Properties of the nucleon-nucleon interaction leading to a standing wave instability in symmetric nuclear matter

Janusz Skalski*
Sołtan Institute for Nuclear Studies, ul. Hoża 69, PL-00 681 Warsaw, Poland
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We examine a recently proposed nucleon-nucleon interaction, claimed by its authors both to be realistic and to lead to a standing-wave instability in symmetric nuclear matter. Contrary to these claims, we find that this interaction leads to a serious overbinding of ^{4}He, ^{16}O, and ^{40}Ca nuclei when the Hartree-Fock method is properly applied. The resulting nuclear densities contradict the experimental data and all realistic Hartree-Fock results.

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Recently, a simple nucleon-nucleon interaction was proposed which claimed to be both realistic and to lead to a standing-wave instability in symmetric nuclear matter [1]. Although, strictly speaking, symmetric nuclear matter is a purely speculative object, it served for years as a testing ground for nuclear many-body theories, and insights into its properties are of considerable interest. The hint that all these theories missed the spatial modulation of the nuclear matter density is provocative. When putting forward such a claim, one has to make sure that the proposed interaction satisfies constraints imposed by our knowledge of nuclear physics.

The interaction considered in Ref. [1] reads

$$V(\mathbf{r}_1,\mathbf{r}_2)=-\alpha C(\mathbf{r}_1-\mathbf{r}_2)^2 e^{-(\mathbf{r}_1-\mathbf{r}_2)^2/s^2}+\beta\sqrt{\langle T\rangle}\,\delta(\mathbf{r}_1-\mathbf{r}_2), \tag{1}$$

where $\langle T\rangle$ is the center-of-mass corrected average kinetic energy:

$$\langle T\rangle=\left(\frac{1-1/A}{A}\right)\frac{\hbar^2}{2m}\sum_{i=1}^{A}|\nabla\phi_i|^2. \tag{2}$$

In the latter equation, single-particle orbitals ϕ_i, relevant for a Hartree-Fock (HF) treatment, are explicitly introduced. The auxiliary constant is $C=2\pi^{-3/2}s^{-5}/3$, while the strength and range of attraction and the strength of contact repulsion are chosen as $\alpha=1690$ MeV fm^3, $s=0.54$ fm, and $\beta=225$ MeV [1]. These parameters were intended to fit the binding energy and equilibrium density of nuclear matter and the binding energy of an alpha particle (but see below). With these parameters, the authors reported reasonable values of the compressibility modulus of nuclear matter and of binding energies of even-even $N=Z$ nuclei.

It is crucial to understand that, although the authors referred to the HF method when describing their calculations for finite nuclei [1], in fact they performed only a very restricted minimization. This restriction is evident in the very small harmonic-oscillator basis that was used. In addition, the exchange integrals were not calculated, but assumed to be a fraction of the direct terms, depending on the average kinetic energy. Therefore, especially in view of the quite important consequences claimed, an independent evaluation of the results of Ref. [1] is called for.

In this Brief Report we report the results of regular HF calculations with interaction (1) by which we determined binding energies of ^{4}He, ^{16}O, and ^{40}Ca nuclei. These binding energies are at variance with Ref. [1] and the obtained matter and charge densities of ^{16}O and ^{40}Ca are highly unusual.

As interaction (1) is spin and isospin independent, one assumes a fourfold degeneracy of the HF orbitals for the even-even $N=Z$ nuclei of interest. There are $A/4$ independent orbitals, and we sum over them to obtain the density $\rho=\Sigma_{i=1}^{A/4}|\phi_i|^2$. Neutron and proton densities are equal, $\rho_n=\rho_p=2\rho$, and the total density is equal to 4ρ. Similarly, the total average kinetic energy $\langle T\rangle$ is quadruple that of the sum of kinetic terms over independent orbitals.

The HF energy reads

$$\begin{aligned}E=\langle T\rangle&+8\int\int d^3r_1 d^3r_2\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)V_a(\mathbf{r}_1-\mathbf{r}_2)\\&-2\sum_{i,j}^{A/4}\int\int d^3r_1 d^3r_2\phi_i^*(\mathbf{r}_1)\phi_j^*(\mathbf{r}_2)\phi_j(\mathbf{r}_1)\phi_i(\mathbf{r}_2)\\&\times V_a(\mathbf{r}_1-\mathbf{r}_2)+6\beta\langle T\rangle^{1/2}\int d^3r\rho^2,\end{aligned} \tag{3}$$

where V_a is the attractive part of Eq. (1). Remembering the differentiation of $\langle T\rangle$, from Eq. 3 we obtain a set of HF equations for the wave functions ϕ_i and single-particle energies ϵ_i,

$$\begin{aligned}-\frac{\hbar^2}{2m^*}\nabla^2\phi_i&+3\beta\sqrt{\langle T\rangle}\rho\phi_i+4\int d^3r_2\rho(\mathbf{r}_2)V_a(\mathbf{r}_1-\mathbf{r}_2)\phi_i\\&-\sum_{j}^{A/4}\int d^3r_2\phi_j^*(\mathbf{r}_2)\phi_j(\mathbf{r}_1)\phi_i(\mathbf{r}_2)V_a(\mathbf{r}_1-\mathbf{r}_2)=\epsilon_i\phi_i,\end{aligned} \tag{4}$$

where the effective mass is given by $m/m^*=(1-1/A)\times[1+3\beta I/(A\sqrt{\langle T\rangle})]$, with $I=\int d^3r\rho^2$.

The numerical solution for ϕ_i is straightforward, but tedious, due to the exchange integrals. For spherically sym-

*Email address: jskalski@fuw.edu.pl

metric completely filled shells, there is, however, a well-known Slater method [2] to obtain the exact exchange potential. Adapting this general argument to the attractive potential V_a we can express the exchange potential, acting on the wave function $\phi_{n'l'm'}(r,\theta,\varphi)=R_{n'l'}(r)Y_{l'm'}(\theta,\varphi)$, as

$$V_{aEx}\phi_{n'l'm'}=Y_{l'm'}\sum_{nl} R_{nl}(r)\left\{\sum_{k=|l-l'|}^{l+l'}\frac{2l+1}{2l'+1}A(k,l,l') \times\int_0^\infty dr_2 r_2^2 R_{nl}(r_2)R_{n'l'}(r_2)V_k(r,r_2)\right\}, \quad (5)$$

where the subshell index (nl) in the summation runs over the occupied orbitals. The coefficients $A(k,l,l')$ are given by

$$A(k,l,n)=\frac{2n+1}{2}\int_{-1}^{1}P_kP_lP_n, \quad (6)$$

where P_i are Legendre polynomials. The functions V_k define the expansion of V_a into spherical harmonics,

$$V_a(\mathbf{r}_1,\mathbf{r}_2)=\sum_k V_k(r_1,r_2)P_k(\cos\theta), \quad (7)$$

$$V_k(r_1,r_2)=-\alpha Cs^2e^{-(r_1^2+r_2^2)/s^2}(2k+1) \times\left[\left(k+1+\frac{r_1^2+r_2^2}{s^2}\right)f_k(z)-zf_{k-1}(z)\right], \quad (8)$$

where f_k are the spherical Bessel functions of the imaginary argument, i.e., $f_k(z)=(-i)^k j_k(iz)=\sqrt{\pi/(2z)}I_{k+1/2}(z)$, with $I_{k+1/2}(z)$ the modified Bessel function [3] and $z=2r_1r_2/s^2$.

In order to check the HF results, we used two different schemes: one spherical, using decomposition (5), and the other three dimensional. Both use wave functions defined over a spatial mesh. The general three-dimensional scheme being more time-consuming practically restricts the mesh size to about 30 points in each direction in one octant of space. The spherical scheme allows radial meshes of 100 points or more, and may easily produce accurate solutions.

We consider magic ^{4}He, ^{16}O, and ^{40}Ca nuclei for which spherically symmetric solutions are expected. The HF problem was solved by the imaginary-time evolution. The convergence is rather slow for density and single-particle energies, especially for ^{40}Ca. This is due to the buildup of a central density peak which costs little energy in the final stages of iteration. The three-dimensional scheme becomes impractical in this case, but still its results tend toward those of the spherical code. Below, we report densities calculated with the faster spherical code on a mesh of 100 points.

As the starting wave functions, we took the results of Ref. [1]. Therefore, we could compare our initial energies and densities with those of Ref. [1]. For ^{4}He we obtain the same energy as in Ref. [1], but for ^{16}O and ^{40}Ca we find differences. These must be attributed to the error in energy introduced in Ref. [1] by an approximate treatment of the exchange integrals. Indeed, the integrals calculated analytically for s- and p-wave functions in ^{16}O agree exactly with the results of our numerical codes. The correct values of the binding energy per nucleon for initial configurations are 8.801 MeV in ^{16}O and 11.137 MeV in ^{40}Ca, to be compared to 8.59 and 10.76 MeV reported in Ref. [1]. Thus the exact calculation of the exchange integrals alone points to the overbinding problem with interaction (1). This problem is magnified if one cares about the HF solutions.

TABLE I. Calculated HF binding energies per nucleon vs results of Ref. [1] and the difference between total quantities (in MeV).

	B/A	B/A in Ref. [1]	$B-B$ [1]
^{4}He	8.08	7.3	3.11
^{16}O	10.85	8.59	36.13
^{40}Ca	14.13	10.76	134.77

The first issue is the binding energy of alpha particle, which bears on the determination of interaction constants [1]. The optimal wave function is more peaked than the Gaussian used there. The HF binding energy per nucleon is 8.076 MeV, i.e., 0.78 MeV more than in Ref. [1], where the experimental value corrected for the Coulomb interaction was used. Thus interaction (1) already overbinds ^{4}He when properly treated.

The results for three nuclei are collected in Table I. As seen there, the overbinding of ^{16}O, and especially ^{40}Ca, is very serious. For ^{16}O, the calculated binding is 173.57 MeV, without Coulomb interaction, while the experimental value is 127.619 MeV [4]. Allowing about 13 MeV for the Coulomb energy (the direct term minus exchange, as it results from any realistic HF treatment), we obtain more than 30-MeV overbinding. For ^{40}Ca, the calculated binding of 565.17 MeV, even after subtraction of about 71 MeV of Coulomb repulsion, is larger than the experimental value of 342.052 MeV by about 152 MeV [4]. In Table I, we also give the difference in total binding (without Coulomb) between our results and those of Ref. [1] to emphasize the importance of proper HF minimization.

The calculated self-consistent nuclear densities are depicted in Fig. 1. The tendency toward a central peak development is evident. It is worth noting that this tendency was already seen in inaccurate results of Ref. [1]. The density of

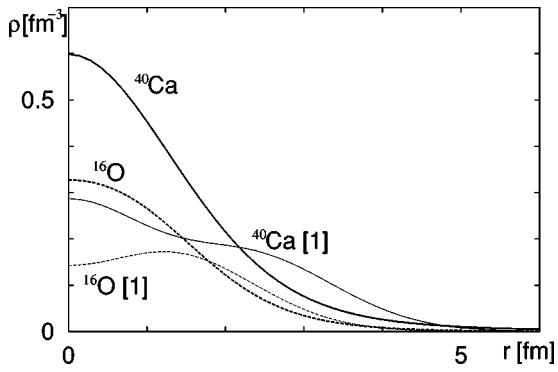

FIG. 1. Total nuclear HF densities (thick lines) and densities from Ref. [1] (thin lines) for ^{16}O (dashed) and ^{40}Ca (solid).

the ^{40}Ca shown there exhibits a strange pileup in the center. However, the HF results shown in Fig. 1 allow one to appreciate that this problem is even more grave: The central density is more than 1.5 times larger in the case of ^{16}O, and three times larger in ^{40}Ca than the experimental one (see, e.g., Ref. [5]).

Exact HF calculations with the recently proposed interaction [Eq. (1)] for magic ^{4}He, ^{16}O, and ^{40}Ca nuclei show a serious overbinding problem. Associated nuclear densities develop central peaks, taking a form unknown in nuclear physics. Both deficiencies grow with increasing mass. In view of the above results, it is clear that the interaction proposed in Ref. [1] is very far from a realistic nucleon-nucleon force. Therefore, assertions about the standing-wave instability in nuclear matter made there, as related to unrealistic interaction, are unfounded.

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