Effects of angular correlations on particle-particle propagation in infinite nuclear matter

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Abstract. The effect of angular correlations on self-consistent solutions for single-particle (sp) potentials in infinite nuclear matter is investigated. To this end we treat explicitly the angular dependence of the particle–particle (pp) propagator in Brueckner–Hartree–Fock (BHF) equation for the $g$ matrix. It is observed that the exact angular dependence of the pp propagator yields highly fluctuating structures, posing stringent difficulties in the actual search of self–consistent solutions for the sp energy. A perturbative approach is presented to evaluate the effect of the angular correlations in the self-consistent solutions. Solutions at Fermi momenta $k_F$ in the range $1.20 - 1.75$ fm$^{-1}$ are reported using Argonne $v_{18}$ nucleon–nucleon potential. Although the sp potentials are sensitive to the treatment of the angular behaviour of the propagator, such sensitivity appears at momenta well above the Fermi surface. As a result, the saturation properties of symmetric nuclear matter differ marginally from those calculated using angle–averaged energy denominators in pp propagators.

1. Introduction

Infinite nuclear matter models have extensively been used for the study of saturation properties [1] as well as for the construction of density-dependent effective interactions to describe nuclear collisions [2]. To lowest order, the BHF approximation is able to account reasonably well for leading order short-range correlations of nuclear matter in normal state. In this model, interacting nucleons are conceived as single particles moving under a sp potential stemming from the interaction with all other nucleons. The determination of the physical properties of the system is reduced to the calculation of the sp potential. At this point, as discussed in Ref. [3], several approximations have been introduced aiming to circumvent difficulties arising from the non–spherical kernel of pp propagation, together with the multi–channel coupling of nucleon–nucleon ($NN$) states with different angular momenta.

In BHF, the propagation of intermediate states is driven by the pp propagator which takes the form $\Lambda \sim Q/e$, where $Q$ is the Pauli blocking operator. The energy denominator $e$ considers two nucleons moving in directions which are in general not identical. Both terms, $Q$ and $e$, exhibit an explicit angular dependence, feature which remains even if multi–channel coupling is neglected. Among the most accurate approximations in use to account for $\Lambda$ we mention the reduction of the propagator $Q/e$ to the ratio of its angular averages, $\langle Q \rangle / \langle e \rangle$. More recently this approximation has been contrasted with the angular average of the ratio, $\langle Q/e \rangle$ [3], where the angular dependence of the energy denominator is retained up to second order in $K \cdot q$, with $K$ and $q$ the total and relative momenta of the interacting nucleons. In this work we examine more closely the approximation $\Lambda \approx \langle Q/e \rangle$, but treating exactly the intrinsic angular dependence of the energy denominator. As we shall see, the effect of this exact treatment manifest itself at high momenta with respect to the Fermi momentum $k_F$, with marginal incidence in the evaluation of the binding energy of the system.
2. Theoretical Framework

In the BHF approximation in Brueckner–Bethe–Godstone theory for infinite nuclear matter at zero temperature, the $g$ matrix depends on the density of the medium, characterized by $k_F$, and a starting energy $\omega$ [1]. In this framework the effective interaction $g$ satisfies the integral equation

$$g(\omega) = v + v \frac{Q}{\omega - \hat{h}_1 - \hat{h}_2 + i\eta} g(\omega),$$  \hspace{1cm} (1)$$

where $v$ denotes the bare $NN$ interaction, $\hat{h}_1$ and $\hat{h}_2$ the single particle energies and $Q$ the Pauli blocking operator. The solution to this equation allows the evaluation of the mass operator

$$M(k; E) = \sum \langle \frac{1}{2} (\mathbf{k} - \mathbf{p}) | g_K(E + \epsilon_p) | \frac{1}{2} (\mathbf{k} - \mathbf{p}) \rangle,$$  \hspace{1cm} (2)$$

where $K = k + p$ represents the total momentum of the interacting pair and $\epsilon_k = k^2/2m + U(k)$ is the sp energy of nucleons of mass $m$ in terms of an auxiliary field $U$. Self–consistency requires that

$$U(k) = \Re \{M(k; \epsilon_k)\}.$$  \hspace{1cm} (3)$$

This condition is achieved iteratively. In the continuous choice this condition is imposed to all momenta $k$. In infinite nuclear matter, the BHF equation takes the following form in momentum representation,

$$\langle \kappa' | g_K(\omega) | \kappa \rangle = \langle \kappa' | v | \kappa \rangle + \int dq \langle \kappa' | v | q \rangle \Lambda(K, q) \langle q | g_K(\omega) | \kappa \rangle.$$  \hspace{1cm} (4)$$

Here, the propagator takes the form

$$\Lambda(K, q) = \frac{Q(K, q)}{\omega + i\eta - \frac{k^2}{2m} - \frac{k^2}{2m} + \Sigma}$$  \hspace{1cm} (5)$$

with

$$\Sigma(K, q, x) \equiv U(k_+) + U(k_-),$$

$$k^2_\pm = \frac{K^2}{4} + q^2 \pm qKx,$$

and $x = \hat{K} \cdot \hat{q}$. Furthermore, the Pauli blocking operator is represented by $Q(K, q) = \Theta(k_+ - k_F)\Theta(k_- - k_F)$.

This operator not only depends on the magnitudes of the momenta, but also on the angle between them.

A common practice to simplify the angular dependence of the propagator $\Lambda(K, q)$ is by treating separately the numerator $Q$ from the denominator $e \equiv \omega - \frac{k^2}{2m} - \frac{k^2}{2m} - \Sigma$. When the energy denominator is angle averaged the propagator takes the form $Q(\epsilon)/\langle \epsilon \rangle$, and the Pauli blocking operator is treated in its full form [5, 6, 7, 8], including multi-channel coupling. The propagator can be approximated even further by angle averaging the Pauli operator [9], i.e. $Q \rightarrow \langle Q \rangle$, with

$$\langle Q \rangle = \frac{1}{4\pi} \int Q(K, q) d\Omega_q = \Delta.$$

Here $\Delta = \min\{1, \max\{0, (K^2/4 - q^2 - k_F^2)/qK\}\}$. In this limit the propagator takes the form of ratio of averages, namely $Q/e \rightarrow \Delta/\langle \epsilon \rangle$. In this work, rather than using the ratio of averages we consider the average of the ratio $Q/e$. This line of thought is motivated after examining the angular behavior of the energy denominator [3]. In Fig. 1 we plot the difference $\delta\Sigma \equiv \Sigma - \langle \Sigma \rangle$, as function of $x$ and $q$. Here $\langle \rangle$ denotes the angular average, $\langle \Sigma \rangle = \int_0^{\pi} \Sigma(K, q, \theta) d\theta/\Delta$, with $\Sigma$ calculated from the self–consistent $U$ obtained within the ratio of the averages approach, using the continuous choice, for the Argonne $v_{18}$ potential (AV18) [4]. Differences between $\Sigma$ and its average $\langle \Sigma \rangle$ become evident. In this work we aim to assess the implications of these differences on the sp fields $U(k)$ when self–consistency is imposed.
2.1. Treatment of the angular dependence of the propagator

In this study we work on the monopole approximation [3], when the propagator takes the form

\[ \lambda(K, q) = \int d\hat{q} Y^0_0(\hat{q}) \frac{Q}{e + i\eta} Y^0_0(\hat{q}) = \frac{1}{2} \int_{-1}^{1} \frac{Q}{e + i\eta} dx, \]

with \( x \) the cosine of the angle between \( K \) and \( q \). If we consider explicitly the form of the Pauli blocking operator \( Q \), the angle–averaged propagator \( Q/e \) reduces to

\[ \lambda(K, q) = \int_0^\Lambda \frac{1}{e + i\eta} du. \]

We have found that the exact angular dependence in the energy denominator leads to highly fluctuating structures, posing severe difficulties in the search of the self–consistent solutions for the sp energy. To overcome these difficulties, we have adopted a perturbative strategy to evaluate the effect of angular correlations in the self–consistent solutions.

In general terms, the equation for the \( g \) matrix is given by

\[ g = v + v\Lambda g, \]

where \( \Lambda \) denotes the exact propagator in the monopolar approximation. Let us denote \( \Lambda_0 \) the pp propagator approximated by the ratio of the averages, \( \Lambda_0 = \Delta/(e) \). Then

\[ g = v + v(\Lambda - \Lambda_0)g + v\Lambda_0 g. \]

Let us define \( \delta\Lambda \equiv (\Lambda - \Lambda_0) \), as a perturbative term and expand \( g \) as an infinite series in orders of \( \delta\Lambda \)

\[ g = g_0 + g_1 + g_2 + \cdots. \]

Combining Eqs. (9) and (10) we obtain

\[ g_0 + g_1 + \cdots = v + v\delta\Lambda(g_0 + g_1 + \cdots) + v\Lambda_0(g_0 + g_1 + \cdots) + \cdots. \]
Equating terms of the same order, we obtain

\begin{align}
  g_0 &= v + v \Lambda_0 g_0 \\
  g_1 &= v \delta \Lambda g_0 + v \Lambda_0 g_1. 
\end{align} 

(12a) (12b)

The first equation represents the BHF equation for \(g_0\), when the ratio of averages is used. Combining Eqs. (12a) and (12b) we obtain

\[ g_1 = g_0 (\delta \Lambda) g_0. \]

(13)

Thus,

\[ g \approx g_0 + g_1. \]

(14)

Therefore, to evaluate \(g_1\) we need to calculate \(g_0\) (following standard procedures) and compute the expectation value \(\langle g_0 \delta \Lambda g_0 \rangle\). This procedure, though simple, exhibits some subtleties which we address in some detail. We denote by \(e_0\) the difference between the starting energy and the kinetic energy of the nucleons

\[ e_0 = \omega - \frac{K^2}{4} - q^2, \]

(15)

and by \(\langle \Sigma \rangle\) the sum of the angle–averaged sp potentials. With these definitions, we can write the exact propagator as

\[ \Lambda = Q \frac{e_0 - \langle \Sigma \rangle + i \eta}{e_0 - \langle \Sigma \rangle + i \eta}, \]

(16)

which is a function of \(q\) and \(x\). For the propagator \(\Lambda_0\) we have

\[ \Lambda_0 = Q \frac{e_0 - \langle \Sigma \rangle + i \eta}{e_0 - \langle \Sigma \rangle + i \eta}, \]

(17)

which is a function of \(q\) but independent of \(x\). The difference \(\delta \Lambda\) then takes the form, when using the monopolar approximation,

\[ \delta \Lambda = 2 \pi \int_{-\Delta}^{\Delta} dx \left( \frac{1}{e_0 - \langle \Sigma \rangle + i \eta} - \frac{1}{1 - e_0 - \langle \Sigma \rangle + i \eta} \right). \]

(18)

By adding and substracting \(\langle \Sigma \rangle\) in the denominator of the first integrand, and defining \(e_0 \equiv e_0 - \langle \Sigma \rangle\), and \(u_x \equiv \Sigma - \langle \Sigma \rangle\), Eq. (18) can be written as

\[ \delta \Lambda = 2 \pi \int_{-\Delta}^{\Delta} dx \left( \frac{1}{e_0 - u_x + i \eta} - \frac{1}{e_0 + i \eta} \right). \]

(19)

Note that \(e_0\) does not depend on \(x\). The real part of \(\delta \Lambda\) reads

\[ \delta \Lambda_R = 2 \pi \frac{e_0}{e_0^2 + \eta^2} \int_{-\Delta}^{\Delta} \frac{u_x (e_0 - u_x)}{(e_0 - u_x)^2 + \eta^2} dx. \]

(20)

Considering

\[ \Lambda_0 = \frac{1}{e_0 + i \eta} = \frac{e_0^2}{e_0^2 + \eta^2} - i \frac{\eta}{e_0^2 + \eta^2}, \]

(21)

then

\[ \delta \Lambda_R = 2 \pi \Re \{ \Lambda_0 \} \times \int_{-\Delta}^{\Delta} \frac{u_x (e_0 - u_x)}{(e_0 - u_x)^2 + \eta^2} dx. \]

(22)
In the case of the imaginary part we have,
\[ \delta \Lambda_I = 2\pi \int_{-\Delta}^{\Delta} \left[ \frac{\eta}{(e_0 - u_x)^2 + \eta^2} - \frac{\eta}{e_0^2 + \eta^2} \right] dx. \]  
(23)

Let us define
\[ f(u_x) = \frac{\eta}{(e_0 - u_x)^2 + \eta^2} - \frac{\eta}{e_0^2 + \eta^2}, \]
(24)

which, after using the Plemelj formula in the limit \( \eta \to 0 \) leads to
\[ f(u_x) = \delta(e_0 - u_x) - \delta(e_0). \]
(25)

Expanding around \( u_x = 0 \), we get
\[ f(u_x) \approx u_x \delta'(e_0) + u_x^2 \frac{1}{2} \delta''(e_0) + O(u_x^3), \]
(26)

and replacing this result in Eq. (23) we obtain
\[ \delta \Lambda_I = 2\pi \int_{-\Delta}^{\Delta} \left[ u_x \delta'(e_0) + u_x^2 \frac{1}{2} \delta''(e_0) \right] dx. \]
(27)

The first term of Eq. (27) vanishes by definition. Therefore
\[ \delta \Lambda_I = \pi \delta''(e_0) \int_{-\Delta}^{\Delta} u_x^2 dx. \]
(28)

Eqs. (22) and (28) can be used to evaluate \( g \), in Eq. (14). With this, the \( g \) matrix is used to calculate the mass operator self–consistently. Convergence is imposed when fluctuations of \( U(k) \) do not exceed 0.05 MeV on three consecutive iterations.

3. Results

We have calculated self–consistent solutions for \( U(k) \) using Argonne \( v_{18} \) potential including all partial waves up to \( J = 7 \). Solutions where found considering the pp propagator in the form of the ratio of angular averages, and the monopole approximation as described above. In the case of SNM we obtained solutions for Fermi momenta between 1.20 and 1.75 \( \text{fm}^{-1} \), in steps of 0.05 \( \text{fm}^{-1} \). We have also investigated pure neutron matter, case in which the solutions where obtained in the range 1.20–1.75 \( \text{fm}^{-1} \). In Fig. 2 we show the on–shell mass operator as a function of \( k \) for different values of \( k_F \). The left–hand side panel shows the real part of the on-shell mass operator, while the right–hand panel shows the imaginary part. Blue (red) curves correspond to \( k_F = 1.25(1.75) \text{fm}^{-1} \).

In Fig. 3 we show a comparison between the self–consistent fields calculated using the angle–averaged propagator (red, continuous) and the ones calculated using the propagator which included the first order correction (blue, dashed). As we can observe, differences between the two are quite moderate and become only noticeable to the eye at momenta over 3.5 \( \text{fm}^{-1} \). Calculation of the pp potentials allowed us to evaluate the energy per nucleon. The saturation points found for both the angle–average and monopolar approximations for the propagator are summarized in Table 1. Here we include the incompressibility of nuclear matter given by
\[ K = k_F^2 \frac{\partial^2 (B/A)}{\partial k_F^2}, \]
(29)

where the second derivative is evaluated at the saturation momentum.
Figure 2. On–shell mass operator calculated using the monopole approximation for the pp propagator. Here $1.25 \leq k_F \leq 1.75 \text{ fm}^{-1}$. Blue (red) curve denotes $k_F = 1.25(0.10)1.75 \text{ fm}^{-1}$.

Figure 3. Comparison between the on–shell mass operator calculated using the angle–averaged propagator versus the ones calculated using $g \sim g_0 + g_1$.

| Solutions       | $k_F$ [fm$^{-1}$] | $B/A$ [MeV] | $K$ [MeV] |
|-----------------|------------------|-------------|-----------|
| Angle–averaged  | 1.520            | -16.691     | 199.4     |
| Monopole        | 1.521            | -16.689     | 202.9     |

Table 1. Saturation properties for SNM found in this work. The third decimal place is shown only to illustrate the differences.

As we can see, the saturation energy and density found are essentially the same when using the angle–
average or the monopole approximation. The nuclear compressibility turned out to be more sensitive to the corrections in the propagator with a 3.5 MeV difference between the two.

In Fig. 4 we show the on–shell mass operator as a function of $k$ for different values of $k_F$ calculated for pure neutron matter. As for the SNM curves, blue (red) corresponds to $k_F = 1.20(1.75)$ fm$^{-1}$. In Fig. 5 we show the comparison between the mass operator calculated using the angle–averaged pp propagator (red, continuous) and the mass operator calculated using the monopolar approximation (blue, dashed). Analogous to the SNM case, the differences between the two become noticeable to the eye at momenta over 3.5 fm$^{-1}$.

**Figure 4.** Same for Figure 2 but for pure neutron matter.

**Figure 5.** Comparison between the self–consistent fields calculated using the angle–averaged propagator versus the ones calculated using the first order correction for neutron matter.
4. Summary and conclusions
We have investigated the effects of angular correlations resulting from considering the angular dependence of the pp propagator of the BHF approximation for symmetric and pure neutron matter. To accomplish this, we calculated the sp potentials for Fermi momenta between 1.20 and 1.75 fm\(^{-1}\) in the continuous choice. The bare NN potential used in this study was the Argonne v\(_{18}\) including all partial waves up to \(J = 7\). The angular dependence of the pp propagator was treated like a perturbation, \(\delta \Lambda = (\Lambda - \Lambda_0)\). The occurrence of possible \(^1S_0\) and \(^3S_1-^3D_1\) bound states was accounted for and its search and regularization was implemented in the calculations using the method outlined in Ref. [11]. Moderate effects are observed in the mass operator at momenta above \(\sim 3.5\) fm\(^{-1}\), when the monopole approximation is used for the pp propagator. We find that both the ratio of angular averages and the average of the ratio yield saturation of nuclear matter at \(k_F = 1.52\) fm\(^{-1}\) and \(B/A = 16.7\) MeV/nucleon. These results confirm that the ratio of averages is a good approximation for the calculation of the sp potentials. The incompressibility, on the other hand, differs by 3.5 MeV between the two solutions. We have also found that the effect of angular correlations in pp propagation in neutron matter is negligible.

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References
[1] Baldo M 1998 Nuclear Methods and the Nuclear Equation of State vol 8 (Singapore: World Scientific) chapter 1 pp 1–116
[2] Amos K et al 2002 Adv. Nucl. Phys. 25 276–536
[3] Arellano H F and Delaroche J-P 2011 Phys. Rev. C 83.4 044306
[4] Wiringa R B et al 1995 Phys. Rev. C 51 38
[5] Sammarruca F, Meng X and Stephenson E J 2000 Phys. Rev. C 62 014614
[6] Suzuki K, Okamoto R, Kohno M and Nagata S 2000 Nucl. Phys. A 665 92
[7] Schiller E, Muther H and Czerski P 1999 Phys. Rev. C 59 2934
[8] Cheon T and Redish E F 1989 Phys. Rev. C 39 331
[9] Brueckner K A and Gammel J L 1958 Phys. Rev. 109 1023
[10] Haftel M I and Tabakin F 1970 Nucl. Phys. A 158.1 1–42
[11] Arellano H F and Delaroche J -P 2015 Eur. Phys. J. A 51 7
[12] Carbone A et al 2013 Phys. Rev. C 88 054326