q_{22} \rangle], \\ &\langle \sum_{i=1}^{A} z_i^2 \rangle = \tfrac{1}{3}[\langle R^2 \rangle + 2(\tfrac{4}{5}\pi)^{1/2} \langle Q_{20} \rangle]. \end{aligned} \tag{8}$$

Upon substituting Eqs. (8) into (7) and expanding, one finds

$$\langle U_D \rangle = \tfrac{1}{2} m\omega_0^{02} [\langle R^2 \rangle^3 - \tfrac{12}{5}\pi \langle R^2 \rangle (\langle Q_{20} \rangle^2 + 2\langle Q_{22} \rangle^2) + 2(\tfrac{4}{5}\pi)^{3/2} (\langle Q_{20} \rangle^3 - 6\langle Q_{20} \rangle \langle Q_{22} \rangle^2)]^{1/3} - \tfrac{1}{2} m\omega_0^{02} \langle R^2 \rangle . \tag{9}$$

The aim is to write (9) as the *Hartree expectation value* of a rotational scalar, involving direct factorization. This means that the expectation value of a product of one-body operators is approximated by the corresponding product of expectation values of these operators. Now, there are only two scalar invariants that can be formed from the quadrupole operators, namely $Q_2 \cdot Q_2 = 5^{1/2}(Q_2 Q_2)_0$ and $(Q_2 Q_2 Q_2)_0$, where $(\cdots)_0$ denotes angular momentum coupling to spin zero. It is a straightforward exercise to show that the Hartree expectation values of these invariants are

$$\langle Q_2 \cdot Q_2 \rangle = \langle Q_{20} \rangle^2 + 2\langle Q_{22} \rangle^2, \quad \langle (Q_2 Q_2 Q_2)_0 \rangle = -(\tfrac{2}{35})^{1/2} (\langle Q_{20} \rangle^3 - 6\langle Q_{20} \rangle \langle Q_{22} \rangle^2). \tag{10}$$

Equation (9) can now be written as the Hartree expectation value of a rotational scalar interaction V,

$$\langle U_D \rangle = \langle V \rangle , \tag{11}$$

in a number of ways, depending on the treatment of the $\langle R^2 \rangle$ terms. The most direct way is to replace $\langle R^2 \rangle$ by R^2 to give

$$\begin{aligned} V &= \frac{m\omega_0^{02}}{2} \left[(R^2)^3 - \frac{12\pi}{5} R^2 (Q_2 \cdot Q_2) - \frac{8\pi}{5} (14\pi)^{1/2} (Q_2 Q_2 Q_2)_0 \right]^{1/3} - \frac{m\omega_0^{02}}{2} R^2 \\ &= \frac{m\omega_0^{02}}{2} \langle R^2 \rangle \left[1 + \frac{(R^2)^3 - \langle R^2 \rangle^3}{\langle R^2 \rangle^3} - \frac{12\pi}{5} R^2 \frac{(Q_2 \cdot Q_2)}{\langle R^2 \rangle^3} - \frac{8\pi}{5} (14\pi)^{1/2} \frac{(Q_2 Q_2 Q_2)_0}{\langle R^2 \rangle^3} \right]^{1/3} - \frac{m\omega_0^{02}}{2} R^2 . \end{aligned} \tag{12}$$

Other possibilities for V are left to a longer publication. The interaction V may be expanded in powers of $\langle R^2 \rangle^{-1}$ as follows:

$$\begin{aligned} V = -\tfrac{1}{2}\chi \Bigg[& Q_2 \cdot Q_2 - \left(\frac{R^2 - \langle R^2 \rangle}{\langle R^2 \rangle} \right) (Q_2 \cdot Q_2) + \frac{2}{3} (14\pi)^{1/2} \frac{(Q_2 Q_2 Q_2)_0}{\langle R^2 \rangle} \\ & + \left(\frac{R^2 - \langle R^2 \rangle}{\langle R^2 \rangle} \right)^2 (Q_2 \cdot Q_2) - \frac{4}{3} (14\pi)^{1/2} \left(\frac{R^2 - \langle R^2 \rangle}{\langle R^2 \rangle} \right) \frac{(Q_2 Q_2 Q_2)_0}{\langle R^2 \rangle} + \frac{4\pi}{5} \frac{(Q_2 \cdot Q_2)^2}{\langle R^2 \rangle^2} + O\left(\frac{1}{\langle R^2 \rangle^3} \right) \Bigg], \end{aligned} \tag{13}$$

where $\chi = 4\pi m\omega_0^{02}/5\langle R^2 \rangle$.

The leading term in the expansion (13) is just the familiar quadrupole-quadrupole interaction with the strength χ appropriate to taking all nucleons into account.[9] The expansion parameter for spherical nuclei is reasonably small, being of the order of the quadrupole zero-point amplitude β_2. The successive terms in the expansion bring in many-body forces of increasingly higher order. Thus, the leading-order quadrupole-quadrupole interaction contains two-body and one-body terms; the next order brings in three-body as well as two- and one-body interactions, etc.

Next, it shall be shown that V gives rise to a self-consistent Hartree potential which is identical to the Nilsson oscillator potential. The first step is to express $U_{\rm osc}$ at equilibrium in terms of appropriate deformation parameters. From the inverse of Eq. (8) together with (6), one obtains

$$\langle Q_{20}\rangle=\left(\frac{5}{16\pi}\right)^{1/2}\left(\frac{2}{\omega_z^{\,2}}-\frac{1}{\omega_x^{\,2}}-\frac{1}{\omega_y^{\,2}}\right)\omega_0^{\,02}\Lambda,\quad \langle Q_{22}\rangle=\langle Q_{2-2}\rangle=\left(\frac{15}{32\pi}\right)^{1/2}\left(\frac{1}{\omega_y^{\,2}}\right)\omega_0^{\,02}\Lambda,$$
$$\langle R^2\rangle=\left(\frac{1}{\omega_x^{\,2}}+\frac{1}{\omega_y^{\,2}}+\frac{1}{\omega_z^{\,2}}\right)\omega_0^{\,02}\Lambda. \tag{14}$$

It is convenient to choose as deformation parameters the ratios σ_0 and σ_2 defined by[10]

$$\sigma_0=(\tfrac{4}{5}\pi)^{1/2}\langle Q_{20}\rangle/\langle R^2\rangle,\quad \sigma_2=(\tfrac{4}{5}\pi)^{1/2}\langle Q_{22}\rangle/\langle R^2\rangle. \tag{15}$$

Then, from (14), (15), and the VC condition (4), one may solve for the oscillator frequencies as functions of σ_0 and σ_2 as follows:

$$\omega_x^{\,2}=(1+2\sigma_0)(1-\sigma_0-6^{1/2}\sigma_2)\omega_0^{\,2},\quad \omega_y^{\,2}=(1+2\sigma_0)(1-\sigma_0+6^{1/2}\sigma_2)\omega_0^{\,2},$$
$$\omega_z^{\,2}=(1-\sigma_0+6^{1/2}\sigma_2)(1-\sigma_0-6^{1/2}\sigma_2)\omega_0^{\,2}, \tag{16}$$

where

$$\omega_0^{\,2}=[(1+2\sigma_0)(1-\sigma_0+6^{1/2}\sigma_2)(1-\sigma_0-6^{1/2}\sigma_2)]^{-2/3}\omega_0^{\,02}. \tag{17}$$

In terms of the parametrization (16), $U_{\rm osc}$ may be written in the form

$$\begin{aligned}U_{\rm osc}&=\tfrac{1}{2}m\omega_0^{\,02}R^2+U_D\\&=\tfrac{1}{2}m\omega_0^{\,2}[(1-\sigma_0^{\,2}-2\sigma_2^{\,2})R^2-(\sigma_0-\sigma_0^{\,2}+2\sigma_2^{\,2})(\tfrac{16}{5}\pi)^{1/2}Q_{20}-\sigma_2(1+2\sigma_0)(\tfrac{16}{5}\pi)^{1/2}(Q_{22}+Q_{2-2})].\end{aligned} \tag{18}$$

If one starts with the nuclear Hamiltonian $H=H_0+V$, the Hartree potential $U_{\rm H}$ arising from V may be defined by

$$U_{\rm H}=\langle\partial V/\partial R^2\rangle R^2+\textstyle\sum_\mu\langle\partial V/\partial Q_{2\mu}\rangle Q_{2\mu}, \tag{19}$$

where $\langle\cdots\rangle$ denotes the Hartree expectation value with respect to the self-consistent ground state. It is a straightforward exercise to show that

$$\langle\partial V/\partial R^2\rangle=\tfrac{1}{2}m\omega_0^{\,2}(1-\sigma_0^{\,2}-2\sigma_2^{\,2})-\tfrac{1}{2}m\omega_0^{\,02},\quad \langle\partial V/\partial Q_{20}\rangle=-\tfrac{1}{2}m\omega_0^{\,2}(\sigma_0-\sigma_0^{\,2}+2\sigma_2^{\,2})(\tfrac{16}{5}\pi)^{1/2},$$
$$\langle\partial V/\partial Q_{22}\rangle=\langle\partial V/\partial Q_{2-2}\rangle=-\tfrac{1}{2}m\omega_0^{\,2}\sigma_2(1+2\sigma_0)(\tfrac{16}{5}\pi)^{1/2}, \tag{20}$$

with all other expectation values vanishing, and with Eq. (15) playing the role of the Hartree self-consistency conditions. From Eqs. (18)–(20) it is seen that U_D and $U_{\rm H}$ are identical in form. It still remains to be proven that the Hartree self-consistency conditions (15) are equivalent to the VC conditions (6). This result easily follows by combining Eqs. (8) with (15) to yield

$$\frac{\langle\sum_{i=1}^{A}x_i^{\,2}\rangle}{1-\sigma_0+6^{1/2}\sigma_2}=\frac{\langle\sum_{i=1}^{A}y_i^{\,2}\rangle}{1-\sigma_0-6^{1/2}\sigma^2}=\frac{\langle\sum_{i=1}^{A}z_i^{\,2}\rangle}{1+2\sigma_0}, \tag{21}$$

which may be converted to (6) with the aid of Eqs. (16). It may therefore be concluded that

$$U_{\rm H}=U_D. \tag{22}$$

The point has often been made that in the Nilsson model, the total energy (apart from the pairing energy) is the expectation value of the independent-particle Hamiltonian, in contrast to the Hartree(-Fock) method in which the energy contains a correction term subtracting $\frac{1}{2}$ of the expectation value of the two-body interaction to prevent double counting.[6,7] Since it has just been shown that the Nilsson model is equivalent to a Hartree approximation, is there a contradiction? The answer is negative for the simple reason that the Hartree potential is arbitrary up to an additive constant, and the choice (19) already tacitly includes the constant which compensates for overcounting many-body interactions. It is worthwhile to understand just how this occurs. From Eq. (13), it is seen first of all that since V contains no pure monopole terms and that since the monopole-quadrupole cross terms depend on powers of $R^2 - \langle R^2 \rangle$, they do not contribute to $\langle V \rangle$ in the Hartree approximation, which therefore contains contributions only from pure quadrupole interactions. Second, the Hartree potential obtained by direct factorization of (13) differs from (19) by the replacement $R^2 \to R^2 - \langle R^2 \rangle$ and therefore this term would give a vanishing expectation value. Hence, in the actual choice of $U_{\rm H}$ given by (19), the constant $\langle \partial V/\partial R^2 \rangle \langle R^2 \rangle$ has been added on already. Since, as follows from (11) and (22), $\langle U_{\rm H} \rangle = \langle V \rangle$, this constant compensates for overcounting of the pure quadrupole interactions in the quadrupole field of $U_{\rm H}$. One must therefore have the identity $\langle V \rangle = \langle \partial V/\partial R^2 \rangle \langle R^2 \rangle + \sum_\mu \langle \partial V/\partial Q_{2\mu} \rangle \langle Q_{2\mu} \rangle$, which is easily established directly.[11]

It can be shown that the rotationally invariant many-body interaction V naturally explains the rotationally noninvariant two-body interactions used in random-phase approximation calculations of deformed nuclei,[12] most recently in connection with the splitting of the giant quadrupole resonance.[13] But this and other possible consequences shall be left to a longer paper.

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[10]In the case of axial symmetry when $\sigma_2 = 0$, the usual Nilsson parameter δ is related to σ_0 by $\delta = 3\sigma_0/2(1+\sigma_0)$.

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