The nature of short-ranged correlations in nuclear systems

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Abstract

We apply ideas of the parquet-diagram and optimized Fermi-hypernetted chain methods to determine the short-range structure of the pair wave function in neutron matter and compare these with Bethe-Goldstone results and those of low-order variational calculations. It is shown that the induced interaction, describing the exchange of density, spin, and tensor fluctuations, has a profound influence on the short-ranged structure of the pair wave function and, hence, on effective interactions in neutron matter.

1. Introduction

It is generally understood that the nature of the wave function in a many-body system is, at short interparticle distances, determined by a Schrödinger-like equation. The prime example for this is the time-honored Bethe-Goldstone equation [1, 2] which is basically a 2-body Schrödinger equation modified by the Pauli principle. Many-body effects are mostly included through the single-particle spectrum. The literature on the subject matter is vast, we cite here only early works [6] and review articles [7, 8].

Similar in spirit is the low-order version of Jastrow-Feenberg theory. The method begins with a variational ansatz for the many-body wave function. One assumes a semi-realistic interaction of the form

$$\hat{v}(i,j) = \sum_{\alpha=1}^{n} v_{\alpha}(r_{ij}) \hat{O}_{\alpha}(i,j),$$

(1.1)

where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ is the distance between particles $i$ and $j$, and the $O_{\alpha}(i,j)$ are operators acting on the spin, isospin, and possibly angular momentum variables of the individual particles. Semi-realistic model potentials use the six base operators are

$$O_1(i,j;\mathbf{r}_{ij}) = \mathbb{1},$$  
$$O_2(i,j;\mathbf{r}_{ij}) = (\sigma_i \cdot \sigma_j),$$  
$$O_3(i,j;\mathbf{r}_{ij}) = \mathbb{S}_{ij}(\mathbf{r}_{ij}) = \mathbb{1} (\sigma_i \cdot \sigma_j) - \sigma_i \cdot \sigma_j,$$

(1.2)

where $\mathbb{S}_{ij}(\mathbf{r}_{ij}) = r_{ij}/r_{ij}$. An appropriate variational wave function is in this case

$$\Psi_{\text{SOP}} = \mathcal{A} \prod_{i<j}^{N} \hat{f}(i,j) \Phi_0,$$

(1.3)

where $\mathcal{A}$ stands for symmetrization, and

$$\hat{f}(i,j) = \sum_{\alpha=1}^{n} f_{\alpha}(r_{ij}) O_{\alpha}(i,j).$$

(1.4)

The need to symmetrize the operator product in (1.3) causes considerable complications and no summation method has been found that comes anywhere close to the diagrammatic richness of the hypernetted-chain (HNC) summation method for bosons [16] and fermions [17, 18, 19, 20] that has been achieved for the case of purely central correlations. The components $f_{\alpha}(r_{ij})$ of the correlation operator $\hat{f}(i,j)$ are therefore often determined by minimization of the two-body approximation of $E_0$, subject to a healing constraint [9]. The method is then referred to as “low order constrained variational method (LOCV)” [10, 11]. The energy expectation value is calculated either in low order, or by partial diagram summations like the “single-operator-chain (SOC)” method [12, 13]. Both the Bethe-Goldstone equation and the LOCV determination of the correlations imply only a minimal inclusion of many-body effects; the fact that they led to rather different answers has caused significant discussions [14, 15].

The situation is much simpler for the case of central correlations. Most importantly, the summation method defines a hierarchy of approximations which permit an unconstrained variational determination of the correlations by minimization of the energy expectation value $E_0$ [21].

$$\frac{\delta E_0}{\delta f(r_1,r_2)} = 0.$$  

(1.5)

For fermions, some care must be taken in the treatment of exchange diagrams to permit an unconstrained variation [22].

A further important insight was that the hypernetted chain summation method together with the unconstrained optimization (1.5) corresponds, for bosons, to a self-consistent summation of both the ring and the ladder diagrams of perturbation theory [23, 24, 25], in other words the Euler equation (1.5) contains both the Bethe-Goldstone equation and the RPA equation. This was already observed by Sim, Buchler, and Woo [26]. The analogy is less systematic for fermions and implies more approximations, but it was similarly proven for the most important classes, namely rings, ladders, and self-energy corrections [27].
Since the Fermi sea defines a preferred reference frame, such information implies the self-consistent summation of both ring- and implies that all two-body functions depend only on the distance. taken, when necessary or appropriate, approximations suggested the response function \( S(q) = -\int_0^\infty \frac{d\omega}{\pi} \frac{\chi_0(q, \omega)}{1 - V_{p-h}(q)} \), \( \chi_0(q, \omega) \) in the basis of the operators \( \hat{V}_{p-h}(q) = \frac{1}{\pi} \int d^3 r \hat{V}(r) \rho(f(r)) \).

In making the connection to FHNC-EL, we must define a pair wave function that is a function of the relative coordinate or momentum, \( \sigma \), i.e. it has the feature that
\[
\langle \mathbf{k}, \mathbf{k}' | \mathbf{h}, \mathbf{h}' \rangle = \frac{1}{N} \langle \mathbf{k} - \mathbf{h} \rangle = \frac{1}{N} \langle \psi(q) \rangle.
\]
Similarly, for local interactions, we should have
\[
\langle \mathbf{k}, \mathbf{k}' | \mathbf{h}, \mathbf{h}' \rangle = \frac{1}{N} \langle v(r) \psi(r) \rangle. \]
where \( \ldots \rangle^F \) stands for Fourier transform. To ensure this, the energy denominator in Eq. \( \psi(r) \) must somehow be approximated by a function of momentum transfer \( q = |k - h| \).

In view of these complications, Smith and Jackson \( \psi \) started from the idea of parquet-diagram summations and implemented the procedure for a fictive system of bosonic nucleons interacting via a vs interaction. We have recently followed up on that idea \( \psi \) and extended it to fermions. In generalizing the parquet equations to fermions, we have used the diagrammatic ideas of the parquet-diagram summations, and taken, when necessary or appropriate, approximations suggested by variational wave functions. Most importantly, the form \( \psi \) implies that all two-body functions depend only on the distance. Since the Fermi sea defines a preferred reference frame, such local functions can be obtained only by specific Fermi-sea averages, we will mention these where appropriate.

2. A brief survey of FHNC-EL and parquet equations

As stated above, the FHNC-EL and parquet diagram summation implies the self-consistent summation of both ring- and ladder diagrams. To be more specific, the ring diagrams are derived from a variational principle (RPA) equation for the response function
\[
\chi(q, \omega) = \frac{\chi_0(q, \omega)}{1 - V_{p-h}(q)\chi_0(q, \omega)}
\]
\( S(q) = -\int_0^\infty \frac{d\omega}{\pi} \frac{\chi_0(q, \omega)}{1 - V_{p-h}(q)\chi_0(q, \omega)}, \]
in terms of a local “particle-hole” interaction \( V_{p-h}(q) \). In the case of state-dependent interactions, \( V_{p-h}(q) \) is a linear combination of local functions \( \tilde{\chi}(p_{-h}(q)) \) and the base operators \( \hat{V}_{p-h}(q) \).

In \( \psi \) it is more convenient to represent \( V_{p-h}(q) \) in the basis of the operators \( \hat{V}_{p-h}(q) \). In \( \psi \) as usual, we define the dimensionless Fourier transform by including a density factor \( \rho \), i.e. \( \tilde{f}(q) = \rho \int d^3 r \tilde{f}(r) \).

The second relevant relationship is the Bethe-Goldstone equation for the pair wave function
\[
\langle \mathbf{k}, \mathbf{k}' | \mathbf{h}, \mathbf{h}' \rangle = \langle \mathbf{k}, \mathbf{k}' | \mathbf{h}, \mathbf{h}' \rangle
\] \( \chi_0(q, \omega) \) by an induced interaction \( \tilde{\psi}(r) \) being defined as the set of particle-hole reducible diagrams. Assuming a particle-hole interaction \( \hat{V}_{p-h}(q) \) of the operator of the form \( \psi \), the sum of these diagrams is a priori an energy-dependent quantity
\[
\tilde{\psi}(q, \omega) = \frac{\tilde{\chi}(p_{-h}(q))}{1 - V_{p-h}(q)\chi_0(q, \omega)} \]
\[ S(q) = -\int_0^\infty \frac{d\omega}{\pi} \frac{\chi_0(q, \omega)}{1 - V_{p-h}(q)\chi_0(q, \omega)} \]
\[ \tilde{\psi}(q, \omega) = \frac{\tilde{\chi}(p_{-h}(q))}{1 - V_{p-h}(q)\chi_0(q, \omega)} \]
\[ \tilde{S}(q) = -\int_0^\infty \frac{d\omega}{\pi} \frac{\chi_0(q, \omega)}{1 - V_{p-h}(q)\chi_0(q, \omega)} \]
Now define an energy independent interaction \( \tilde{\psi}(q, \omega(q)) \) by demanding that it gives the same static structure function,
This energy independent interaction $\hat{v}_I(q) \equiv \hat{v}_I(q, \omega(q))$ is then taken as a correction to the interaction in the Bethe-Goldstone equation. For state-dependent interactions it is again understood that $\hat{v}_I(q, \omega)$ is a linear combination of local functions and operators of the form (1.1). For solving the Bethe-Goldstone equation, it is convenient to write both the interaction and the induced interaction as a linear combination of the spin-singlet projector $\hat{P}_s = (1 - \sigma_1 \cdot \sigma_2)/4$, and the spin-triplet projectors $\hat{P}_{+} = (3\mathbb{1} + \sigma_1 \cdot \sigma_2 + S_{12}(\mathbf{r}))/6$ and $\hat{P}_{-} = (3\mathbb{1} + \sigma_1 \cdot \sigma_2 - 2S_{12}(\mathbf{r}))/12$.

We also mention briefly the connection to the FHNC-EL summation method. Diagrammatically we can identify the pair wave function $\psi(\mathbf{r})$ with the direct correlation function $\Gamma_{dd}(\mathbf{r})$

$$\psi(\mathbf{r}) = \sqrt{1 + \Gamma_{dd}(\mathbf{r})}. \quad (2.8)$$

The equation determining the short-ranged structure of $\psi(\mathbf{r})$ or $\sqrt{1 + \Gamma_{dd}(\mathbf{r})}$ is slightly different from Eq. (2.3), see Eq. (3.33) of Ref. 27, we found, however, in our numerical applications that the numerical solutions are very close. We shall, therefore, not elaborate on this issue any further.

3. Short-ranged structure

Let us now go through a step-by-step analysis of the influence of the induced interaction and the consequences for other quantities for a specific example. We have chosen the Reid $v_6$ interaction [32] in the parametrization of Day [33] for neutron matter at the relatively low density $k_F = 1 \text{ fm}^{-1}$. We have carried out a sequence of calculations

1. Simply set $\hat{v}_I(\mathbf{r})$ zero. That correspond to the Bethe-Goldstone equation and, in a sense, also to LOCV.
2. Use the state-dependent theory, Eq. (2.7) [30].
3. Use the FHNC-EL (or parquet) version for purely central correlations as described, for example, in Refs. 27 or 34. This implies that only the central component of the interaction operator (1.1) is kept.
4. Take the spin-singlet component of the interaction operator in the Bethe-Goldstone equation but use the induced interaction from the state-independent calculation.

4. Results

Turning to the key message of our paper, we emphasize that the essential additional quantity provided by parquet theory or FHNC-EL is the induced interaction $\hat{v}_I(q)$. FHNC-EL or parquet offers the prescriptions (2.7) for calculating this quantity. Fig. 1 shows the the singlet component if the induced interactions $w_I(\mathbf{r})$ coming from a state-dependent and state-independent parquet calculation, along with the resulting pair wave functions (2.8). Since the central part of the Reid potential is less attractive than the singlet projection, the pair wave function for the state-independent case has no pronounced nearest neighbor peak.

To isolate the relevance of the induced interaction, we have also carried out a calculation taking the spin-singlet projection in the Bethe-Goldstone equation, but the induced interaction from the state-independent calculation. The result is shown in blue in Fig. 1. This calculation is somewhat inconsistent at the state-independent parquet-level because there the correlations should be determined by the central part of the of the interaction operator. The resulting pair wave function is close to the one obtained by simply omitting the induced interaction. However, taking the spin-singlet component of the interaction in a full parquet calculation does not lead to self-consistent solutions of the parquet equations even at very low densities. Hence, it is very important to include the induced interaction to guarantee the stability of the system.

We have also tried the original version of Bethe and Goldstone, setting the center of mass momentum to zero. The results are very similar to those shown in Fig. 1 in particular the key message of our paper on the importance of the induced interaction remains unchanged.

Pair wave functions are auxiliary quantities, effective interactions are more directly relevant for dynamic properties and pairing phenomena. The essential input is always the particle-hole interaction, which also determines the induced interaction $w_I(\mathbf{r})$. It is therefore important to both verify the validity of our analysis and to determine the importance of the pair wave function for these interactions. In terms of the quantities introduced above, the simplest version, dubbed FHNC-EL/0, has the form

$$v_{\alpha}(\mathbf{r}) = \left[1 + \Gamma_{dd}(\mathbf{r})\right]v_{\alpha}(\mathbf{r}) + \Gamma_{\alpha}(\mathbf{r})w_I(\mathbf{r}).$$

$$\rho_{\alpha}(\mathbf{r}) = \frac{\hbar^2}{m} \left| \nabla \sqrt{1 + \Gamma_{dd}(\mathbf{r})} \right|^2.$$

where $\alpha$ stands for the spin-singlet and the two spin-triplet projections, and $\rho_{\alpha}(\mathbf{r})$ is the 2-body part of the “Clark-Westhaus” kinetic energy [11]. In the state-independent approximation, all
in other words, the 2-body interaction is close to developing a
effect of the effective interaction due to the enhanced nearest
peak as shown in Fig. 1. Such an enhancement can,
energy term
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found effect. After all, the well-depth of the spin-singlet Reid
small correction to the bare interaction can have a rather pr o-
important and have been included in our calculation as described in Refs. [27 and 30].

The expression (4.1) shows nicely the physical effects that contribute to the particle-hole interaction. These were described by Aldrich and Pines [36, 37]:

1. Local screening of the short-ranged repulsion of the bare interaction. This is described by the factor $1 + \Gamma_{\text{dd}}^{(a)}(r)$, which goes to zero at short distances.

2. The cost in kinetic energy to bend down the wave function. This leads to some repulsion and a “swelling” of the core. The effect is described by the kinetic energy term $t_{\text{CW}}^{(a)}(r)$.

3. An enhancement of the attraction due to the presence of other particles. Again, the factor $1 + \Gamma_{\text{dd}}^{(a)}(r)$ describes this effect, note that an attractive interaction generates a high nearest neighbor peak in the pair wave function and, hence, enhances the attractive part of the interaction.

4. The last term $\Gamma_{\text{dd}}^{(a)}(r)\psi_{j}^{(a)}(r)$ describes the modification of the interactions through the exchange of density or spin fluctuations.

Returning to Fig. 1, one might wonder why a relatively small correction to the bare interaction can have a rather profound effect. After all, the well-depth of the spin-singlet Reid interaction is of the order of 100 MeV. One of the reasons for the sensitive dependence of the pair wave function on the induced interaction is that the bare singlet interaction has almost a bound state, the S-wave scattering length is $-18.7$ fm [35], in other words the 2-body interaction is close to developing a bound state and small changes of the interaction can cause large changes in the pair wave function.

The most important issue for our discussion is the enhancement of the effective interaction due to the enhanced nearest neighbor peak as shown in Fig. 1. Such an enhancement can, for example, have significant effects on pairing phenomena in neutron matter which depend sensitively on the interaction strength. To see this effect, we show in Fig. 2 the bare singlet interaction and the components of the particle hole interaction [4.1]

The most pronounced effect is evidently the enhancement of the interaction by the peak in the pair wave function. The kinetic energy term $t_{\text{CW}}^{(a)}(r)$ basically causes the “swelling” of the core, but is not strong enough to compensate for the enhancement of the attraction.

The long-wavelength limits of the components of the particle-hole interactions can be related to Landau’s Fermi-liquid parameters,

\[ \psi_{p-h}^{(a)}(0+) = mc_{F}^{2}F_{0}^{s}, \quad \psi_{p-h}^{(\sigma)}(0+) = mc_{F}^{2}F_{0}^{\sigma}, \quad (4.2) \]

where $c_{F}^{2} = \sqrt{\frac{\hbar^{2}k_{F}^{2}}{2m^{*}}} \approx \text{speed of sound of the non-interacting Fermi gas with the effective mass } m^{*}$, and $F_{0}^{s,\sigma}$ are Landau’s Fermi liquid parameters.

The two Landau parameters can also be obtained by derivatives of the equation of state as a function of density and spin-polarization, for example we have for the incompressibility

\[ mc^{2} = \frac{d}{d\rho} \rho \frac{d}{d\rho} E = mc_{F}^{2}(1 + F_{0}^{d}). \quad (4.3) \]

Predictions for the Fermi-liquid parameters derived from hydrodynamic derivatives and from effective interactions agree only in an exact theory [22, 38]; good agreement is typically reached only at very low densities [27].

Fig. 3 shows the calculated Fermi-Liquid parameters $F_{0}^{d}$ and $F_{0}^{s}$ for the Reid $V_{0}$ model potential as obtained from Eqs. (4.2) and (4.3). Note that the results for $F_{0}^{d}$ differ slightly from those of Ref. [32] due to improved numerics.

A relationship similar to Eq. (4.3) can be derived for $F_{0}^{a}$ by calculating the equation of state of a partially spin-polarized system. Such a calculation goes beyond the scope of this paper, we note however that our results indicate that $F_{0}^{a}$ is positive and
of the order of 1 which agrees with several previous calculations. 39, 40, 41.

Returning to the full particle-hole interaction, we show in Figs. 4 and 5 a comparison between $\tilde{V}_{p-h}^{(d)}(q)$ for the central and the spin-channel for both the state-dependent and the state-independent theory. Recall that in the state-independent approximation, all $V_{p-h}^{(d)}(r)$ are the same, and we get simply $V_{p-h}^{(d)}(r) = \left[ 1 + \Gamma_{d\sigma}(r) \right] v_0(r)$. Evidently the agreement between results from state-dependent and state-independent calculations is at most qualitative.

![Figure 4](image4.png)

Figure 4: (Color online) The figure shows, for the Reid $v_R$ interaction, the central channel of the particle-hole interaction obtained by the full-parquet calculation (red, solid lines) and the state-independent approximation (black, dashed lines). The interaction strength is given in units of the Fermi energy of the non-interacting system, $\hbar^2 k_F^2/(2m)$.

![Figure 5](image5.png)

Figure 5: (Color online) Same as Fig. 4 for the spin-channel interaction $\tilde{V}_{p-h}^{(s)}(q)$.

5. Summary

We have in this paper highlighted the importance of the exchange of density and spin fluctuations for the short-ranged structure of correlations in neutron matter and their immediate relevance for effective interactions. We have chosen the example of neutron matter because this is next to electrons and perhaps cold gases away from the uniform limit – one of the simplest realistic many-body systems. The reason for this simplicity is that neutron matter is, as opposed to liquid $^3$He and nuclear matter, not self-bound. A self-bound Fermi system has necessarily at least two spinodal points below saturation density which have the immediate consequence that the equation of state is a non-analytic function of the density. These complications do not exist in neutron matter and we can focus on the problem at hand, namely the importance and the treatment of operator-dependent correlations.

Immediate applications are foreseeable, among others, for pairing properties of neutron matter which has been discussed for decades, for a collection of recent review articles, see Ref. 42. Similarly important is the response of neutron matter which has been discussed over the years, 43, 44, 45.

A completely open issue, which must be resolved before these phenomena are examined, is the importance of non-parquet diagrams corresponding to the commutator diagrams in the wave function $\langle \hat{\rho} \rangle$. There is evidence 28 that these diagrams can be very important whenever the core size of the interaction is very different in different interaction channels. This is the case for both the Reid and the Argonne interactions.

Acknowledgment

This work was supported, in part, by the College of Arts and Sciences of the University at Buffalo, SUNY. Encouragement for this work was derived from a workshop on Nuclear Many-Body Theories: Beyond the mean field approaches at the Asia Pacific Center for Theoretical Physics in Pohang, South Korea, in July 2019. We thank J. W. Clark for numerous comments and suggestions on this manuscript. One of us (JW) thanks the Austrian Marshall Plan Foundation for support during the summer 2018 and Robert Zillich for discussions.

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