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

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We examine a recently proposed nucleon-nucleon interaction, claimed by its authors both realistic and leading 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.

I. INTRODUCTION

Recently, a simple nucleon-nucleon interaction was proposed which is claimed both realistic and leading 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 new 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 claim, one has to make sure that the proposed interaction satisfies constraints imposed by our knowledge of nuclear physics.

The interaction considered in [1] reads

\[
V(r_1, r_2) = -\alpha C(r_1 - r_2)^2 e^{-(r_1 - r_2)^2/s^2} + \beta \sqrt{< T >} \delta(r_1 - r_2),
\]

where \( < T > \) is the center-of-mass corrected average kinetic energy:

\[
< T > = \left(1 - \frac{1}{A}\right) \frac{\hbar^2}{2m} \sum_{i=1}^{A} | \nabla \phi_i |^2.
\]

In the latter equation, single-particle orbitals \( \phi_i \) relevant for the Hartree-Fock (HF) treatment are explicitly introduced. The auxiliary constant \( C = 2\pi^{-3/2}s^{-5/3} \), while the strength and range of attraction and the strength of contact repulsion are chosen as \( \alpha = 1690 \text{ MeV fm}^3 \), \( s = 0.54 \text{ fm} \), \( \beta = 225 \text{ MeV} \). These parameters were intended to fit the binding energy and the equilibrium density of nuclear matter and the binding energy of 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 refer to the HF method when describing their calculations for finite nuclei [1], they performed in fact only a very restricted minimization. This restriction is evident in a very small harmonic oscillator basis that has been 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 quite important consequences claimed, an independent evaluation of the results of Ref. [1] is called for.

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

II. HARTREE-FOCK METHOD

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

\[
E = < T > + 8 \int d^3r_1d^3r_2 \rho(r_1) \rho(r_2) V_a(r_1 - r_2) - 2 \sum_{i,j}^{A/4} \int d^3r_1d^3r_2 \phi^*_i(r_1) \phi^*_j(r_2) \phi_j(r_1) \phi_i(r_2) V_a(r_1 - r_2) + 6 \beta < T >^1/2 \int d^3r \rho^2,
\]

(3)

where \( V_a \) is the attractive part of (1). Remembering about differentiation of \( < T > \), we obtain from (3) a set of HF equations for the wave functions \( \phi_i \) and single-particle energies \( \epsilon_i \)

\[
-\frac{\hbar^2}{2m^*} \nabla^2 \phi_i + 3\beta \sqrt{< T >} \rho \phi_i + 4 \int d^3r_2 \rho(r_2) V_a(r_1 - r_2) \phi_i - \sum_{j}^{A/4} \int d^3r_2 \phi^*_j(r_2) \phi_j(r_1) \phi_i(r_2) V_a(r_1 - r_2) = \epsilon_i \phi_i,
\]

(4)

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

The numerical solution for \( \phi_i \) is straightforward, but tedious due to the exchange integrals. For spherically symmetric 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

\[
V_{aEx}(\phi_{n'l'm'}) = Y_{l'm'} \sum_{nl} R_{nl}(r) \left\{ \frac{2l+1}{2l' + 1} A(k, l, l') \int_0^\infty dr_2 r_2^2 R_{nl}(r_2) R_{n'l'}(r_2) V_a(r_1, r_2) \right\},
\]

(5)

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

\[
A(k, l, n) = \frac{2n+1}{2} \int_{-1}^{1} P_k P_l P_n,
\]

(6)

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

\[
V_a(r_1, r_2) = \sum_k V_k(r_1, r_2) P_k(\cos \theta),
\]

(7)

\[
V_k(r_1, r_2) = -\alpha C \rho^2 e^{-\left(r_1^2 + r_2^2\right)/s^2} (2k + 1)[(k + 1 + \frac{r_1^2 + r_2^2}{s^2}) f_k(z) - z f_{k-1}(z)],
\]

(8)

where \( f_k \) are the spherical Bessel functions of the imaginary argument, i.e. \( f_k(z) = (-i)^k j_k(i z) = \sqrt{\pi/(2z)} I_{k+1/2}(z) \), with \( I_{k+1/2}(z) \) the modified Bessel function [3] and \( z = 2r_1 r_2 / s^2 \).

III. RESULTS AND DISCUSSION

In order to have a check on the HF results we used two different schemes, one spherical, using decomposition [3], 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 \( ^4\text{He} \), \( ^{16}\text{O} \) and \( ^{40}\text{Ca} \) nuclei for which the 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 \( ^{40}\text{Ca} \). This is due to the buildup of central density peak which costs little energy in final stages of iteration. The three-dimensional scheme becomes impractical in this case but still its results tend to those of the spherical code. Below, we report densities calculated with the faster spherical code on the mesh of 100 points.
As the starting wave functions we took the results of [1]. Therefore we could compare our initial energies and densities with those of [1]. We obtain for $^4$He the same energy as in [1], but for $^{16}$O and $^{40}$Ca we find differences. These must be attributed to the error in energy introduced in [1] by the 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 MeV and 10.76 MeV reported in [1]. Thus, the exact calculation of the exchange integrals alone points to the overbinding problem with the interaction (1). This problem is magnified if one cares for the HF solutions.

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 [1] where the experimental value corrected for Coulomb interaction was used. Thus, the interaction (1) overbinds already $^4$He when properly treated.

The results for three nuclei are collected in Table 1. As seen there, the overbinding of $^{16}$O, and especially $^{40}$Ca, is really serious. For $^{16}$O, the calculated binding is 173.57 MeV without Coulomb while the experimental value is 127.619 MeV [4]. Allowing about 13 MeV for Coulomb energy (the direct term minus exchange, as it results from any realistic HF) we get 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 by about 152 MeV (!) larger than the experimental value of 342.052 MeV [4]. In Table 1, we also give the difference in total binding (without Coulomb) between our results and those of [1] to emphasise the importance of proper HF minimization.

The calculated self-consistent nuclear densities are depicted in Figure 1. The tendency towards central peak development is evident. It is worth noting that this tendency is already seen in inaccurate results of [1]. The density of the $^{40}$Ca shown there exhibits a strange pile-up in the center. However, the HF results shown in Figure 1 allow 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. [5]).

IV. CONCLUSIONS

The exact HF calculations with the recently proposed interaction (1) for magic $^4$He, $^{16}$O and $^{40}$Ca nuclei show a serious overbindig 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 (1) is very far from a realistic nucleon-nucleon force. Therefore, the assertions about the standing wave instability in nuclear matter made there, as related to unrealistic interaction, are unfounded.

[1] A. E. Pozamantir and A. W. Overhauser, Phys. Rev. C 64 (2001) 014302, and 014303
[2] J.C. Slater, Phys. Rev. 81 (1951) 85, and in Quantum Theory of Atomic Structure, Vol. 1 and 2 (Mc Graw - Hill, New-York, Toronto, London, 1960)
[3] A. Abramowitz and I. A. Stegun eds., Handbook of mathematical functions (National Bureau of Standards, 1964)
[4] G. Audi and A. H. Wapstra, Nuclear Physics 595 (1995) 409
[5] C. J. Batty et al., Advances in Nuclear Physics, Vol. 19 (1989) p.1
TABLE 1 - Calculated HF binding energies per nucleon vs. results of [1] and the difference between total quantities (in [MeV]).

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

Figure caption

Figure 1

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