Planar Theory Made Variational

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Within the framework of boson parquet-diagram summations in perturbation theory, we show analytically that several simple approximations lead inevitably to the radial distribution function $g(r)$ which would be obtained with the Jastrow hypernetted-chain variational method. This is the first derivation of the Jastrow result from perturbation theory. Without mentioning pair-correlation functions, we have a clear interpretation of $g(r)$ and the structure function, $S(k)$, in terms of diagram sums.

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Successful microscopic descriptions of quantum fluids have been based usually either on a variational wave function or on a partial summation of Feynman (or Goldstone) diagrams. While each of these approaches has had forceful advocates, one essential point has remained obscure: The physical content of successful variational and diagrammatic calculations is essentially identical. This point has been addressed from time to time with varying degrees of rigor. Here, we shall demonstrate an *exact equivalence* for Bose systems between one popular and successful variational theory, based on the hypernetted-chain (HNC) approximation, and a well-defined approximation to the parquet class of diagrams. We believe this to be the first demonstration of such an equivalence. Thus, these approaches offer practitioners a choice of *language* but not of *substance* as is commonly believed.

The HNC variational calculation starts with a wave function of the Jastrow form, i.e., a product of pair-correlation functions $f(r_{ij})$. Energy calculations require the related radial distribution function, $g(r_{12})$. The static liquid structure function, $S(k)$, is defined as $1+\rho F[g-1]$ where F denotes a Fourier transform. Exact determination of g from f is complicated. The hypernetted-chain assumption provides a simple and useful approximate relation between these quantities.[1,2] Introduction of the HNC approximation in the related variational energy functional and the requirement of stationarity give[3-5] the Euler-Lagrange equation for g:

$$(-\nabla^2+V+W[g])\sqrt{g}=0, \tag{1}$$

where the Fourier transform of $W[g]$ is given by

$$F[W]=-\omega_k[2S(k)+1][S(k)-1]^2/2\rho S^2(k), \tag{2}$$

with $\omega_k=k^2/2$. For a wide range of potentials and densities, solutions to Eqs. (1) and (2) provide a local minimum in the approximate energy functional and a reasonable description of both the energy and liquid structure function.[6] We proceed to a diagrammatic derivation of these equations.

We treat bosons as fermions with high degeneracy, ν. For fixed density, $\rho=\nu k_F^3/6\pi^2$, we let $k_F\to 0$. In this limit, exchange diagrams vanish and each closed loop contains exactly one particle line in the zero-momentum condensate. (General rules for perturbation theory are given by Fetter and Walecka.[7]) In the parquet theory the fundamental quantity is the two-body vertex, $\Gamma=V+L+C$, where V is a set of irreducible diagrams (approximated here by the bare potential), L is the set of particle-particle reducible (ladder) diagrams, and C is the set of particle-hole reducible (chain or ring) diagrams. When V contains strong short-range repulsion, ladder diagrams must be summed to describe g at small r. The description of phonon effects and the behavior of S for small k require summation of the chain diagrams. The simultaneous retention of both limits requires the self-consistent summation of ladder and chain diagrams. This defines the set of parquet diagrams which are summed by the nonlinear integral equations depicted in Fig. 1.[8,9] Γ is a function of three independent

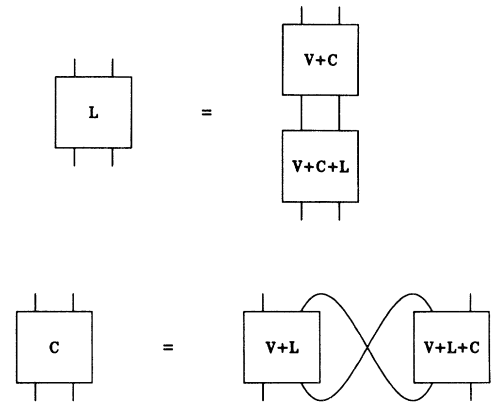

FIG. 1. The form of the parquet equations for the determination of Γ.

four-momenta. Although rotational invariance reduces the number of independent variables to nine, vigorous approximations are required to obtain a tractable scheme. For local interactions, V is a function of the magnitude of a three-momentum transfer only. This, and the structure of Eqs. (1) and (2), suggest local approximation of L and C. Suitable local forms can be obtained by requiring that the resulting approximate parquet equations reproduce pure ladder- and pure ring-diagram contributions to $S(k)$. This determination is almost unique. Various routes from Γ to the static structure function, equivalent for an exact parquet description of Γ, are rendered distinct by such

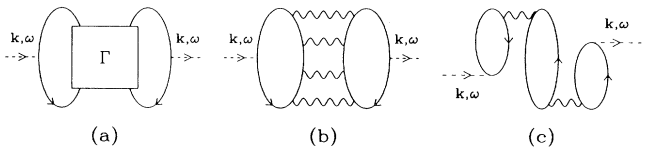

FIG. 2. Contributions to $S(k,\omega)$ from (a) the general vertex, (b) ladders, and (c) rings.

local approximations. Previously, we considered a route which went from Γ to the proper self-energy (by closing two external particle lines) to the energy of the system (by closing the remaining lines) to S (by a functional differentiation with respect to the bare interaction). This allowed us to see that Eqs. (1) and (2) contain approximations to precisely the parquet class of diagrams but did not indicate a more detailed equivalence. Here, we shall proceed directly from Γ to $S(k)$. In this case $S(k)-1$ is obtained by the closing off of each Γ diagram to get $S(k,\omega)$, as illustrated by Fig. 2(a), and integration over ω. The contribution to $S(k)$ from $V(k)$ is $-\rho V(k)/\omega_k$.

We wish to sum ladder contributions to $S(k)$, such as Fig. 2(b), with the assumptions that V is local and that a local approximation to C is known. Only diagrams with condensate lines located symmetrically contribute to $S(k)$. They may be inside the vertex or outside. By first summing ladders, $\tilde{L}$, in which no condensate line occurs, we obtain the sums $\tilde{L}$ and X needed for an exact evaluation of ladder contributions to S:

$$\tilde{L}(k)=\int d^3q\,(2\pi)^{-3}[V+C]_{|k+q|}[V+C+\tilde{L}]_q/(-2\omega_q), \tag{3}$$

$$X(k)=-\int d^3q\,(2\pi)^{-3}[V+C+\tilde{L}]_{|k+q|}[V+C+\tilde{L}]_q/4\omega_q\omega_{|k+q|}. \tag{4}$$

Given the locality of V and C, the local form of Eq. (3) is not an approximation. Rather, the exact calculation of S in this case involves only ladder sums in which one end of each $\tilde{L}$ has both legs at zero momentum. The contribution to S from ladders with two or more rungs is

$$S_L(k)=(-\rho/\omega_k)[\tilde{L}(k)+X(k)]. \tag{5}$$

Our local approximation to the parquet equations will be to use Eqs. (3) and (4) for *all* ladder sums including those required for the construction of the driving term for the chain equations.

For a local link, $V(k)+\tilde{L}(k)+X(k)$, ring diagrams generate contributions to C with explicit k and ω dependence:

$$C(k,\omega)=\frac{[V(k)+\tilde{L}(k)+X(k)](\epsilon_k^2-\omega_k^2)}{(\omega-\epsilon_k+i\eta)(\omega-\epsilon_k-i\eta)}, \tag{6}$$

$$\epsilon_k^2=\omega_k^2+2\rho\omega_k[V(k)+\tilde{L}(k)+X(k)]. \tag{7}$$

The full random-phase approximation structure function, containing terms such as Fig. 2(c), is simply $S=\omega_k/\epsilon_k$. We seek a local approximation, $C(k)$. As in Ref. 8, we define $C(k)=C(k,\bar{\omega}_k)$ where $\bar{\omega}_k$ is chosen to give the exact random-phase- approximation structure function:

$$S(k)=1-(\rho/\omega_k)[V(k)+\tilde{L}(k)+X(k)+C(k)]$$
$$=\omega_k/\epsilon_k. \tag{8}$$

Here, chains with a single link, given by Eq. (5), are also included. This gives $\bar{\omega}_k^2=-\omega_k^2\epsilon_k/(2\omega_k+\epsilon_k)$ and the desired local approximation to C which can be expressed in terms of S as

$$C(k)=\frac{-\omega_k[2S(k)+1][S(k)-1]^2}{2\rho S^2(k)}. \tag{9}$$

This result of the local approximation to the parquet diagrams is identical in form to the induced interaction, Eq. (2), arising in HNC theory.

This establishes our local approximation to the par-

quet sums. Equations (6) and (7) with $\omega=\bar{\omega}_k$ are to be used to set $C(k)$. Equations (3) and (4) are to be used for $\tilde{L}(k)$ and $X(k)$. These equations must be solved self-consistently for $\tilde{L}$, X, and C. Such self-consistency, readily obtained numerically, guarantees the preservation of both the small-k behavior of S and the small-r behavior of g. For example, the complete contribution to the structure function is given by Eq. (8) which yields $S=\omega_k/\epsilon_k$ by construction.

Defining $\Gamma(k)=V(k)+\tilde{L}(k)+C(k)$ and $\bar{\Gamma}(k)=-\Gamma(k)/2\omega_k$, we observe that X can be expressed as the convolution $X(k)=-\rho\bar{\Gamma}*\bar{\Gamma}$. Similarly, $S-1=2\bar{\Gamma}+\bar{\Gamma}*\bar{\Gamma}$. Fourier transformation of this to coordinate space gives an algebraic equation which is solved to give

$$F[\bar{\Gamma}]=\sqrt{g}-1. \tag{10}$$

Expressing the ladder summation of Eq. (3) in terms of Γ and $\bar{\Gamma}$, we find

$$-k^2\bar{\Gamma}=[V+C]+[V+C]*\bar{\Gamma}. \tag{11}$$

Fourier transformation of Eq. (11) yields Eq. (1) exactly. This indicates that the approximate parquet equations lead to the desired correlations in g at short distances where repulsion in V dominates W. Of greater importance, the fact that Eqs. (9) and (11) are identical to Eqs. (1) and (2) proves our assertion that HNC variational calculations have a physical content identical to that of a local approximation to the parquet diagrams. Evaluation of the energy of the system is straightforward in HNC calculations. In the parquet approach, it is necessary to invoke the Feynman-Hellman theorem and perform a suitable coupling-constant integration. With the present approximations, HNC and parquet energies are also identical.[10]

Clearly, the parquet theory contains HNC but is not identical. HNC emerges only with the well-defined approximations above. This set of approximations necessarily leads to a degradation of the exact sums of the parquet equations. For example, inclusion of the X term in the driving term of the chain equation causes counting errors. Adjacent X links lead to more than one condensate line in closed loops and should be excluded. Tractable approximation schemes which count diagrams better have been constructed and represent an obvious improvement over optimized HNC.[11]

The constructive nature of the present results, which places HNC in the framework of a more general theory, reveals the similarity of content of variational and diagrammatic theories in spite of superficial differences. It supports the choice of kinetic energy functional implicit in Eq. (2). By relating g to Γ explicitly, Eq. (10) offers opportunities for making reliable diagrammatic analyses of other constructs which arise in variational theory. Immediately, one can see that the HNC has none of the self-energy corrections which a more fully consistent parquet approximation would have. The inclusion of spin-dependent forces is simple and unambiguous in parquet theory.[12] This is not the case in HNC. Finally, the full parquet theory offers guidance for the systematic improvement of the approximations made here; a discussion of such corrections has been published elsewhere.[11]

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[1]J. M. J. van Leeuwen, J. Groeneveld, and J. de Boer, Physica (Utrecht) **25**, 792 (1959).

[2]T. Morita, Prog. Theor. Phys. **20**, 920 (1958).

[3]C. E. Campbell and E. Feenberg, Phys. Rev. **188**, 396 (1969).

[4]L. J. Lantto and P. J. Siemens, Phys. Lett. **68B**, 315 (1977).

[5]A. Kallio and R. A. Smith, Phys. Lett. **68B**, 315 (1977).

[6]L. C. Castillejo, A. D. Jackson, B. K. Jennings, and R. A. Smith, Phys. Rev. B **20**, 3631 (1979).

[7]A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).

[8]A. D. Jackson, A. Lande, and R. A. Smith, Phys. Rep. **86**, 55 (1982).

[9]A. Lande and R. A. Smith, Phys. Lett. **131B**, 253 (1983).

[10]A. D. Jackson, E. Krotscheck, A. Lande, and R. A. Smith, to be published.

[11]A. D. Jackson, A. Lande, and R. A. Smith, Phys. Rev. B **31**, 403 (1985).

[12]R. A. Smith and A. D. Jackson, to be published.