Dispersion energies and excitation parameters in fermion fluids

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Certain physical mechanisms contributing to the Brueckner pair dispersion energy W_2^D are reviewed. This W_2^D is found to appear also in the Iwamoto-Yamada cluster expansion if the same Brueckner state- and momentum-dependent correlation operators are used. It does not appear in the two-body Iwamoto-Yamada energy, however, but in the three-body energy. Up to this point, a Brueckner triplet dispersion energy W_3^D has not yet appeared. This W_3^D depends on a triplet excitation parameter κ_3, which is calculated using Jastrow correlation functions. We find that κ_3 is small when κ_2 is small ($\lesssim 0.1$), and large when κ_2 is large ($\gtrsim 0.4$). Since $\kappa_2 \approx 0.2$ in nuclear matter, there is hope that both Brueckner and Iwamoto-Yamada expansions converge to the same answer at fairly low orders.

[NUCLEAR STRUCTURE Fermion fluids, nuclear matter; compared Brueckner and IY expansions; calculated triplet excitation parameter.]

I. INTRODUCTION

For a number of years, attempts[1-7] have been made to understand the relationship between variational theories of fermion fluids and the more familiar Brueckner theory (BT).[8] At the lowest order (LO), i.e., independent pair, level, the Iwamoto-Yamada[9] (IY) pair energy E_2 can be related to the Brueckner pair energy W_2 if the same pair (Bethe-Goldstone) correlation operator is used in both theories. It was then found[2] that E_2 differs from W_2 in the absence of a repulsive pair dispersion energy W_2^D. (This energy is one manifestation of a pair dispersion effect, which also prevents the pair correlation function from becoming too long range.[2]) The result $E_2 \approx W_2 - W_2^D$ holds also for realistic potentials in nuclear matter (NM).[10]

Although missing in E_2, W_2^D could appear in the IY three-body cluster energy E_3. This is indeed the case, but it is there canceled formally and completely by another part of E_3 when the state-independent Jastrow correlation function (cfn) is used.[3] This cancellation gives rise to the belief that the pair dispersion effect is "spurious."

We would like to point out in this paper that the cancellation occurs only because the Jastrow cfn is state and momentum independent. (Here we use the term "state dependence" in the broad sense, or many-body context, to include the effects of specific time ordering of operators and specific excitations in the many-body intermediate states. The two-body partial-wave dependence of a cfn may be called a "two-body state dependence" whenever only this type of state dependence is under consideration. In contrast, the state dependence of a *two-body* potential is necessarily a two-body state dependence.) If state- and momentum-dependent correlation operators are used in the IY expansion, the cancellation is incomplete. Then W_2^D appears, not at the two-body level, but at the three-body level. At this three-body level, the IY energy still differs from the Brueckner energy, because a Brueckner triplet dispersion energy W_3^D has not yet appeared in the IY expansion. These results are described in Sec. II.

The importance of W_3^D depends on a triplet excitation parameter κ_3 for the simultaneous excitation of three fermions above the Fermi sea. In Sec. III we calculate κ_3 for a number of Jastrow cfn's. We find that κ_3 is correlated with κ_2; it is very small when κ_2 is small, and large when κ_2 is large. Using κ_2 as an indicator, we argue that NM at and below normal density appears to be a low- to medium-density fermion fluid. Consequently, the Brueckner expansion may remain useful.

The last section contains brief concluding remarks.

II. DISPERSION ENERGIES

The Brueckner pair dispersion energy W_2^D appears because there is a change of the interaction potential energy of a fermion with the surrounding medium when it is excited out of the Fermi sea. We write

$$W_2^D(\Delta U) = \Delta U \kappa_2, \quad \Delta U = U_p - U_h \ , \tag{2.1}$$

where U_p and U_h are average single-particle (s.p.) potentials for a particle and a hole, respectively,

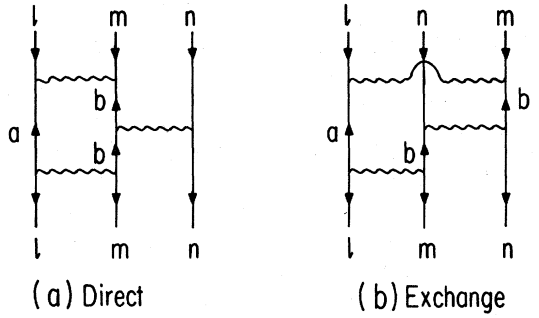

FIG. 1. Third-order bubble insertion diagrams on a particle line.

and κ_2 is the pair excitation parameter.

Since $\kappa_2 > 0$, W_2^D vanishes only if $\bar{U}_p = \bar{U}_h$. In the simplest picture where U is defined in terms of pair interactions only, the cancellation occurs if (i) the effective two-body interaction (the reaction matrix G or its variational analog $f^2 v$, where f is the two-body correlation function) is state independent, and (ii) the exchange part of the two-body matrix element (TBME) is neglected. When G is state independent, the direct TBME and consequently the Hartree s.p. potential are momentum independent. As a result, there is no contribution to $\Delta\bar{U}$. (The Hartree part of ΔU is often small even for state-dependent potentials. However, there are many potentials of interest in nuclear physics for which the state dependence is substantial. Examples are interactions acting only in relative S states.) The exchange TBME is momentum dependent, however, as shown explicitly in the second term of the following simplified expression for a state-independent interaction $v_{\rm eff}(r)$:

$$\langle ij|v_{\rm eff}|ij-ji\rangle \propto \int d^3r v_{\rm eff}(r)(1-\exp[-2i\vec{k}\cdot\vec{r}]) \ , \qquad (2.2)$$

where $\vec{k}$ is the relative momentum. Consequently, the Fock s.p. potential is also momentum dependent. This momentum dependence contributes to dispersion energies.

To see how this effect contributes to W_2^D, we show in Fig. 1 the direct and exchange diagrams of the third-order bubble insertion process on a particle line drawn in the Rajaraman convention.[21] Down arrows and symbols $l, m, n, \ldots$, label hole lines, while up arrows and symbols $a, b, c, \ldots$, label particle lines. We see that the exchange diagram differs from the direct diagram not only in the labeling of the upper external lines, but also in the exchange TBME, $-\langle bn|G|nb\rangle$, which because of the momentum dependence shown in Eq. (2.2), differs from the exchange TBME ($-\langle mn|G|nm\rangle$) before the $m \to b$ excitation. Since the relative momentum $k_{bn} > k_{mn}$, $-\langle bn|G|nb\rangle$ is less attractive or more repulsive than $-\langle mn|Gnm\rangle$ for most potentials. This means that the $\bar{U}_p$ part of W_2^D is less attractive or more repulsive than the $\bar{U}_h$ part. Consequently $W_2^D \neq 0$ obtains. This exchange effect is absent for Boltzmann particles and is probably less important for boson fluids. (Also exchange diagrams for bosons are ring-type diagrams, which may have to be treated differently.[22])

There is another contribution to the dispersion effect involving the middle G matrix of these bubble insertion diagrams in addition to that arising from the momentum dependence of its exchange, and in general also its direct, TBME. This concerns the effect of off-the-energy-shell propagation,[23] i.e., the fact that the intermediate state for the middle G matrix contains an additional particle-hole excitation, thus making its TBME more repulsive. However, it is known[23] that for the bubble insertion on a hole line, this G matrix can be put on the energy shell by generalized time ordering. This cannot be done for the bubble insertion on a particle line. Consequently, this mechanism contributes to $\Delta\bar{U}$.

The situation is different in the usual variational calculations. One starts with a state- and momentum-independent Jastrow correlation function

$$F = \prod_{i<j} f_{ij}, \quad f_{ij} \equiv f(r_{ij}) \ , \qquad (2.3)$$

rather than a correlation *operator*. This assumption is equivalent to a neglect of the time ordering of interactions and, in our present context, to the approximation of $\langle bn|G|nb\rangle$ by $\langle mn|G|nm\rangle$. Consequently $\Delta U = 0$ obtains, and the pair dispersion energy vanishes.

There is thus no doubt that a pair dispersion energy should appear when only the third-order bubble insertion processes are included. The situation is not so clear if other processes are also included. It is therefore interesting to compare the theories to higher orders.

A direct comparison between Brueckner and IY expansions at the next, i.e., three-body, level is possible if one uses the same Bethe-Faddeev (BF) triplet correlation operator (as well as the same Bethe-Goldstone pair correlation operator) in both theories. It is then found[4,5] that the IY cluster energy up to three-body terms is

$$E \approx \frac{3}{10}\frac{\hbar^2}{M}k_F^2 + [W_2 - W_2^D(\lambda^{(2)})] - \bar{U}_h\kappa_2 + E_3^{hh} + [W_3 - W_3^D(\lambda^{(3)})] \ , \qquad (2.4)$$

where E_3^{hh} is the three-body hole-hole interaction energy. The BF three-body cluster energy W_3 includes the third-order bubble insertion on a particle line (as well as the third-order ring diagram). The two terms inside each square bracket are the

Brueckner components of an IY energy. (A brief derivation of the second square bracket is reproduced in the Appendix for the reader's convenience.) One of these components is the negative of the n-body dispersion energy

$$W_n^D(\lambda^{(n)}) = \lambda^{(n)}\kappa_n/(n-1)! \ . \tag{2.5}$$

This energy is proportional to the multiplet excitation parameter

$$\kappa_n = \frac{1}{N}\sum_{ij\cdots} \langle ij\cdots|\chi^\dagger_{12\ldots n}\chi_{12\ldots n}|ij\cdots\rangle_a \tag{2.6}$$

for the simultaneous excitation of n fermions out of the Fermi sea, as described by the multiplet excitation operator $\chi_{12\ldots n}$. (N is the number of fermions in the system.) It also depends on the Lagrange multiplier[5] $\lambda^{(n)}$, which is introduced formally via a constraint on the size of κ_n. It is ultimately determined by the choice of s.p. potentials, as in BT. (It is also related to the renormalization of s.p. occupation probabilities.[4]) Therefore we may use the Brueckner expression

$$\lambda^{(n)} \approx \overline{U}_p^{(n)} - \overline{U}_h^{(n)} \ , \tag{2.7}$$

and interpret it as an average change of the s.p. potential energy when a fermion is excited out of the Fermi sea. The choice of s.p. potentials $U_p^{(n)}$ and $U_h^{(n)}$ appropriate for the n-plet excitation is of course an important dynamical question which affects both the cfn's and the overall qualitative picture. However, we are not concerned with this question in this paper.

On the other hand, the Brueckner energy up to three-body terms differs from Eq. (2.4) in the absence of the last term $-W_3^D(\lambda^{(3)})$, which cancels the three-body dispersion energy in W_3.

We should point out parenthetically that Eq. (2.4) contains an explicit illustration of that special feature of Brueckner theory that each s.p. potential $\overline{U}_p^{(n)}$ is chosen for the cancellation of certain terms in *higher orders*. The illustration involves W_2^D of which a $\overline{U}_p^{(2)}\kappa_2$ part comes originally from W_3 in Eq. (2.4). (We may include the choice of $\overline{U}_p^{(2)} = 0$ as a special case of the above.) We can thus identify in Eq.(2.4) an *original* W_2^D energy made up of this $\overline{U}_p^{(2)}\kappa_2$ and the $-\overline{U}_h\kappa_2$ terms. This original W_2^D is canceled by $-W_2^D(\lambda^{(2)})$ of the first square bracket. This leaves a dispersion energy W_2^D in W_2. Thus pair dispersion terms $\pm W_2^D$ appear 3 times in Eq. (2.4).

The same situation may obtain for W_n^D, so that the energy expression may appear complicated for general choices of $U_p^{(n)}$. It is in this context that the conceptual simplicity of the choice $\overline{U}_p^{(n)} = 0$ can be appreciated, although this choice does not necessarily give the fastest convergence of the energy expansion.

To render further analysis more definite, let us make this simple approximation

$$\overline{U}_p^{(n)} = 0, \quad \lambda^{(n)} = -\overline{U}_h^{(n)} = -\overline{U}_h \ , \tag{2.8}$$

which corresponds to the compact-cluster expansion of Brandow[11] and the recommended procedure in the exp-S method.[12] Then the Brueckner and IY energies both contain the pair dispersion energy $W_2^D(-\overline{U}_h)$. They still differ, but now by the triplet dispersion energy

$$W_3^D(-\overline{U}_h) = -\tfrac{1}{2}\overline{U}_h\kappa_3 \ . \tag{2.9}$$

It would be interesting to see if W_3^D will eventually appear in the four-body energy of the IY expansion.

How serious is the discrepancy W_3^D at this three-body level? At low densities, we expect $\kappa_3 \ll \kappa_2$. Hence there is reason to hope that these theories agree at relatively low orders. However, as the density increases, the "break-even" point ($\kappa_3 \approx 2\kappa_2$ in the present approximation) may be reached and passed. The situation then becomes quite complicated.

It is therefore useful to study κ_3 in order to gain some insight into W_3^D.

III. TRIPLET EXCITATION PARAMETER

In this section, we calculate κ_3 and κ_2 and study their relationship. For simplicity, we use Jastrow cfn's (2.3) which often give values of κ_2 in close agreement with those obtained in Brueckner calculations.[1,2] Also great accuracy is not needed in the present semiquantitative study.

For these cfn's, we find that

$$\begin{aligned} &\chi_{123} = \chi_{12}\chi_{13} + \chi_{12}\chi_{23} + \chi_{13}\chi_{23} + \chi_{12}\chi_{13}\chi_{23} \ , \\ &\chi_{ij} = f_{ij} - 1 \ . \end{aligned} \tag{3.1}$$

The following forms of $f(r)$ are used in the calculation.

(i) BCC form (Ref. 1):

$$f(r) = \begin{cases} 0, & \text{for } r < c \\ \{1 - \exp[-\mu_1(r-c)]\}\{1 + \gamma\exp[-\mu_2(r-c)]\}, & \text{for } r \geq c \end{cases} \tag{3.2}$$

with the parameters of Chakkalakal, Yang, and Clark[13] (their Tables 10a and 12a).

(ii) Pandharipande (PP) form (Ref. 14):

Function $f(r)$ heals smoothly to 1 at and beyond the cutoff distance d. Typically $k_f d \approx 2$. We use the analytic approximation of Alexandrov, Moszkowski, and Wong[15]:

$$f(r)=\begin{cases}0, & \text{for } r<c\\ 1-\dfrac{c}{r}\left(\dfrac{d-r}{d-c}\right)^{p}, & \text{for } c\le r\le d\\ 1, & \text{for } r>d\end{cases} \tag{3.3}$$

with $p=2$.

(iii) CMW form (Ref. 16):

$$f(r)=\exp\left(-\frac{b}{2r}\,e^{-r/b}\right) \tag{3.4}$$

with the parameters of Krotscheck and Takahashi.[17]

The excitation parameter κ_3 is then given by the integral

$$\kappa_3=\rho^2\int\int d^3r_{12}d^3r_{23}(3\chi_{12}^2\chi_{23}^2+6\chi_{12}^2\chi_{23}\chi_{31}+6\chi_{12}^2\chi_{23}^2\chi_{31}+\chi_{12}^2\chi_{23}^2\chi_{31}^2)\left[1-\frac{1}{\nu}(l_{12}^2+l_{23}^2+l_{31}^2)+\frac{2}{\nu^2}\,l_{12}l_{23}l_{31}\right], \tag{3.5}$$

where

$$l_{12}\equiv l(k_Fr_{12})=\frac{3}{k_Fr_{12}}\,j_1(k_Fr_{12}) \tag{3.6}$$

is the Slater function for the Pauli exchange part of the pair correlation function, and ν is the degeneracy of the fermion s.p. spatial state (2 for neutron matter, 4 for NM). We note that if χ_{ij} is very short range, then $l_{ij}\approx 1$ when $\chi_{ij}\neq 0$. Then κ_n is proportional to $\nu(\nu-1)\cdots(\nu-n+1)/\nu^n$. Consequently $\kappa_n\approx 0$ for $n>\nu$. If χ_{ij} is reasonably long range, κ_n is non-negligible for $n>\nu$. We also note for the sake of completeness that

$$\kappa_2=\rho\int d^3r\chi^2(r)\left[1-\frac{1}{\nu}l^2(k_Fr)\right]. \tag{3.7}$$

Figure 2 gives $2\kappa_2$ (broken curves) and κ_3 (solid curves) in neutron matter for CMW cfn's (open circles) and BCC cfn's (solid circles). The CMW functions used were originally obtained for the repulsive part of the $^1S_0$ Reid potential of the "homework problem,"[24] while the BCC functions were obtained for the standard hard-core potential (SHCP) in even states and the pure hard core ($c=0.4$ fm) in odd states. These two potentials are rather similar. The resulting κ_n are very different, however, because the CMW function is long range (e.g., $f(b)=0.83$ and $b\approx 2$ fm). It is not completely clear to what extent the CMW cfn is inferior to shorter-range Bethe-Goldstone, BCC, PP, and other cfn's. The fact that the pair dispersion effect cuts down long-range correlation[2] is very suggestive in this connection.

Figure 3 shows results in NM for the BCC and PP functions. They give comparable results for the SHCP, except at the higher densities where the PP parameters are smaller because the corresponding cfn's have shorter ranges. (The PP functions are cut off at $r=d$, where $d\approx 1.7/k_F$.) For the IY potential[18] with its larger core radius ($c=0.6$ fm), similar values of κ_n appear at values of k_F smaller than those for the SHCP by $\approx 20\%$.

These results show an interesting correlation between the values of κ_2 and κ_3. We recall that the true (pair) excitation probability is not κ_2, but[10,11]

$$f_2=[(1+4\kappa_2)^{1/2}-1]/[(1+4\kappa_2)^{1/2}+1]\,. \tag{3.8}$$

This is approximated by κ_2 adequately for small κ_2 ($\lesssim 0.1$), but differs significantly from the latter for large κ_2 ($\gtrsim 0.4$, which is just below the break-even point). Traditionally κ_2 is used as an expansion parameter. We find here that κ_3 is indeed very small when κ_2 is small, and large when κ_2 is large. Therefore the use of κ_2 as an expansion parameter appears quite justified.

Thus for each potential and each correlation function, we can distinguish a low-density region of small κ_2 and κ_3, where a simple hole-line expansion appears sensible, a medium-density re-

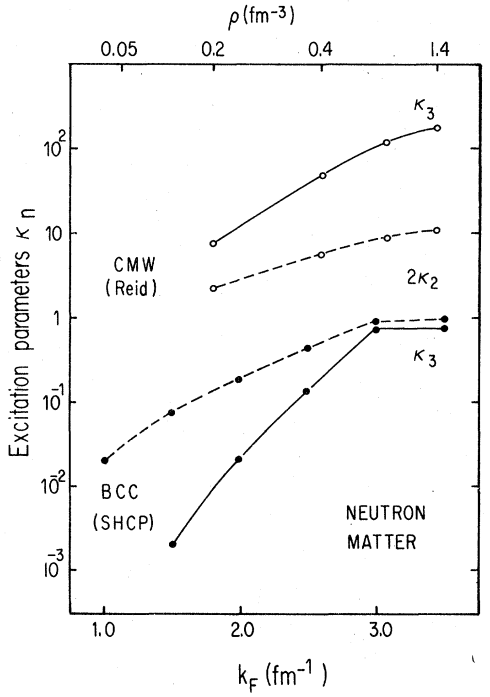

FIG. 2. Multiplet excitation parameters κ_3 (solid curves) and $2\kappa_2$ (broken curves) for CMW cfn's (Reid potential) and BCC cfn's (SHCP potential) in neutron matter.

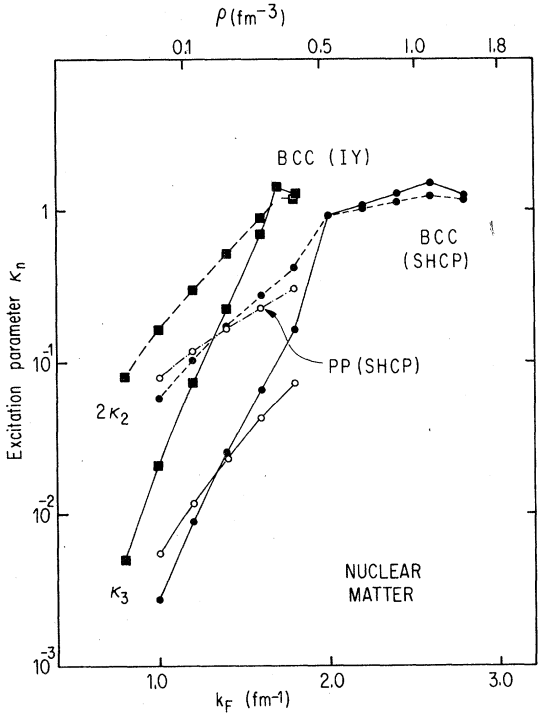

FIG. 3. Multiplet excitation parameters κ_3 (solid curves) and $2\kappa_2$ (broken curves) for BCC cfn's (SHCP potential), PP cfns (SHCP potential) and BCC cfns (IY potential) in nuclear matter.

gion, and a high-density region of large κ_2 and κ_3 where many-body correlations become significant and the Fermi liquid features become manifest.

If the above qualitative picture is valid, knowledge of κ_2 is quite valuable. For example, consider NM at or below normal density ($\rho_0 = 0.15$ fm^{-3}). From Brueckner calculations we obtain $\kappa_2 \lesssim 0.2$ for the IY potential, and $\kappa_2 \lesssim 0.13$ for the SHCP (in even states plus the hard core in odd states). The results are quite insensitive to the choice of $\lambda^{(2)}$ (Ref. 2). For these potentials, the density of NM does not appear high.

The situation is more complicated for realistic nuclear potentials because of tensor forces. It is quite likely that the same qualitative relation holds between κ_2 and κ_3, since κ_3 is made up of successive pair excitations, and a major effect of tensor forces is already included in κ_2. We find that for $\rho \leq \rho_0$, κ_2 ranges from 0.07 (UG3 potential) to 0.19 (HJ potential) in a "standard" Brueckner calculation with $\bar{U}_p = 0$.[10] The situation is then rather similar to that for simple potentials.

Realistic potentials do differ from simple potentials in at least one respect: κ_2 is sensitive to the choice of $\bar{U}_p$. For example, a lowering of $\bar{U}_p$ by 50 MeV causes κ_2 to increase by 0.1 at ρ_0 for the HJ potential,[10] leading to higher estimates of $\kappa_2 \approx \kappa_3 \approx 0.3$. These values are rather large and indicate that the comparison between theories should then be carried to higher orders.

Even at the three-body level, quantitative comparisons between Brueckner results, IY results for Brueckner (i.e., state dependent) cfn's and IY results with Jastrow (i.e., state independent) cfn's for realistic nuclear potentials are probably of considerable value.

Finally, we can visualize higher n-plet dispersion energies involving n-plet excitation parameters. The results of this section suggest that κ_n will decrease rapidly with n when the density and κ_2 are small. Then W_n^D becomes progressively less important. On the other hand, if both density and κ_2 are large, κ_n and W_n^D may remain large. Under the worst of circumstances, the difference between Brueckner and IY truncation points may remain substantial to any finite order of perturbation. When this occurs, special techniques will be needed to sum the perturbation series.

IV. CONCLUDING REMARKS

The Brueckner theory identifies explicit mechanisms which can contribute to the dispersion energies W_n^D, both at the two-body level and at the three-body level. To the extent that their contributions are significant, the resulting dispersion effects can be considered to be physically meaningful. It can also happen, especially at high densities, that there are so many important higher-order contributions that the isolation of one class of effects for special treatment is not useful. Even so, the fact remains that the effects are present and can be calculated.

A pair dispersion energy W_2^D also appears in the IY expansion if the same state- and momentum-dependent Brueckner cfn's are used. Then the IY expansion appears to differ from the Brueckner expansion only in the truncation point. For example, W_2^D appears only at the three-body level, but W_3^D has not yet appeared.

In contrast, dispersion energies are entirely absent when state-independent Jastrow cfn's are used.[3] This is a simple consequence of the state independence of these simple trial functions.

We cannot rule out the possibility that simple state-independent Jastrow cfn's are actually better than Brueckner cfn's, pernaps for certain potentials at certain densities. However, if they are better, we ought to understand why they are better in spite of the many state- and momentum-dependent effects which appear so readily. Similarly, the rejection of the pair dispersion energy should have an explicit, dynamical justification. No such justification has been given in the literature.

There is a related problem in the comparison between Brueckner and variational energies. Being variational in character, Jastrow functions do not have to be very realistic to be useful for estimating energy upper bounds. Since calculated variational energies[19,20] are already much lower than the results of LOBT, significant attractive contributions should appear in higher-order Brueckner calculations if the calculated variational energies are indeed upper bounds. This possibility does not necessarily imply that dispersion effects are spurious.

There is no doubt that we need reliable energy comparisons between theories. The present work suggests that qualitative comparisons between Brueckner and IY expansions will also help if continued to the four-body level, at least for relatively low-density fermion fluids such as nuclear matter at or below normal density.

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APPENDIX: THREE-BODY DISPERSION FORMULA

The structure of the first bracket in Eq. (2.4) is well known and was first derived in Ref. 2. The three-body terms have been analyzed in Refs. 4 and 5. Of these terms, the part of greatest importance in the present discussion is the second square bracket. Although its structure has been derived before,[4,5] we believe that the reader will find it convenient to have summarized below in this Appendix the major steps involved in the analysis. We follow the derivation of Ref. 4.

The IY cluster energy in question is

$$C_3 = \frac{1}{3!N}\sum_{ijk}\left[\langle ijk|\Omega_{123}^{\dagger}(t_{123}+v_{123}-t_i-t_j-t_k)\Omega_{123}|ijk\rangle_{\mathcal{A}} - 3\delta_{k\bar{k}}\langle ij|\Omega_{12}^{\dagger}(t_{12}+v_{12}-t_i-t_j)\Omega_{12}|ij\rangle_{\mathcal{A}}\right] . \tag{A1}$$

Here

$$t_{12} = t(1)+t(2) ,$$
$$t_{123} = t(1)+t(2)+t(3) ,$$
$$v_{123} = v_{12}+v_{23}+v_{31} \tag{A2}$$

are kinetic-energy and potential operators, $\Omega_{12} = 1+\chi_{12}$ is the usual Bethe-Goldstone pair correlation operator, and

$$\Omega_{123} = 1+\chi_{12}+\chi_{13}+\chi_{23}+\chi_{123} \tag{A3}$$

is the triplet Bethe-Faddeev (BF) wave operator. The latter is defined by the three-body equation

$$\chi_{123} = -\frac{Q_{123}}{e_{123}}v_{123}\Omega_{123} , \tag{A4}$$

where Q_{123} is the Pauli operator for the simultaneous excitation of three fermions out of the Fermi sea. The energy denominator

$$e_{123} = t_{123}+U_{123}-\epsilon_i-\epsilon_j-\epsilon_k \tag{A5}$$

is defined in terms of the s.p. potential operator

$$U_{123} = U(1)+U(2)+U(3) \tag{A6}$$

and the s.p. energies t_i and $\epsilon_i = t_i+U_i$ of the normally occupied s.p. state i. (For simplicity of notation, we shall not distinguish between the s.p. potentials $U_i^{(3)}$ and plain U_i.) The symbol $\bar{k}$ labels the s.p. state of particle 3 in the antisymmetrized set $\mathcal{A}(ijk)$.

Part of the first term in Eq. (A1) is

$$\begin{aligned} -W_3^D &= \frac{1}{6N}\sum_{ijk}\langle ijk|\chi_{123}^{\dagger}(t_{123}+v_{123}-t_i-t_j-t_k)\Omega_{123}|ijk\rangle_{\mathcal{A}} \\ &= \frac{1}{6N}\sum_{ijk}\langle ijk|\chi_{123}^{\dagger}(U_i+U_j+U_k-U_{123})\Omega_{123}|ijk\rangle_{\mathcal{A}} \\ &= -\tfrac{1}{2}\lambda^{(3)}\kappa_3 , \end{aligned} \tag{A7}$$

where

$$\lambda^{(3)} \approx \Delta\bar{U} = \bar{U}_p - \bar{U}_h .$$

The crucial step leading to line 2 requires an application of the wave Eq. (A4).

The remainder of Eq. (A1) can be simplified by separately examining its kinetic- and potential-energy contributions. The former,

$$\frac{1}{6N}\sum_{ijk}\left[\langle ijk|(1+\chi_{12}^{\dagger}+\chi_{23}^{\dagger}+\chi_{31}^{\dagger})(t_{123}-t_i-t_j-t_k)\Omega_{123}|ijk\rangle_{\mathcal{A}} - 3\delta_{k\bar{k}}\langle ij|\Omega_{12}^{\dagger}(t_{12}-t_i-t_j)\Omega_{12}|ij\rangle_{\mathcal{A}}\right] = 0 , \tag{A8}$$

vanishes because the first term in Eq. (A8) cancels the second. The remaining, potential-energy term is

$$W_3 = \frac{1}{6N}\sum_{ijk}\left[\langle ijk|(1+\chi_{12}^{\dagger}+\chi_{23}^{\dagger}+\chi_{31}^{\dagger})T|ijk\rangle_a - 3\delta_{k\bar{k}}\langle ij|\Omega_{12}^{\dagger}G_{12}|ij\rangle_a\right] , \tag{A9}$$

where we have used the definitions

$$G_{12} = v_{12}\Omega_{12}, \quad T = v_{123}\Omega_{123} = T_1 + T_2 + T_3 \tag{A10}$$

for the two- and three-body reaction matrices. The component T matrix T_i is that part of T in which particle i is not involved in the last G interaction.[21] We may write

$$T = G_{23} + G_{31} + G_{12} + [(T_1 - G_{23}) + (T_2 - G_{31}) + (T_3 - G_{12})] , \tag{A11}$$

and note that the contributions from the G_{ij} parts of T to the first term of Eq. (A9) exactly cancel its second term. This leaves

$$W_3 = \frac{1}{6N}\sum_{ijk}\langle ijk|3\chi_{12}^{\dagger}[(T_1 - G_{23}) + (T_2 - G_{31}) + (T_3 - G_{12})]|ijk\rangle_a . \tag{A12}$$

The last term of this equation vanishes, because the third particle is already excited out of the Fermi sea in $(T_3 - G_{12})|ijk\rangle_a$. The remaining two terms contribute equally. Using the definition

$$T_1 - G_{23} = -G_{23}Z_1 , \tag{A13}$$

where Z_1 is the BF operator introduced by Bethe,[21] we obtain finally the familiar expression

$$W_3 = -\frac{1}{N}\sum_{ijk}\langle ijk|\chi_{12}^{\dagger}G_{23}Z_1|ijk\rangle_a \tag{A14}$$

of Bethe.[21] Thus the form

$$C_3 = W_3 - W_3^D \tag{A15}$$

is obtained for the second square bracket in Eq. (2.4).

The result (A14) was first obtained by da Providencia and Shakin.[4] In repeating their derivation, we hope to have made particularly clear how the "two-sided" IY energy expression (with its two Ω operators) is reduced to the "one-sided," model expression of the Brueckner theory, i.e., through the fact that Ω_{123} satisfies the wave Eq. (A4).

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