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Correlations in fully-spin-polarized liquid ^{3}He: Ladders, rings, and the particle-hole irreducible interaction

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We investigate the relative contribution of ladder and ring diagrams to the single-particle self-energy in fully-spin-polarized liquid ^{3}He (^{3}He$^\uparrow$). Ladder diagrams are summed to all orders of the bare ^{3}He-^{3}He interaction using the Galitskii-Feynman-Hartree-Fock (GFHF) analysis. Previous studies of ^{3}He$^\uparrow$, using GFHF analysis, have neglected the part of the GFHF self-energy coming from the correlation potential, V_{co}. These calculations produced ground-state energies in fair agreement with values obtained from variational Monte Carlo (VMC) calculations. However, properties such as Landau parameters, which are directly related to long-range correlations, tend to differ considerably from known values. In the present work we have evaluated V_{co} and found it to have an appreciable effect on the single-particle excitation energies, $\varepsilon(k)$ and the ground-state energy: Including V_{co} significantly reduces the ground-state energy. As a further refinement over previous GFHF calculations, we have used a more accurate center-of-mass momentum, P, dependence for the Galitskii-Feynman t matrix in the self-energy calculation. Again we find an undesirably large decrease in the ground-state energy. Finally, upon including a contribution from a summation of ring diagrams, we find a ground-state energy that is once again in fair agreement with the VMC values. The ring diagrams are driven by a local particle-hole interaction obtained by the method of correlated basis functions (CBF). Ring diagrams are then summed within a random-phase approximation. Our final $\varepsilon(k)$ is used to calculate the particle-hole irreducible interaction $I_{p\text{-}h}$. In the long-wavelength limit we find that our $I_{p\text{-}h}$ is in much better agreement with the CBF $I_{p\text{-}h}$ when our $\varepsilon(k)$ includes contributions from V_{co}, Σ_R, and the refined self-energy calculation.

I. INTRODUCTION

The important role that many-body correlations have in determining the properties of quantum fluids, such as liquid ^{3}He, has long been recognized. A standard means for obtaining a proper theoretical description of ^{3}He, that deals directly with these correlations, begins by evaluating the single-particle self-energy, $\Sigma(\mathbf{k},\omega)$. From $\Sigma(\mathbf{k},\omega)$ the single-particle excitation energies, spectral functions, momentum distribution, effective mass, and binding energy can be derived.[1] For a highly correlated quantum system, such as ^{3}He, the calculation of $\Sigma(\mathbf{k},\omega)$ requires an appropriately defined "effective" interaction. Various methods have been employed to determine a suitable effective interaction. These methods may be semiempirical as in the case of polarization potential theories[2] and induced-interaction models[3] or based on first principles alone. First-principles calculations restrict the input of the theory to the bare ^{3}He-^{3}He interaction and the bare ^{3}He mass. Variational Euler-Lagrange,[4] correlated basis function (CBF),[5] coupled cluster,[6] and Green's-function perturbation methods[1,7] are all examples of first-principles approaches. In these theories, the effective interaction is obtained by a proper renormalization of the bare interaction. The mechanisms responsible for renormalizing the bare interaction are the statistical and dynamical correlations. In CBF and Green's function perturbation approaches these correlations are represented by scattering processes involving particles (p) and holes (h).

Independent of the method from which it is determined, the effective interaction should have the correct short- and long-range behavior before certain elementary properties of the system can be described. It has become conventional to speak of the interaction as being appropriately short- and long-ranged screened.

Short-range screening is necessary to renormalize the steeply repulsive core of the bare interaction. In variational Euler-Lagrange and CBF approaches the repulsive core is handled by choosing an appropriate trial wave function. The most successful choice is the well-known (properly symmetrized) Feenberg wave function.[4,5] In Green's-function perturbation theory, short-range screening is accomplished by summing ladder diagrams to all orders of the bare interaction.[1] In terms of a scattering process, the ladders represent multiple scattering of a pair of particles (p-p) or a pair of holes (h-h). For scattering processes involving large momentum transfers $\mathbf{Q}$, where long-range correlations are negligible, the ladder sum completely determines the systems dynamics[8] as is manifested in the dynamic structure function $S(\mathbf{Q},\omega)$.

Long-range screening is necessary to ensure that the appropriate behavior will be obtained in the Landau limit

($Q \rightarrow 0$). This leads to the correct long-wavelength behavior for quantities such as the static structure function $S(\mathbf{Q})$, Landau parameters, and the zero-sound dispersion curve. Fermi-surface properties such as the quasiparticle strength, z_{k_F}, which is the discontinuity in the momentum distribution at k_F, are strongly influenced by the long-range correlations. This was observed to be the case in nuclear matter by Poggioli and Jackson.[9] In Green's-function perturbation theory long-range screening is accomplished by summing particle-hole (p-h) ring diagrams. The ring diagram summation is usually done within a random-phase approximation (RPA).[10] In CBF theory this is done using a correlated version of the RPA (CRPA).[11]

In spite of the rather complete conceptual understanding of the correlations important in ^{3}He, far fewer attempts have been made for a full numerical evaluation of the ladder and ring summations. In the present work we use standard Green's-function perturbation theory, where ladder and ring diagrams appear explicitly and naturally. The problem, of course, remains of how to evaluate the ladders and rings. In principle, one could follow the parquet formalism.[12] For practical matters this formalism, albeit certainly appealing, has always been simplified by introducing local approximations for the four-point vertex functions. These approximations are necessary, since the goal of parquet is to treat ladders and rings on equal footing: Ladder vertex functions drive the ring series and vice versa. Unfortunately, it presently appears to be prohibitively difficult to introduce nonlocal interactions back into the parquet while maintaining this goal.

The present work represents a more modest but tractable calculation. Rather than attempting to sum large classes of diagrams consistently, we use a nearly complete calculation of the ladder diagrams that has recently been used to study the ground-state and dynamical properties of spin-polarized liquid deuterium.[13] This study is based on the Galitskii-Feynman t matrix.[14] Galitskii-Feynman-Hartree-Fock (GFHF) theory is reviewed in Sec. II. The GFHF self-energy Σ_L is calculated directly from the t matrix. Introducing local approximations for the t matrix are unnecessary in this calculation. The calculation of Σ_L described in Ref. 13 supersedes that of previous calculations by including the so-called correlation potential $V_{\rm co}$. $V_{\rm co}$ involves scattering to intermediate two-hole, one-particle states (2h-1p). Further discussion of $V_{\rm co}$ is given in Sec. II. GFHF theory is itself a first-principles theory, and one can define a single-particle excitation energy $\varepsilon(\mathbf{k})$ from the GFHF self-energy:

$$\varepsilon(\mathbf{k})=\frac{k^2}{2m}+\mathrm{Re}\Sigma_L((\mathbf{k},\varepsilon(\mathbf{k}))\ . \qquad (1)$$

Recent calculations[15] of spectral functions and the momentum distribution for fully-spin-polarized liquid ^{3}He have shown that both $V_{\rm co}$ and an accurate center-of-mass momenta dependence for the t matrix are necessary to achieve qualitatively correct values for those quantities. Consequently, part of Sec. II is devoted to an explanation of a refined treatment of the center-of-mass momenta of the t matrix in the evaluation of Σ_L.

The analysis necessary to evaluate the ring diagram contribution to the self-energy Σ_R is given in Sec. III. The ring diagrams are summed within a RPA. Σ_R has the same form as that used by Blaizot and Friman[16] in nuclear-matter calculations. This same expression has been used by Krotscheck,[11] and Friman and Krotscheck[17] for normal ^{3}He, by Krotscheck, Clark, and Jackson[18] for spin-polarized ^{3}He, and recently by Dave, Clark, and Panoff[19] for spin-polarized deuterium. The evaluation of Σ_R requires a driving interaction and a single-particle excitation energy. In the present work, we use the local particle-hole interaction of Ref. 18, and the excitation energy comes from our self-consistent GFHF calculation [cf. Eq. (1)]. Proceeding in this way introduces a certain amount of "overcounting" of distinct diagrams. We comment on this in Sec. III. Adding the two self-energies results in our final expression for $\varepsilon(\mathbf{k})$,

$$\varepsilon(\mathbf{k})=\frac{k^2}{2m}+\mathrm{Re}\Sigma_L(\mathbf{k},\varepsilon(\mathbf{k}))+\mathrm{Re}\Sigma_R(\mathbf{k},\varepsilon(\mathbf{k}))\ . \qquad (2)$$

Here, we consider an N-particle system of fully spin-polarized liquid ^{3}He ($^3\mathrm{He}^\uparrow$). We choose this system both for its intrinsic interest[20] and also to avoid unnecessary complications due to state-dependent effects. We are interested in assessing the role that ring and ladder diagrams have in determining, for example, $\varepsilon(\mathbf{k})$. As is well known, $\varepsilon(\mathbf{k})$ is a quantity of fundamental interest. For on-shell calculations, it directly contains information about the effective mass and the binding energy. It is also primary input to four-point vertex functions such as the t matrix and the particle-hole irreducible interaction $I_{p\text{-}h}$. $I_{p\text{-}h}$ is the interaction that drives the dynamic structure function. Further, a local approximation to $I_{p\text{-}h}$ is used to evaluate Σ_R as described above. For Q less than the Fermi momentum k_F, $I_{p\text{-}h}$ should provide a good indication for the importance of long-range screening. Consequently, in Sec. IV we review the analysis necessary to calculate $I_{p\text{-}h}$.

In Sec. V we present and discuss our results. The $\varepsilon(\mathbf{k})$ are compared for the various cases: ladder contributions without $V_{\rm co}$, ladder contributions including $V_{\rm co}$, and ladder contributions including $V_{\rm co}$ plus ring contributions. In $^3\mathrm{He}^\uparrow$ we find that including $V_{\rm co}$ requires that a ring contribution be included as well. That is, the full contribution of the ladders tends to reduce substantially the binding of the system. Including the rings largely cancels this effect. The need for adding a ring contribution was not as evident in the deuterium study of Ref. 13. Our $I_{p\text{-}h}$ is compared to the CBF calculation of Ref. 18. This comparison is made for ladder contributions only and then ladder plus ring contributions. The full evaluation of the ladders with the rings greatly improves the agreement with the CBF result for small momentum transfer.

Before proceeding to the discussion of GFHF analysis, we mention that this work should be regarded as somewhat preliminary in the sense that the the final form for the excitation energy is no longer self-consistent. To go beyond the present calculation would require substantial numerical effort, however. Nevertheless, our experience with this formalism makes us confident that a self-consistent calculation will produce the same qualitative results observed for the excitations and $I_{p\text{-}h}$. This point will be discussed further in Sec. VI.

II. LADDER DIAGRAM CONTRIBUTION TO THE SELF-ENERGY

In this section we provide a brief review of GFHF theory with emphasis on the self-energy, self-consistency, the center-of-mass momentum dependence of the t matrix and the self-energy, and the application to spin-polarized $^3\text{He}^{\uparrow}$. Further discussion can be found in Refs. 13 and 14. The primary interaction in GFHF theory is the Galitskii-Feynman t matrix. It is obtained by summing ladder diagrams to all orders of the bare ^{3}He-^{3}He interaction $V(\mathbf{r})$. This summation leads to the Bethe-Salpeter equation for the t matrix:

$$T(k_1,k_2,k_3,k_4)=V(\mathbf{k}_1-\mathbf{k}_3)+i\int\frac{d^4k_5}{(2\pi)^4}V(\mathbf{k}_1-\mathbf{k}_5)G(k_5)G(k_1+k_2-k_5)T(k_5,k_1+k_2-k_5,k_3,k_4)\ , \tag{3}$$

where $V(\mathbf{k})$ is the Fourier transform of $V(\mathbf{r})$. In the present work $V(\mathbf{r})$ is the potential of Aziz *et al.*[21] (Note that we have adopted the notation that all vectors are four-vectors unless otherwise specified).

The single-particle Green's function $G(\mathbf{k},\omega)$ is taken to have the form

$$G(\mathbf{k},\omega)=\frac{1-n(\mathbf{k})}{\omega-\varepsilon(\mathbf{k})+i\eta}+\frac{n(\mathbf{k})}{\omega-\varepsilon(\mathbf{k})-i\eta}\ , \tag{4}$$

where $n(\mathbf{k})\equiv\theta(k_F-k)$ is single-particle momentum distribution and $\varepsilon(\mathbf{k})$ is the single-particle excitation energy:

$$\varepsilon(\mathbf{k})=\frac{k^2}{2m}+\text{Re}\Sigma_L(\mathbf{k},\varepsilon(\mathbf{k}))\ . \tag{5}$$

Here m is the bare mass and $\text{Re}\Sigma(\mathbf{k},\varepsilon(\mathbf{k}))$ is the real part of the (on-shell) GFHF self-energy. For an instantaneous pair potential, T depends on the frequency only through $E=\omega_1+\omega_2$ and the frequency integral in (3) can be performed:

$$T(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4,E)=V(\mathbf{k}_1-\mathbf{k}_3)+\int\frac{d^3k_5}{(2\pi)^3}V(\mathbf{k}_1-\mathbf{k}_5)\left[\frac{(1-n_5)(1-n_{1+2-5})}{E-\varepsilon_5-\varepsilon_{1+2-5}+i\eta}-\frac{n_5n_{1+2-5}}{E-\varepsilon_5-\varepsilon_{1+2-5}-i\eta)}\right]$$
$$\times T(\mathbf{k}_5,\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_5,\mathbf{k}_3,\mathbf{k}_4,E)\ , \tag{6}$$

where $n_p\equiv n(\mathbf{k}_p)$ and similarly for ε_p.

The GFHF self-energy $\Sigma_L(\mathbf{k},\omega)$ is a generalization of the Hartree-Fock self-energy in which the bare interaction is replaced by the exchange symmetrized t matrix T^{sy}:

$$T^{\text{sy}}(k_1,k_2,k_3,k_4)=T(k_1,k_2,k_3,k_4)-T(k_1,k_2,k_4,k_3)\ . \tag{7}$$

Explicitly,

$$\Sigma_L(\mathbf{k}_1,\omega_1)=-i\int\frac{d^4k_2}{(2\pi)^4}T^{\text{sy}}(k_1,k_2,k_1,k_2)G(k_2)\ . \tag{8}$$

Equations (3)–(8) form a closed set of equations, which must be iterated until self-consistent. The ω_2 dependence may be integrated out of (8). This is done by invoking the analytical properties of the t matrix and $G(\mathbf{k},\omega)$. We simply state the result.[13,14]

$$\text{Re}\Sigma_L(\mathbf{k}_1,\omega_1)=\int\frac{d^3k_2}{(2\pi)^3}\left[\text{Re}T^{\text{sy}}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_1,\mathbf{k}_2,\omega_1+\varepsilon(\mathbf{k}_2))n(\mathbf{k}_2)-\text{P}\int_{-\infty}^{2\mu}\frac{dE}{\pi}\frac{\text{Im}T^{\text{sy}}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_1,\mathbf{k}_2,E)}{\omega_1+\varepsilon(\mathbf{k}_2)-E}\right]\ , \tag{9}$$

$$\text{Im}\Sigma_L(\mathbf{k}_1,\omega_1)=\int\frac{d^3k_2}{(2\pi)^3}\text{Im}T^{\text{sy}}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_1,\mathbf{k}_2,\omega_1+\varepsilon(\mathbf{k}_2))[\theta(\mu-\varepsilon(\mathbf{k}_2)-\theta(2\mu-\omega_1-\varepsilon(\mathbf{k}_2))]\ , \tag{10}$$

where $\mu=\varepsilon(k_F)$ is the chemical potential.

The first and second terms of $\text{Re}\Sigma_L$ are referred to as the Brueckner-Hartree-Fock (BHF) term, and the correlation potential V_{co}, respectively. V_{co} involves intermediate scattering processes to two-hole one-particle (2h-1p) states.[22] Previous calculations[14] using GFHF theory, done in normal and spin-polarized ^{3}He, have dropped V_{co}, although both terms in $\text{Im}\Sigma_L$ were retained. On the basis of the hole-line expansion[23] it was logical to assume that V_{co} should contribute substantially less than the BHF term in (9), which has a strong component coming from 2p-1h states. Nevertheless, V_{co} has been included in recent calculations done on liquid atomic deuterium[13] and, while qualitatively the hole-line argument seems to be correct, it was found that V_{co} is significant. This is also found to be true for $^3\mathrm{He}^{\uparrow}$.

An exact solution of the t matrix for general momenta is not technically feasible, and an angle-averaged approximation for the center-of-mass momentum is often used.[14] The angle average approximation is made in the solution of the Bethe-Salpeter equation (6) for the t matrix. Conservation of momentum reduces the number of independent momenta in T to a relative incoming $\mathbf{k}$, relative outgoing $\mathbf{k}'$, and center-of-mass momentum $\mathbf{P}$. The transformation equations are

$$\begin{aligned}
&\mathbf{k}=\tfrac{1}{2}(\mathbf{k}_1-\mathbf{k}_2)\ ,\\
&\mathbf{k}'=\tfrac{1}{2}(\mathbf{k}_3-\mathbf{k}_4)\ ,\\
&\mathbf{P}=\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4\ ,\\
&E=\omega_1+\omega_2=\omega_3+\omega_4\ ,
\end{aligned} \tag{11}$$

where for completeness we included a statement of energy conservation. To reduce the number of variables in T to a tractable number we assume that T depends only on the magnitude of $\mathbf{P}$, while the direction cosines defined by $\mathbf{P}$ and the relative momenta are angle averaged. In this approximation the t matrix reduces to

$$T(k_1,k_2,k_3,k_4)\approx T(\mathbf{k},\mathbf{k}',|\mathbf{P}|,E)\ . \tag{12}$$

We refer the reader to Refs. 14 and 24 for discussions of this approximation.

The angle-averaged approximation is likely to work best for on-shell energy calculations. An important example is the BHF term in (9) when the self-energy is evaluated on-shell, $\Sigma_L(\mathbf{k}_1,\varepsilon(\mathbf{k}_1))$. This observation is easily explained. In the on-shell BHF calculation one may argue that a relatively simple evaluation of the t matrix is sufficient. In that case, the frequency dependence for the t matrix is simply $E=\varepsilon(k_1)+\varepsilon(k_2)$. Transforming to relative and center-of-mass momenta, the total energy becomes $E=\varepsilon(\mathbf{P}/2+\mathbf{k})+\varepsilon(\mathbf{P}/2-\mathbf{k})$ and the energy denominator in (6) for the t matrix is $\varepsilon(\mathbf{P}/2+\mathbf{k})+\varepsilon(\mathbf{P}/2-\mathbf{k})-\varepsilon(\mathbf{P}/2+\mathbf{k}'')-\varepsilon(\mathbf{P}/2-\mathbf{k}'')\pm i\eta$, where $\mathbf{k}''\equiv\mathbf{P}/2-\mathbf{k}_5$ is a momentum corresponding an intermediate state. For $\varepsilon(k)$ with quadratic momentum dependence there is a cancellation of $\mathbf{P}$ from the energy denominator. Since interacting Fermi liquids have $\varepsilon(k)$ with approximately this property, the role of $\mathbf{P}$ is not expected to be too important in the energy denominator of the t matrix. Parenthetically, shifting the spectrum by a constant amount will leave the on-shell t matrix unchanged.[14] In principle, angle averaging is then required only in the remaining dependence of T on $\mathbf{P}$ through the occupation numbers in (6). For this reason it was found[14] that even taking $\mathbf{P}=0$ is a reasonable approximation for BHF ground-state energy calculations.

On the other hand, when considering V_{co}, even for on-shell self-energies, the above arguments no longer hold, and the role of the $\mathbf{P}$ in V_{co} can be expected to be important. The work in Ref. 15 has demonstrated that maintaining the angle-averaged $\mathbf{P}$ dependence in (9) and (10) is sufficient to obtain the correct qualitative behavior of $\mathrm{Im}\Sigma_L$ near the Fermi surface. For example, we know from Luttinger[25] that

$$\mathrm{Im}\Sigma(k,\omega)=(\omega-\mu)^2\mathrm{sgn}(\mu-\omega)$$

as $\omega\to\mu$. For this reason, we have done the calculation in which the dependence of T on $\mathbf{P}$ is retained in the self-energy calculation. More explicitly, the relative momentum and $\mathbf{k}_2$ in (9) and (10) can be expressed in terms of P,k_1 and the cosine of the angle between them, $\cos\theta_{P,k_1}$:

$$\begin{aligned}
&k=[k_1^2+(P/2)^2-k_1P\cos\theta_{P,k_1}]^{1/2}\ ,\\
&k_2=(k_1^2+P^2-2k_1P\cos\theta_{P,k_1})^{1/2}\ .
\end{aligned} \tag{13}$$

The integration is then done over P and $\cos\theta_{P,k_1}$. In addition to giving the correct behavior of $\mathrm{Im}\Sigma_L$, removing the $\mathbf{P}=0$ approximation also results in a substantial positive shift in the single-particle energies, as we discuss in Sec. V.

III. RING DIAGRAM CONTRIBUTION TO THE SELF-ENERGY

In this section we develop the necessary formalism to include contributions to the self-energy, which build in long-range screening. There are two issues for which we will be primarily concerned. The first issue deals with the choice of the interaction used to drive the ring diagrams. The second issue deals with the problem of overcounting of distinct diagrams.

As in Refs. 11 and 17–19, we choose the driving interaction in the ring diagram series to be the particle-hole irreducible interaction $I_{p\text{-}h}$. In fact, the spirit of the present calculation is very similar to that of those references: The full self-energy consists of a generalized Hartree-Fock term plus a ring contribution, which is driven by $I_{p\text{-}h}$. The diagrammatic representation of the p-h ring series is displayed in Fig. 1. Replacing the four-point interaction $I_{p\text{-}h}$ with a local interaction is equivalent to summing the ring series in an RPA. Krotscheck, Clark, and Jackson[18] have used CBF theory to calculate a local approximation to $I_{p\text{-}h}$ in $^3\mathrm{He}^{\uparrow}$. With this approximation for the interaction we may algebraically sum the ring series. The result for the self-energy is

$$\Sigma_R(\mathbf{k},\omega)=i\int\frac{d^4Q}{(2\pi)^4}I_{p\text{-}h}^2(\mathbf{Q})\chi(\mathbf{Q},\omega_Q)G(\mathbf{k}-\mathbf{Q},\omega-\omega_Q)\ , \tag{14}$$

where the RPA expression for the dynamic susceptibility $\chi(\mathbf{Q},\omega_Q)$ is

$$\chi(Q)=\frac{\chi^0(Q)}{1-I_{p\text{-}h}(Q)\chi^0(Q)}\ . \tag{15}$$

In this equation χ^0 is a generalized Lindhard function:

$$\chi^0(Q)=-i\int\frac{d^4p}{(2\pi)^4}G(p+Q)G(p)\ . \tag{16}$$

In these expressions, $G(\mathbf{k},\omega)$ is the full single-particle Green's function given by (4). Consequently, single-particle excitation energies are needed to evaluate (14) and (16). In our calculation we take these from our self-consistent GFHF theory [cf. Eq. (5)].

The ω_Q can be integrated from (14) with the result:

$$\mathrm{Re}\Sigma(\mathbf{k},\omega)=\int\frac{d^3Q}{(2\pi)^3}I_{p\text{-}h}^2(\mathbf{Q})\left[\mathrm{Re}\chi(\mathbf{Q},\omega-\varepsilon(\mathbf{k}-\mathbf{Q}))n(\mathbf{k}-\mathbf{Q})-P\int_0^\infty\frac{dE}{\pi}\frac{\mathrm{Im}\chi(\mathbf{Q},E)}{\omega-\varepsilon(\mathbf{k}-\mathbf{Q})-E}\right], \tag{17}$$

$$\mathrm{Im}\Sigma(\mathbf{k},\omega)=\int\frac{d^3Q}{(2\pi)^3}I_{p\text{-}h}^2(\mathbf{Q})\mathrm{Im}\chi(\mathbf{Q},\omega-\varepsilon(\mathbf{k}-\mathbf{Q}))[\theta(\varepsilon(k_F)-\varepsilon(\mathbf{k}-\mathbf{Q}))-\theta(\omega-\varepsilon(\mathbf{k}-\mathbf{Q}))] . \tag{18}$$

As mentioned in Sec. I, this expression has been used extensively in nuclear matter,[16] liquid-helium,[11,17,18] and liquid-deuterium calculations.[19]

We now return to the issues mentioned above. Rather than using $I_{p\text{-}h}$ in the ring diagrams we could have chosen a local approximation to the t matrix. $I_{p\text{-}h}$ appears to be the better choice for several reasons. First, a diagrammatic analysis[26] shows that $I_{p\text{-}h}$ contains many diagrams that are not contained in the t matrix. One example of the diagrams missed would be those with p-h rings in the rungs of the ladders. This type of diagram can be expected to be important, since it has a direct screening effect on the bare interaction. Secondly, $I_{p\text{-}h}$ is considerably more repulsive than the t matrix for low values of momentum. It is well established[18,27,28] that a repulsive interaction in (15) is necessary to effectively push the zero-sound mode up out of the particle-hole band in $^3\mathrm{He}^\uparrow$. $I_{p\text{-}h}$ is sufficiently repulsive to achieve this, while the t matrix is not. Consequently, for collective effects to be included in the self-energy, (15) must be driven by $I_{p\text{-}h}$. This does not preclude using the t matrix for the two vertex functions flanking the χ in Fig. 1 and accounting for the $I_{p\text{-}h}^2$ in (14). We settled this issued by performing a numerical calculation and comparing the results. The result of that study showed that the t matrix gave substantially inferior results for spectra $\varepsilon(\mathbf{k})$, compared to those obtained by using $I_{p\text{-}h}$.

We now discuss the over counting introduced by adding (14) to the GFHF self-energy. We refer to the terms in Fig. 1 that are second order in $I_{p\text{-}h}$ by $\Sigma_R^{(2)}$. It is clear that keeping $\Sigma_R^{(2)}$ introduces over counting even at second order in $V(\mathbf{k})$. This is immediately obvious by noting that one set of diagrams in $I_{p\text{-}h}$ are the ladder diagrams. The T approximation for $I_{p\text{-}h}$, discussed in the next section, is an example. One can choose to eliminate $\Sigma_R^{(2)}$ altogether, but this introduces problems. First, eliminating $\Sigma_R^{(2)}$ would remove unique diagrams that are not contained in Σ_L. Further, this approach produces erroneous results. The important point is that $I_{p\text{-}h}\chi I_{p\text{-}h}$ uses a fully long- and short-range screened interaction in the "crossed" particle-hole channel and is fully long-range screened (because of χ) in the "direct" particle-hole channel. A term with the χ^0 appearing explicitly, for example, $I_{p\text{-}h}\chi^0 I_{p\text{-}h}$ is only short-range screened in the direct particle-hole channel. Subtracting these terms destroys the long-range screening, which we are trying to build into our effective interaction in the first place. Consequently, and this was verified numerically, it is far better to keep the over counting of diagrams than to reintroduce an unscreened quantity.[29] This general behavior is common in many-body theory. The most famous example is that of the logarithmic divergences encountered in dielectric studies in the degenerate electron gas.[1,10] Because of the singular nature of the Coulomb potential, individual terms in the ring series yield energy contributions that diverge at every order. However, when summed to all orders, the ring series produces a physically meaningful contribution to the energy. While in the present work we do not encounter divergences, exposing single unscreened terms leads to spectra with nonphysical properties. Finally, it should be mentioned that a strength of the parquet method over the present work is that it avoids overcounting problems.

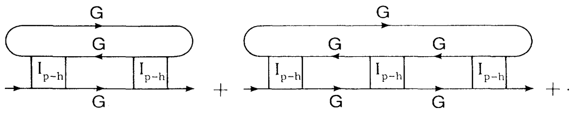

FIG. 1. Diagrammatic representation of Σ_R. $I_{p\text{-}h}$ is the particle-hole irreducible interaction, and G is the single-particle Green's function.

IV. THE PARTICLE-HOLE IRREDUCIBLE INTERACTION

In the preceding section, it was shown that the calculation of $\chi(\mathbf{Q},\omega)$ and Σ_R require $I_{p\text{-}h}$ as input. A knowledge of $I_{p\text{-}h}$ is also important because of the well-known relation that exists between $\chi(\mathbf{Q},\omega)$ and the experimentally measured dynamic structure function $S(\mathbf{Q},\omega)$:

$$S(\mathbf{Q},\omega)=-\frac{1}{n\pi}\mathrm{Im}\chi(\mathbf{Q},\omega) , \tag{19}$$

where n is the particle number density.

In Green's-function perturbation theory $I_{p\text{-}h}$ can be determined from a method proposed by Baym and Kadanoff.[30] Given an approximation to the actual self-energy and the corresponding single-particle Green's function, an approximate $I_{p\text{-}h}$ that conserves particle number, energy, and momentum can be obtained as follows:

$$I_{p\text{-}h}(1,2,3,4)=i\frac{\delta\Sigma(1,3)}{\delta G(4,2)} , \tag{20}$$

where $1=(x_1,t_1,\sigma_1)$. The nonlocal nature of $I_{p\text{-}h}$ is clear from this expression.

The Baym-Kadanoff method has recently been used in conjunction with GFHF analysis[28] to study the dynamical properties of normal and spin-polarized ^{3}He. Applying (20) to Σ_L results in the "T approximation" for $I_{p\text{-}h}$. The analysis necessary to reduce $I_{p\text{-}h}$ to a local approximation is rather lengthy, and we refer the reader to Ref. 28 for the details. We simply state the results. The T approximation, expressed in a momentum space representation, is

$$I_{p\text{-}h}(p_1+Q,p_2,p_1,p_2+Q)=T(p_1+Q,p_2,p_1,p_2+Q)+i\int\frac{d^4p}{(2\pi)^4}T\left[p_1+Q,p-\frac{q}{2},p_2+Q,p+\frac{q}{2}\right]G\left[p+\frac{q}{2}\right]\times G\left[p-\frac{q}{2}\right]T\left[p+\frac{q}{2},p_2,p-\frac{q}{2},p_1\right]\ . \qquad (21)$$

We have introduced the vector $\mathbf{q}=\mathbf{p}_1-\mathbf{p}_2$. In (21) the first and second terms are referred to as the direct and induced terms, respectively. Our local approximation for $I_{p\text{-}h}$ is obtained by closing the four-vertices of $I_{p\text{-}h}$ with single-particle Green's functions and integrating the internal momentum $\mathbf{p}_1$ and $\mathbf{p}_2$:

$$I_{p\text{-}h}(\mathbf{Q},\omega)\equiv\frac{1}{\chi^0(\mathbf{Q},\omega)^2}\int\frac{d^4p_1}{(2\pi)^4}\int\frac{d^4p_2}{(2\pi)^4}G(p_1)G(p_1+Q)I_{p\text{-}h}(p_1+Q,p_2,p_1,p_2+Q)G(p_2+Q)G(p_2)\ . \qquad (22)$$

As discussed in Ref. 28, up to the T approximation, this local approximation to $I_{p\text{-}h}$ makes $\chi(\mathbf{Q},\omega)$ exact to first order in $I_{p\text{-}h}$. Equations (21) and (22) are our approximate $I_{p\text{-}h}$ studied in this work. We consider the static limit ($\omega=0$) only. Our $I_{p\text{-}h}$ is compared to the CBF $I_{p\text{-}h}$ in the next section, where further comments about the T approximation are made.

V. RESULTS

We now present our results for the single-particle spectra $\varepsilon(k)$, ground-state energies, and the particle-hole irreducible interaction $I_{p\text{-}h}(\mathbf{Q})$ in $^3\mathrm{He}^{\uparrow}$. Figure 2 shows our spectra as a function of k at a density $n=0.0172$ Å^{-3} ($V=35.1$ cm^3/mol). The Fermi momentum at this density is $k_F=1.005$ Å. The totally self-consistent spectra ε_1 and ε_2 are solutions of (5). ε_2 has the V_{co} term in the self-energy (9), while ε_1 does not. ε_2 represents the full GFHF approximation, while ε_1 is essentially the BHF $\varepsilon(k)$. In both cases the center-of-mass momentum $\mathbf{P}$ is set equal to zero. ε_3 is obtained by keeping the V_{co} contribution and also using the $\mathbf{P}$ dependence of the t matrix in the evaluation of (9) and (10). Once again, within the GFHF analysis, ε_3 is fully self-consistent. Finally, ε_4 is the solution of (2), i.e., it has a ring contribution in the self-energy. It is no longer fully self-consistent, as will be discussed in Sec. VI.

Contrasting ε_1 and ε_2, we find that including V_{co} increases $\varepsilon(k)$ significantly for 0.4 Å$^{-1}<k<1.8$Å^{-1}. This increase is similar to that observed in liquid deuterium.[13] An increase in the low-momentum values of $\varepsilon(k)$ leads to a reduction in the binding of the system as is apparent from the independent-particle approximation[14,15,31] for the ground-state energy:

$$\frac{E}{N}=\frac{3}{5}\varepsilon_F^0+\frac{3}{2k_F^3}\int_0^{k_F}dk\,k^2\mathrm{Re}\Sigma(k,\varepsilon(k))\ . \qquad (23)$$

The observed increase in $\varepsilon(k)$ is undesirable, since the ground-state energy calculated using ε_1 (without V_{co}) was already in fair agreement with the variational Monte Carlo values of Lhuillier and Levesque.[32] In Fig. 3 the ground-state energies as a function of the molar volume are shown for various cases: E_1 is the ground-state energy when V_{co} is not included. At $V=35.1$ cm^3/mol it is the ground-state energy obtained by evaluating (23) using ε_1 as input. Similarly, E_2 is the ground-state energy when V_{co} is included. In both cases, the $\mathbf{P}=\mathbf{0}$ approximation was always invoked. The variational Monte Carlo (VMC) values of Ref. 32 are also shown. It is immediately obvious that V_{co} decreases the binding in the system, while shifting the zero pressure state to higher volumes. In Table I numerical values for the ground-state energy are given for $V=35.1$ cm^3/mol.

Another effect caused by including V_{co} is a decrease in the effective mass at k_F. Recall that the effective mass is related to the reciprocal of the slope:

$$m^*(k)=k\left[\frac{d\varepsilon(k)}{dk}\right]^{-1}\ . \qquad (24)$$

In Table I values of $m^*(k_F)/m$ are given. For comparison, we have included a CBF on-shell effective mass[18] and one taken from an induced-interaction model calculation.[33] (Both are extrapolations from other densities.)

Next consider ε_3. From Fig. 2 it is obvious that the $\mathbf{P}$ dependence of the t matrix- and self-energy is extremely important when V_{co} is added. Recall from the discussion

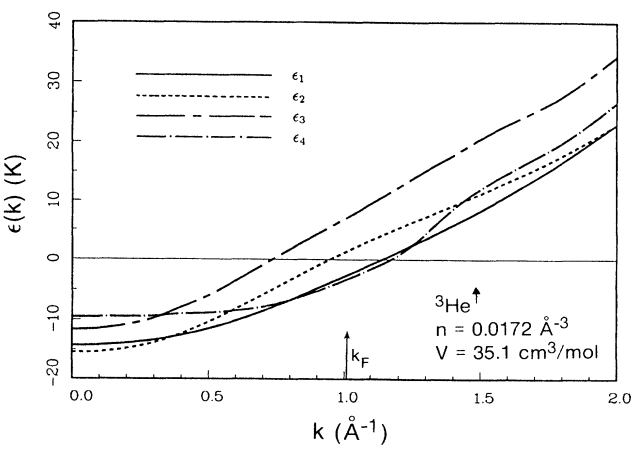

FIG. 2. Single-particle excitation energies: ε_1, ε_2, ε_3, and ε_4 in $^3\mathrm{He}^{\uparrow}$ at 0.0172A^{-3} ($V=35.1$ cm^3/mol). ε_1 and ε_2 are the *GFHF* excitation energies obtained without and with V_{co}, respectively. ε_3 is simlar to ε_2 but is calculated with an improved evaluation of the center-of-mass momenta dependence of the t matrix in the self-energy calculation. ε_4 is the full GFHF plus the ring diagram term.

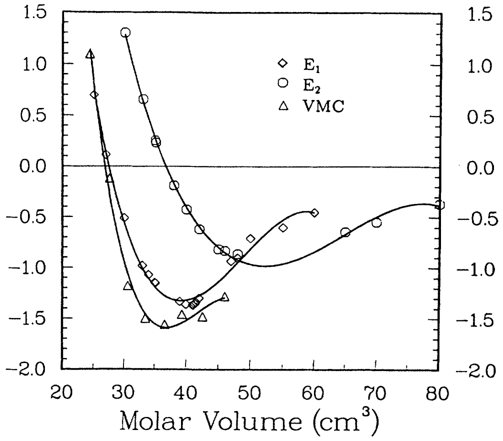

FIG. 3. Ground-state energies in ${}^3\mathrm{He}^{\uparrow}$. E_1 (E_2) is calculated from self-consistent GFHF theory and omits (includes) the V_{co} contribution to the self-energy. In both cases the center-of-mass momentum in the t matrix is set equal to zero. *VMC* is the variational Monte Carlo ground-state energy from Ref. 32.

in Sec. II that earlier work,[14] which kept only the BHF term in (9), found the role of **P** for on-shell calculations to be much less important. The ground-state energy and effective mass ratio differ substantially from the VMC and CBF calculations (cf. Table I). Nevertheless, from the point of view of satisfying certain fundamental properties[15] of the full off-shell self-energy, ε_3 is superior to ε_1 and ε_2.

As we now discuss, the contribution from the full V_{co} (including the **P** dependence) is largely canceled by the ring contributions. To calculate Σ_R, we used the local approximation to $I_{p\text{-}h}$ obtained from CBF calculations (cf. Fig. 4). (This $I_{p\text{-}h}$ was actually calculated at $n=0.0166$ Å^{-3} and not $n=0.0172$ Å^{-3}, but for the present calculation the difference is negligible.) $I_{p\text{-}h}$ is used as input in both (14) and (15). To evaluate the generalized Lindhard function a spectrum is needed as input. The generalized Lindhard function is rather insensitive to the spectrum, since the spectrum appears only through an energy difference $[\varepsilon(\mathbf{p}+\mathbf{Q})-\varepsilon(\mathbf{p})]$. Consequently, ε_1 and ε_2 yield similar values for χ^0. The important point is that the final spectrum, including ring contributions, is given by

$$\varepsilon_4 \equiv \frac{k^2}{2m} + \mathrm{Re}\Sigma_L(\mathbf{k},\varepsilon(\mathbf{k})) + \mathrm{Re}\Sigma_R(\mathbf{k},\varepsilon(\mathbf{k})) \ , \qquad (25)$$

where Σ_L is calculated with V_{co} included ($\varepsilon_4=\varepsilon_3+\mathrm{Re}\Sigma_R$). This spectrum is displayed in Fig. 2. It is immediately obvious that the full V_{co} and Σ_R nearly cancel near k_F. Consequently, including Σ_R and V_{co} produces only a modest reduction in the ground-state energy from ε_1 (cf. Table I).

The effective-mass ratio $m^*(k_F)/m$ calculated from ε_4 is enhanced over that calculated from ε_2, and ε_3 and is in reasonable agreement with ε_1. As can be seen from Table I, this value of $m^*(k_F)/m$ is also in agreement with that calculated in CBF theory[18] and calculations based on the induced interaction model.[33] An enhancement in m^* is obtained from ε_4 near $k=1.6$ Å^{-1}. This is caused by a coupling to the collective excitations (zero-sound mode) observed in our theoretical calculations.[28] A further discussion of this enhancement can be found in Ref. 17.

TABLE I. Ground-state energies and effective-mass ratios in ${}^3\mathrm{He}^{\uparrow}$ at $n=0.0172$ Å^{-3} ($V=35.1$ cm³/mol). Ground-state energies are calculated from Eq. (23) using the spectra ε_1 through ε_4 from Fig. 2 as input. The effective-mass ratios are calculated from Eq. (24) from these spectra. VMC is the ground-state energy obtained from a variational Monte Carlo calculation (Ref. 32). KCJ and BQ are the effective-mass ratios obtained from CBF (Ref 18) and induced-interaction model (Ref. 33) calculations. Both are extrapolations from other densities.

	Ground-state energy (K)	$m^*(k_F)/m$
ε_1	−1.16	0.82
ε_2	0.229	0.75
ε_3	2.73	0.61
ε_4	−0.86	0.87
VMC	−1.5	
KCJ		0.8
BQ		0.82

We now turn to $I_{p\text{-}h}$ given by (21) and (22). In Fig. 4, $I_{p\text{-}h}$ as a function of momentum transfer **Q**, is displayed for the same density as above. The CBF result of Krotscheck, Clark, and Jackson[18] is widely accepted as a good local approximation to $I_{p\text{-}h}$. The curve labeled $I_{p\text{-}h}(L)$ is $I_{p\text{-}h}$ calculated in the T approximation discussed in Sec. IV using the spectrum ε_1. For complete-

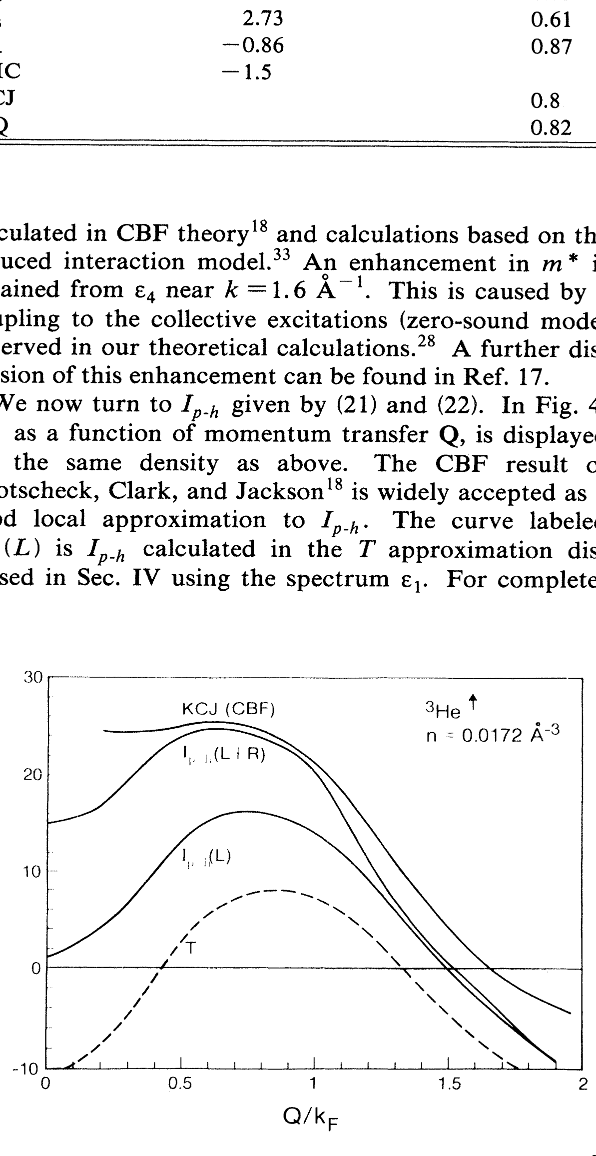

FIG. 4. Particle-hole interaction, $I_{p\text{-}h}$, in ${}^3\mathrm{He}^{\uparrow}$ at 0.0172 Å^{-3}. $I_{p\text{-}h}(L)$ is the direct plus induced term calculated in the T approximation (Ref. 28) using the GFHF ladder (L) self-energy, Σ_L. For this case, T is the direct term only (dashed line). $I_{p\text{-}h}(L+R)$ is calculated in the T approximation using the present ladder plus ring (R) self-energy $\Sigma=\Sigma_L+\Sigma_R$. KCJ is the CBF result of Kotscheck, Clark, and Jackson (Ref. 18). The KCJ density is 0.0166 Å^{-3}.

ness, we have included a plot of the direct term contribution to $I_{p\text{-}h}(L)$ (curve T in Fig. 4). Recall that the direct term is essentially a local approximation for the t matrix and is given by the first term in (21). $I_{p\text{-}h}(L+R)$ is $I_{p\text{-}h}$ in the T approximation calculated using ε_4. When $\varepsilon_4(k)$ is used in the T approximation we find a new $I_{p\text{-}h}$, which lies much closer to the CBF result. The Landau limit corresponds to the small-Q limit.[28,34] It is seen in Fig. 4 that including Σ_R with the full calculation of V_{co} has the largest effect in the Landau limit. This is in complete agreement with the discussion given in Sec. I.

We conclude this section with a discussion of the T approximation. According to the Baym-Kadanoff scheme, the approximate $I_{p\text{-}h}$ calculated depends on the approximation used for the self-energy. When Σ_L is used in (20) the result is the T approximation. If, for example, $\Sigma_L+\Sigma_R$ is used in (20), then a higher-order expression for $I_{p\text{-}h}$ will result. In principle, then, we should calculate a new expression for $I_{p\text{-}h}$. However, based on the work of Ref. 28, we know that, while the T approximation is only semiquantitatively correct,[35] including higher-order diagrams in the "cross channel" will produce only a moderate change in $I_{p\text{-}h}$ for $^3\text{He}^\uparrow$. We are confident that truncating $I_{p\text{-}h}$ at the level of the T approximation is completely sufficient for the present work, where our goal is to determine the effects of ring diagrams on the long-wavelength limit of $I_{p\text{-}h}$.

VI. CONCLUSIONS

In this work we have investigated the role of ladder and ring diagrams in the self-energy for liquid $^3\text{He}^\uparrow$. Ladder diagrams were summed to all orders of the bare ^{3}He-^{3}He interaction by using GFHF analysis. The present calculation includes the part of the GFHF self-energy coming from the correlation potential V_{co}. When V_{co} is added, we found that the center-of-mass momentum dependence of the t matrix has an important effect in the ladder self-energy. Similar to recent findings for liquid deuterium, V_{co} makes a significant contribution to the self-consistent single-particle spectra. We found that a full evaluation of the ladder contribution to the self-energy including V_{co} reduced the binding energy in $^3\text{He}^\uparrow$ by an undesirable amount.

To evaluate Σ_R we have used a local interaction obtained by CBF theory. We found a substantial cancellation of the full V_{co} and Σ_R. Including Σ_R largely corrects the unbinding of the system discussed above and yields an effective-mass ratio in good agreement with other calculations. We then used the resulting $\varepsilon(k)$ to evaluate the T approximation to $I_{p\text{-}h}$. We found that our $I_{p\text{-}h}$ is in much better agreement with the CBF result in the Landau limit, when our $\varepsilon(k)$ includes the effects of both V_{co} and Σ_R.

We conclude that we have shown that it is possible for a first-principles calculation, based on Green's-function perturbation theory, to obtain a qualitatively reasonable value for the ground-state energy and effective mass. We also find a reasonable behavior for the particle-hole irreducible interaction in the limit of small momentum transfer. In spite of this success, we regard this work as a preliminary but necessary step for future calculations. One would like to achieve a completely self-consistent theory. At the present, this calculation is self-consistent only at the level of the GFHF theory. The close agreement of our $I_{p\text{-}h}$ and the CBF $I_{p\text{-}h}$ (Fig. 4) is strongly suggestive that the T approximation to $I_{p\text{-}h}$ can be used as input in the next iteration in the evaluation of (14). This represents a substantial numerical calculation as one would first need to extend our local approximation to $I_{p\text{-}h}$ to large values of momentum. At the present, our T approximation developed in Ref. 28 gives meaningful results for momentum not exceeding $2k_F$. Secondly, one would like to extend these calculations to the entire range molar volumes of interest. In this way the density dependence of the ground-state energy and effective masses could be studied. Again, this represents a substantial numerical task. The present work is meant to stimulate further research in these areas.

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[35] By semiquantitatively correct we mean that the T approximation fails in certain cases such as not satisfying stability conditions for ferromagnetic ordering in normal ^{3}He.