Single particle spectrum and binding energy of nuclear matter

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Abstract. In non-relativistic Brueckner calculations of nuclear matter, the self-consistent single particle potential is strongly momentum dependent. To simplify the calculations, a parabolic approximation is often used in the literature. The variation in the binding energy value introduced by the parabolic approximation is quantitatively analyzed in detail. It is found that the approximation can introduce an uncertainty of 1-2 MeV near the saturation density.

PACS: 21.65.+f , 24.10.Cn , 45.50.Jf , 21.30.-x , 26.60.+c

1. Introduction

It is one of the fundamental issue in nuclear physics to evaluate the nuclear matter binding energy and saturation properties, starting from a realistic nucleon-nucleon (NN) interaction with no free parameter. This old project requires the solution of a complex many-body problem, and has received several contributions and improvements along the years, beginning as far back as the middle of the last century. One of the main approaches to this long standing problem is the so-called hole-expansion or Bethe-Brueckner-Goldstone (BBG) theory [1]. The first real breakthrough in this scheme was the introduction of the self-consistent single particle potential at the two hole-line level of approximation, which is then usually referred as the Brueckner-Hartree-Fock (BHF) approximation [2, 1]. The introduction of the self-consistent potential drastically improves the results. In particular, the binding energy and saturation density, which otherwise would turn out unreasonable, move to values which can be considered an acceptable starting approximation. The remaining discrepancy could be summarized in the celebrated “Coester band” [1], along which the saturation points for different NN interactions were clustering and which misses the empirical region (corresponding approximately to a binding energy per nucleon of -16 MeV and a nucleon density of 0.17 \( fm^{-3} \)). Later, the Liége group stressed [5] the relevance of the choice of the single particle potential. In particular they suggested the use of the “continuous choice”, which indeed appears to move the saturation point towards the empirical one, but still missing it [5, 6]. A period of major developments took place in the latest two decades. Starting from the works by B.D. Day [3], the hole-line expansion was analysed up to the three hole-line level of approximation. A strong indication of convergence of the expansion was obtained [3, 7]. Furthermore, BHF calculations with the continuous choice seem to get a substantially smaller corrections from three-body correlations [7]. The results confirm that the empirical saturation point is
still missed, and therefore that three-body forces are needed in the nuclear hamiltonian [3]. In the meanwhile the relativistic Dirac-Brueckner (DB) method was developed [8], which already at the two hole-line level of approximation appears to be able to reproduce the empirical saturation point. The main relativistic correction introduced by the DB method is due to the structure of the Dirac 4-spinors, which in the medium appear “rotated” with respect to the free ones. The non-relativistic three-body forces and this relativistic effect of the DB approach are probably two faces of the same dynamical effect [9]. The many-body theory has reached, therefore, such a precision that it is possible to test the nuclear hamiltonian. Because of that, the time seems to be appropriate to check the reliability of the approximations which are commonly employed in BBG calculations of nuclear matter.

In this letter we consider the BHF in the continuous choice and we analyze quantitatively the uncertainty of the results which comes out by approximating the single particle self-consistent potential with a parabolic form. This approximation is quite popular, since it allows to calculate the potential, at each iteration, only for few momenta, thus reducing drastically the computer time. The single particle potential, as obtained from fully self-consistent BHF calculations, is indeed strongly momentum dependent and not necessarily so simple as a parabola.

2. Sketch of the formalism

In the BHF approximation, the nuclear matter total energy \( E \) is obtained from the Brueckner G-matrix \( G(\omega) \) according to the equation

\[
E = \sum_{k_1<k_F} \frac{\hbar^2 k_1^2}{2m} + \frac{1}{2} \sum_{k_1,k_2<k_F} \langle k_1 k_2 | G(e_{k_1} + e_{k_2}) | k_3 k_4 \rangle_A
\]

(1)

with \( |k_1 k_2\rangle_A = |k_1 k_2\rangle - |k_2 k_1\rangle \). Here \( k_F \) is the Fermi momentum, the summation over the momenta \( k_i \) include spin and isospin variables. The single particle energies \( e_k \), appearing in the entry energy of the G-matrix, are given by

\[
e(k) = \frac{\hbar^2 k^2}{2m} + U(k)
\]

(2)

where the single particle potential \( U(k) \) is determined by the self-consistent equation

\[
U(k) = \sum_{k'<k_F} \langle kk'| G(e_{k_1} + e_{k_2}) | kk' \rangle
\]

(3)

The self-consistency is coupled with the integral equation for the G-matrix

\[
\langle k_1 k_2 | G(\omega) | k_3 k_4 \rangle = \langle k_1 k_2 | v | k_3 k_4 \rangle +
\]

\[
+ \sum_{k_3' k_4'} \langle k_1 k_2 | v | k_3' k_4' \rangle \frac{(1-\Theta_F(k_3'))(1-\Theta_F(k_4'))}{\omega-e_{k_3'}-e_{k_4'}} \langle k_3' k_4' | G(\omega) | k_3 k_4 \rangle
\]

(4)

where \( \Theta_F(k) = 1 \) for \( k < k_F \) and is zero otherwise. The product \( Q(k, k') = (1 - \Theta_F(k))(1 - \Theta_F(k')) \), appearing in the kernel of Eq. (4), enforces the scattered momenta
to lie outside the Fermi sphere, and it is commonly referred as the “Pauli operator”. The
self-consistent set of equations are usually solved by an iteration procedure. The G-matrix
can be expanded in partial waves, according to the classification of two-nucleon channels
\[1\]. To avoid coupling between different two-body channels, the Pauli operator \( Q \), as
well as the two-body energies \( e_{k'} + e_{k''} \) in the denominator, are averaged over the angle
between the relative momentum \( q = (k'_3 - k'_4)/2 \) and the total momentum \( P = k'_3 + k'_4 \).
Despite this approximation, which has been tested recently in ref. \[10\], the numerical
solution of the coupled equations (3),(4) is quite time consuming, since the single particle
potential \( U(k) \) must be calculated in a wide range of momenta with a fine enough grid. If
one assumes that the potential \( U(k) \), or equivalently the single particle energy \( e(k) \), has
approximately a quadratic form
\[
e(k) \approx e_0 + \frac{h^2 k^2}{2m^*} \tag{5}
\]
then one can calculate the potential, at each iteration step, in few points only and inter-
polate the obtained values with a parabola. The approximation of Eq. (5) is usually
called the effective mass approximation, since then the spectrum has the same shape as
the free one but with an “effective mass” \( m^* \).

In order to test this approximation, we have performed a set of BHF calculations fully
self-consistently without any assumption about the potential shape, as well as by forcing
the potential to a parabolic shape by means a fitting procedure, and then compared the
results.

3. Results and discussion

The performed BHF calculations include all two-body channels up to total angular mo-
momentum \( J = 11\hbar \). In a set of calculations we adopted the Argonne v18 \[11\] potential as
the NN interaction. This potential belong to a new generation of realistic NN potentials,
with an improved fit of the scattering data, which give similar results and cluster closely
together in the Coester band \[12\]. The self-consistent single particle potential \( U(k) \) was
calculated up to the momentum cut-off \( k_{max} = 7.5 fm^{-1} \), which turns out to be large
enough in the considered density range \[13\]. The potential, for the Fermi momentum
\( k_F = 1.4 fm^{-1} \), is displayed in Fig. 1 (full circles). It is numerically calculated with a grid
step of \( 0.1 fm^{-1} \) from the G-matrix, Eq. (3), and inserted as the entry potential at each
iteration step, until convergence is reached, i.e. the potential and the binding energy are
stable under iteration with good accuracy. Stability within few KeV of the binding was
systematically reached. The numerical method is described in ref. \[6\]
The quadratic approximation, at each step of the iteration procedure, is introduced by
fitting the potential up to a certain maximum momentum \( k_{FIT} \). For definiteness, we have
considered in detail two choices, namely \( k_{FIT} = 2k_F \) and \( k_{FIT} = k_{max} \). At each iteration
step, the potential \( U(k) \) coming directly from the G-matrix calculation is fitted with a
parabola, which is then used as the entry potential for the next iteration. Convergence is
reached when both potentials remain stable under this procedure. In this procedure one
obtains, therefore, two potentials, one calculated from the G-matrix with the parabolic
input, and one from the parabolic fit to this potential. Of course, if the potential coming directly from the G-matrix were indeed parabolic, the two potentials would closely agree. For the choice \( k_{FIT} = 2k_F \), in Fig. 1 the two potentials at convergence are displayed. In principle, one can calculate the nuclear matter binding energy from both potentials, but the result will be in general slightly different. As one can see, the fully self-consistent potential, obtained without any fitting procedure, as specified above, does not coincide with anyone of the two previous potentials, and these differences give a quantitative indication of the uncertainty introduced by the parabolic approximation. The corresponding saturation curves are reported in Fig. 2a. The parabolic potential produces a saturation curve in fair agreement with the one reported e.g. in ref. [10]. Around saturation the parabolic approximation introduces a shift in the binding of 1-2 MeV. The two choices for the potentials, discussed above, give different binding, since \( U(k) \) is not really parabolic, and the fitting procedure introduces necessarily an approximation. Another uncertainty is coming from the choice of \( k_{FIT} \), as can be seen in Fig. 2b, where the results for \( k_{FIT} = k_{max} \) are reported. In this case the discrepancy are larger for lower density, since then the potential \( U(k) \) becomes indeed flatter at momenta below \( k_F \). A more complete account of the dependence on the fitting range is reported in Fig. 3, where the binding at \( k_F = 1.4 \text{fm}^{-1} \) is reported as a function of \( k_{FIT} \).

In all cases the saturation curves appear distorted, and the saturation point shifted. Even if in some cases the saturation point seems to be “improved”, this does not have any physical meaning, since, anyhow, it is mainly a spurious effect.

Completely similar results are obtained with the “old” potential Argonne v14 [14].

In conclusion, we have shown that the parabolic approximation for the single particle potential \( U(k) \) in the self-consistent Brueckner scheme introduces an uncertainty of 1-2 MeV near the saturation density, and therefore it cannot be used in accurate calculations. The full momentum dependence has to be retained, which prevents the use of a constant effective mass approximation. However, the uncertainty is not dramatic, and for approximate estimates of nuclear binding it can be useful.
Figure captions

Fig. 1.- Single particle potential as function of momentum. The full circles indicate the results of the fully self-consistent calculation, where the potential is taken at each iteration step as calculated from the Brueckner G-matrix. The solid line is the result of the parabolic approximation. The parabolic potential, used as input for the G-matrix, produces the potential indicated by the squares.

Fig. 2.- Saturation curves as obtained for the fully self-consistent calculation (full circles), from the parabolic fit (triangles) and from the single particle potential obtained from the parabolic input (squares). Panel a corresponds to $k_{FIT} = 2k_F$, panel b to $k_{FIT} = k_{max}$.

Fig. 3.- Dependence of the binding energy from the value of $k_{FIT}$, using either the parabolic fit potential (triangles), or the parabolic input (squares) potential. The arrows indicate the value of the binding energy obtained in the fully self-consistent calculation, where no fitting procedure is introduced.
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Fig. 1

Potential \( k_{\text{fit}} = 2k_f \)

- Parabolic fit
- Parabolic input
- Self-consistent

\( k_f = 1.4 \text{ fm}^{-1} - \text{Argonne V}_{18} \)
Binding energy - $k_{\text{fit}} = 2k_F$

Argonne $V_{18}$

Binding energy - $k_{\text{fit}} = k_{\text{max}}$

Argonne $V_{18}$
Fig. 3

Binding energy as a function of $k_F$.

- Parabolic input
- Parabolic Fit

$k_F = 1.4$ fm$^{-1}$ – Argonne $V_{1s}$