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Effective interactions, linear response, and correlated rings: A study of chain diagrams in correlated basis functions

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We study the connections between the chain summations of variational theories of Fermi fluids and those generated by ring-diagram summations in the correlated-basis-functions (CBF) perturbation theory. The effective interactions of CBF theory and the random-phase-approximation (RPA) equations in the correlated basis are rewritten in an irreducible form. We discuss local approximations to the irreducible vertex which are sympathetic with the use of variational wave functions. They allow contact to be made with conventional formulations of the RPA, to weak-coupling, pseudopotential, or "local-screening" theories. Our studies lead also to consistency requirements between variational calculations of ground-state properties and the effective interactions used in CBF theory.

I. INTRODUCTION

The random-phase approximation (RPA) has in the past been applied successfully to the study of elementary excitations in various many-body systems such as finite nuclei, nuclear matter, or terrestrial quantum fluids like the electron gas. The important class of perturbation-theory diagrams generated by the RPA equations is also used to compute corrections to the ground-state energy of many-body systems, and to study the coupling of excited states to the particle-hole excitations and the collective modes of the medium.

In the case where the microscopic interaction between two particles is strong, the conventional formulation of the RPA relies on phenomenological or semimicroscopic models for the particle-hole interaction (for example, Skyrme-type forces or local approximations for the *G* matrix) which have only indirect connections with the bare force between two particles. Clark and collaborators have recently demonstrated[1-3] how this problem may be circumvented by the use of correlated wave functions, which, roughly speaking, build in the core exclusion. The study of low-lying excitations in a basis of correlated wave functions led, in an analysis patterned after conventional derivations of the RPA equations, to the so-called "correlated RPA theory" (CRPA).

In this paper we will examine the meaning and potential applications of the CRPA theory from various points of view. In contrast to earlier work, which was formulated sufficiently generally to be applicable to finite nuclei and quantum liquids, we emphasize here the case of an infinitely extended system. This will allow us to take advantage of the far more developed formalisms and computational possibilities.

To give some motivation for the present studies, it is worth illuminating the conceptual differences between the CRPA and the conventional RPA. Conventional RPA is usually formulated in terms of a particle-hole-irreducible interaction, which has a direct resemblance to the quasiparticle interaction. This is no longer true in the CRPA: Here, the effective interactions[4] entering the formalism also contain diagrams that may be classified as particle-hole reducible. (These diagrams are usually referred to as "chain diagrams" in variational theories of quantum liquids.[5]) The task of the correlated RPA consists, in essence, in the inclusion of propagator corrections and state dependence which were not built into the variational wave function. As a consequence, the effective interaction entering the CRPA equations becomes energy dependent. There is still some formal connection with the quasiparticle interaction. This connection, however, relies on a cancellation of chain diagrams in the limit of zero momentum transfer. The identification of the quantities entering the CRPA equations with the finite-momentum extension of the quasiparticle interaction is no longer permitted.

It is one of the purposes of this paper to examine the connection between the correlated RPA and conventional formulations of the RPA. To this end, in Sec. II we briefly discuss the correlated-basis-functions (CBF) theory and the structure of the effective interactions. Section III discusses the

CRPA equations and the representation of the two-body Green's function in the correlated basis. We will reformulate the CRPA equations in terms of a suitably defined particle-hole-irreducible interaction. It turns out that this in fact simplifies the equations and largely eliminates the energy dependence of the interaction. In other words, the CRPA will emerge in a form and interpretation identical to conventional RPA. The essential (and most important) difference is that unique prescriptions are provided for the computation of the particle-hole interaction from the underlying microscopic two-body potential.

In Sec. IV we study the perturbation expansion for the ground-state energy in the correlated basis. The expansion is represented in terms of Goldstone-type diagrams containing effective one-, two-, three- , . . . , n-body operators. Topological comparison with Goldstone diagrams allows the identification of the class of "ring diagrams" in CBF theory. We draw the connections between these ring diagrams and those generated by iteration of the (C)RPA equations. It is worth noting here that there is no *a priori* reason that there should be a complete agreement: Studies of the CBF perturbation theory within the framework of the correlated-coupled-cluster theory[6] have shown that diagrams of similar topology emerge from both high-order diagrams containing the effective two-body interaction and reducible low-order diagrams arising from effective four-, six- , . . . , $2n$-body interactions. Since the CRPA is based on the effective two-body interaction alone, one need not expect that such effects are included properly. Nevertheless, we will verify up to fourth order that the CRPA equations sum the CBF ring diagrams correctly. Beyond this order, there are no new mechanisms for generating topologically equivalent diagrams.

In Sec. V we return to the variational calculations of the irreducible vertex function and give explicit working formulas for the particle-hole interaction, which are based on variational wave functions and can be used in conjunction with the conventional RPA. Despite the somewhat formal appearance of the studies of Secs. II – V, the results are quite practical in nature. The determination of the most general irreducible vertex requires no more effort than the computation of the full effective interaction; it essentially requires a different combination of precalculated quantities.

Of course, one can continue to analyze the CBF perturbation series and the effective interaction at the same time. In principle, it must be possible to eliminate the correlation operator systematically and to arrive ultimately at an ordinary Goldstone perturbation expansion. Such a procedure is, of course, not only impractical, but also against the spirit of CBF theory: The power of CBF lies in the fact that it makes it possible to sum large arrays of diagrams in an approximate way, which would be out of reach in any conventional (e.g., Brueckner-Bethe-Goldstone or Bethe-Faddeev-type) theory. One does not want to undo this. On the other hand, if a certain subclass of CBF diagrams is summed by a systematic procedure, it is necessary to consider the relationship between this subclass of diagrams and ones which were already (approximately) included in a preceding variational calculation. One result of this study is a requirement for consistency between the approximations used for the variational calculation of the physical observable under consideration (e.g., the ground-state energy or the optical potential) and those used for the effective interaction entering the CBF expansion.

To be definite, the RPA sums certain classes of ring diagrams, whose obvious counterparts are the chain diagrams of variational theories.[7,8] On the other hand, it should be clear that RPA does not sum the equivalents of those chain diagrams in which a "ladder diagram" acts as the driving term. We will exploit the correspondence between the chain diagrams of variational theories and those generated by the iteration of the (C)RPA equations at a practical level which clearly shows the connections to polarization potentials and conventional RPA, and allows study of the most interesting physical effects.

In order to make contact to phenomenological theories, we study in Sec. VI simple models for the vertex function. The reader with only casual interest who skims through the technical Secs. II – V will find here the simplest applications and the interpretation of our results. An averaging procedure which is sympathetic with the use of variational wave functions defines a local approximation of the effective interaction. The averaging is related to the "fluid-dynamic approximation,[8,9]" or the "quasiboson approximation.[10]" Our local approximation for the vertex function is readily identified with the pseudopotential model of Aldrich and Pines[11] or with a screened interaction in the Hubbard model.[12] The most important feature of these studies is that to the extent that a local approximation is adequate, the pseudopotential $U(q)$ may be obtained algebraically from the RPA relation

$$1/S^2(q)=1/S_F^2(q)+4mU(q)/(\hbar^2q^2) \qquad (1.1)$$

in the fluid-dynamic approximation. $S_F(q)$ is the static structure function of the noninteracting Fermi system. Note that Eq. (1.1) is to be understood in a way opposite to what one usually does in RPA: Normally, RPA is used to determine the static structure function $S(q)$ from a given, local weak interaction $U(q)$. Here, Eq. (1.1) serves to determine $U(q)$ from a structure function $S(q)$ that was calculated previously for a strongly interacting system. The only additional prerequisite for Eq. (1.1) is that the local correlations were determined by minimization of the energy expectation value; the relation is somewhat more complicated for nonoptimal correlation functions. The local $U(q)$ may, in turn, be used to determine the response function, the dynamic structure factor, the self-energy, etc., essentially via equations commonly available in textbooks.

Section VII concludes by summarizing the consequences of our studies in a broader framework. We discuss some of the stringent consistency requirements for variational-CBF calculations for the elementary excitations in quantum liquids.

II. CBF THEORY AND THE EFFECTIVE INTERACTION

The literature now contains many descriptions of the correlated-basis-functions[13] theory; we can restrict ourselves therefore to a very brief review of the theory and to a definition of the nomenclature used below. CBF theory uses a correlation operator F to generate a correlated basis $\{ | \psi_m \rangle \}$ of the Hilbert space from a basis $\{ | \phi_m \rangle \}$ of noninteracting particle states by

$$| \psi_m \rangle = F | \phi_m \rangle / I_{mm}^{1/2}, \quad I_{mm} = \langle \phi_m | F^\dagger F | \phi_m \rangle \ . \tag{2.1}$$

The uncorrelated states $| \phi_m \rangle$ are, in the case of infinite matter under consideration here, Slater determinants of plane waves characterized by a set of quantum numbers $m = (m_1, \ldots, m_A)$. The filled Fermi sea carries the subscript 0. The choice of the basis (2.1) generally sacrifices the orthogonality of the basis states, on the other hand, all relevant matrix elements are, given a sensible choice of the correlation operator F, *a priori* finite. Actually, for many of the considerations to follow, no particular choice of the correlation operator needs be made. However, the *Jastrow choice*

$$F = \prod_{i<j} f(r_{ij}) \tag{2.2}$$

for F is the only one for which we currently have sufficient mastery of the formal structure of the ingredients of CBF theory and reliable algorithms[4] for the accurate computation of the relevant matrix elements. We expect, however, that the essential conclusions of our work will remain valid for state-dependent correlations, and in finite systems.

The first quantity to be computed using the correlated basis states $| \psi_m \rangle$ is, of course, the energy expectation value,

$$H_{00} = \langle \psi_0 | H | \psi_0 \rangle \ . \tag{2.3}$$

Further quantities of interest are the particle-hole excitation energies and off-diagonal matrix elements of the Hamiltonian and the unit operator. The single-particle energies are computed from the energy difference of a $1p$-$1h$ "excited" state

$$\begin{aligned} | \psi_{ph} \rangle &= F a_p^\dagger a_h | \phi_0 \rangle / I_{ph}^{1/2} \ , \\ I_{ph} &= \langle \phi_0 | a_h^\dagger a_p F^\dagger F a_p^\dagger a_h | \phi_0 \rangle \ , \end{aligned} \tag{2.4}$$

and the correlated ground state

$$e(p) - e(h) = \langle \psi_{ph} | H - H_{00} | \psi_{ph} \rangle \ . \tag{2.5}$$

The variational single-particle energies are a generalization of the Hartree-Fock single-particle spectrum to correlated wave functions. They are of the form

$$e(k) = \hbar^2 k^2 / 2m + u_v(k) \ , \tag{2.6}$$

where $u_v(k)$ is the average field seen by a single particle.

Off-diagonal matrix elements between two correlated states $| \psi_m \rangle$ and $| \psi_n \rangle$ are usually classified by the number d of orbitals in which $| \psi_m \rangle$ and $| \psi_n \rangle$ differ. They are most conveniently expressed in terms of antisymmetrized plane-wave matrix elements of d-body operators, e.g.,

$$\langle \psi_{ph} | \psi_{p'h'} \rangle = \langle ph' | \mathscr{N}(12) | hp' \rangle_a \ , \tag{2.7}$$

$$\begin{aligned} \langle \psi_{ph} | H - H_{00} | \psi_{p'h'} \rangle &= \langle ph' | \mathscr{V}(12) | hp' \rangle_a \\ &= \langle ph' | \mathscr{W}(12) | hp' \rangle_a + \tfrac{1}{2}[e(p) + e(p') - e(h) - e(h')] \, \langle ph' | \mathscr{N}(12) | hp' \rangle_a \ . \end{aligned} \tag{2.8}$$

The last two lines in Eq. (2.8) are structural decompositions of the effective two-body interaction $\mathcal{V}(12)$: The two-body operators $\mathcal{W}(12)$ and $\mathcal{N}(12)$ are Hermitean, whereas $\mathcal{V}(12)$ is not.[4] In a more general environment, the single-particle energies in Eq. (2.8) have to be taken with a positive sign for particle states and with a negative one for hole states.[6] The subscript a indicates antisymmetrization.

For future reference, we also define the ratio of normalization integrals

$$z_m=(I_{mm}/I_{00})^{1/2},\quad z_{ph}=(I_{ph}/I_{00})^{1/2}\ . \tag{2.9}$$

The analytic form and the most important properties of the operators $\mathcal{V}(12)$, $\mathcal{W}(12)$, and $\mathcal{N}(12)$ has been discussed in various places, see, e.g., Ref. 4. For the formal study of the CBF ring diagrams and the CRPA equations performed in the next two sections, we need only assume that these quantities can be calculated reliably. In order to make contact with the quasiparticle interaction, however, it is necessary to analyze the CBF interaction in more detail.

To this end, we first study the diagrammatical structure of the two-body operator $\mathcal{N}(12)$. Once this is determined, $\mathcal{W}(12)$ may be generated by "diagrammatical differentiation," as described in Ref. 4. To be definite, we assume the Jastrow ansatz (2.2) for the correlation operator. For a convenient representation, we utilize the diagrammatical language introduced for Jastrow correlations.[5] With the use of this diagrammatic scheme, $\mathcal{N}(12)$ is expanded in

$$\mathcal{N}(12)=\sum_i(\Delta\mathcal{N})_{(i)}(12)\ , \tag{2.10}$$

where the subscript (i) refers, e.g., to the number of correlation factors present in a cluster contribution $(\Delta\mathcal{N})_{(i)}(12)$. Each term may be represented diagrammatically by (dashed) "correlation lines" describing a function $h(r)=f^2(r)-1$, and (solid, oriented) "exchange lines", describing an exchange function

$$l(rk_F)=A^{-1}\sum_k n(k)\exp(i\vec{k}\cdot\vec{r})\ , \tag{2.11}$$

where $n(k)$ is the Fermi distribution.

In configuration space, the two-body operator $\mathcal{N}(12)$ has the form of a four-point function:

$$\begin{aligned}\mathcal{N}(12)&=\mathcal{N}(\vec{r}_1,\vec{r}_2;\vec{r}\,'_1,\vec{r}\,'_2)\\&=\mathcal{N}_{dd}(\vec{r}_1,\vec{r}_2;\vec{r}\,'_1,\vec{r}\,'_2)+\mathcal{N}_{dcc}(\vec{r}_1,\vec{r}_2;\vec{r}\,'_1,\vec{r}\,'_2)\\&\quad+\mathcal{N}_{ccd}(\vec{r}_1,\vec{r}_2;\vec{r}\,'_1,\vec{r}\,'_2)\\&\quad+\mathcal{N}_{cc,cc}(\vec{r}_1,\vec{r}_2;\vec{r}\,'_1,\vec{r}\,'_2)\end{aligned}$$

with (2.12)

$$\mathcal{N}_{dd}(\vec{r}_1,\vec{r}_2;\vec{r}\,'_1,\vec{r}\,'_2)=\mathcal{N}_{dd}(r_{12})\delta(\vec{r}_1-\vec{r}\,'_1)\delta(\vec{r}_2-\vec{r}\,'_2)\ ,$$

$$\mathcal{N}_{dcc}(\vec{r}_1,\vec{r}_2;\vec{r}\,'_1,\vec{r}\,'_2)=\mathcal{N}_{dcc}(\vec{r}_1;\vec{r}_2,\vec{r}\,'_2)\delta(\vec{r}_1-\vec{r}\,'_1)\ .$$

The configuration-space functions appearing in (2.12) are all symmetrical under the exchange $\vec{r}_i\leftrightarrow\vec{r}\,'_i$. Typical diagrams depicting cluster contributions to the distinct portions of $\mathcal{N}(12)$ are shown in Fig. 1. The absence of a unique particle-hole structure in the cluster expansion of the operators $\mathcal{N}(12)$ [and $\mathcal{W}(12)$] leaves possible ambiguities as to just which contributions to $\mathcal{N}(12)$ should be classified as particle-hole reducible. One procedure is to isolate all those contributions that vanish in the Landau limit

$$\lim_{q\to0}\langle\vec{k},\vec{k}'+\vec{q}\,|\mathcal{N}(12)|\,\vec{k}+\vec{q},\vec{k}'\rangle_a\ . \tag{2.13}$$

Following this scheme, some direct matrix elements of the diagrams shown in Fig. 1 may in an obvious manner be classified as particle-hole reducible. These include not only the chain diagrams of the first line of Fig. 1, but also the separable diagrams shown in the second and third lines. These terms may be explicitly represented in a Goldstone-type manner involving sums over particle-hole loops. For example, the second *plus* the third diagram can be written as

$$\sum_{p,h}\langle ip\,|\,h(r)\,|\,jh\rangle\langle kh\,|\,h(r)\,|\,lp\rangle=\langle ik\,|\,(\Delta\mathcal{N}_{dd})_2(r)\,|\,jl\rangle\ , \tag{2.14}$$

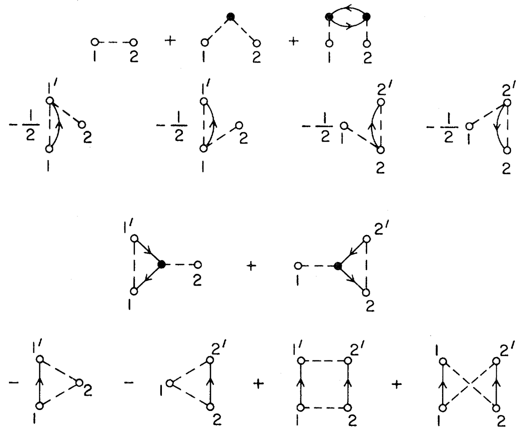

FIG. 1. Configuration-space representation of the leading terms of $\mathcal{N}(12)$. The dashed line represents a correlation factor $f^2(r)-1$, the oriented, solid line an exchange line $l(rk_F)$. Open circles represent the "external points" $\vec{r}_i,\vec{r}\,'_i$, closed circles indicate coordinate-space integration.

where p and h refer to internal particle and hole labels.

The identification becomes less clear in the case of the diagrams shown in the last line of Fig. 1. The first one may be generated either as a piece of a particle-particle ladder,

$$\sum_{p,p'} \langle ik \mid h(r) \mid pp' \rangle \langle pp' \mid h(r) \mid jl \rangle \ , \tag{2.15}$$

or of a particle-hole ladder,

$$\sum_{p,h} \langle ih \mid h(r) \mid pj \rangle \langle pk \mid h(r) \mid lh \rangle \ . \tag{2.16}$$

Note that (2.15) generates an additional diagram not shown in Fig. 1. This contains factor $h^2(r)$, which does not occur in $\mathcal{N}(12)$ and corresponds, in higher orders, to parallel-connected diagrams.

In order to introduce a formal definition of particle-hole-irreducible diagrams we define a correlation matrix of the form

$$C = \begin{bmatrix} \langle ph' \mid \mathcal{N}(12) \mid hp' \rangle_a & \langle pp' \mid \mathcal{N}(12) \mid hh' \rangle_a \\ \langle hh' \mid \mathcal{N}(12) \mid pp' \rangle_a & \langle hp' \mid \mathcal{N}(12) \mid ph' \rangle_a \end{bmatrix} = \begin{bmatrix} C_{ph,p'h'} & C_{ph,h'p'} \\ C_{hp,p'h'} & C_{hp,h'p'} \end{bmatrix} , \tag{2.17}$$

and a matrix of particle-hole irreducible diagrams

$$X = \begin{bmatrix} X_{ph,p'h'} & X_{ph,h'p'} \\ X_{hp,p'h'} & X_{hp,h'p'} \end{bmatrix} , \tag{2.18}$$

which is defined by the relation

$$C = X + \tfrac{1}{2} C X \ . \tag{2.19}$$

We will later give further motivation for the definition (2.19). At present, it is sufficient to state that the iteration of Eq. (2.19) generates from the bare correlation $h(r)$ all chain diagrams. By including the exchange terms, we also recover the factorizable diagrams shown in the second and third lines of Fig. 1, and the exchange terms arising from the last line with a factor of $\frac{1}{2}$. Since the definition of the correlation matrix C does not rely on notions of reducibility we consider Eq. (2.19) as a definition of the matrix X. We stress that rather than computing $X = (1 + \frac{1}{2}C)^{-1} C$, we use Eq. (2.19) to identify and *eliminate* diagrams contributing to C but not to X. At the two-line level, the construction of X from C via Eq. (2.19) eliminates all direct matrix elements of the two-line diagrams displayed in lines 1 to 3 of Fig. 1, and half of the exchange matrix elements of the diagrams shown in the last line.

Once the steps for identifying the particle-hole-irreducible diagrams are determined, it is straightforward to extend them to analyze the effective interaction $\mathcal{W}(12)$. A cluster expansion of $\mathcal{W}(12)$ is generated from the corresponding expansion for $\mathcal{N}(12)$ by replacing, in turn, each correlation factor $h(r)$ by a screened interaction $f^2(r) v_{\mathrm{JF}}(r)$, where

$$v_{\mathrm{JF}}(r) = v(r) - (\hbar^2/2m) \nabla^2 \ln f(r) \tag{2.20}$$

is the Jackson-Feenberg potential, and $v(r)$ is the bare two-body interaction. (Similar equations have been derived for alternative forms of the kinetic energy.[4]) In addition, $v_{\mathrm{JF}}(r)$ must be supplemented by kinetic-energy terms involving derivatives of the exchange function $l(rk_F)$. Explicit formulas for the construction of $\mathcal{W}(12)$ may be found in various places[4,14]; we will return to this question in Sec. V. At present, we generalize the algorithm (2.19) to handle the two-body operator $\mathcal{W}(12)$. Again, writing the matrix elements of $\mathcal{W}(12)$ in the two particle-hole channels in the supermatrix form

$$W = \begin{bmatrix} \langle ph' \mid \mathcal{W}(12) \mid hp' \rangle_a & \langle pp' \mid \mathcal{W}(12) \mid hh' \rangle_a \\ \langle hh' \mid \mathcal{W}(12) \mid pp' \rangle_a & \langle hp' \mid \mathcal{W}(12) \mid ph' \rangle_a \end{bmatrix} = \begin{bmatrix} W_{ph,p'h'} & W_{ph,h'p'} \\ W_{hp,p'h'} & W_{hp,h'p'} \end{bmatrix} , \tag{2.21}$$

we define the particle-hole-irreducible piece X' through

$$W = (1 + \tfrac{1}{2} C) X' (1 + \tfrac{1}{2} C) \ , \tag{2.22}$$

where X', like W, is a supermatrix of the form

$$X' = \begin{bmatrix} X'_{ph,p'h'} & X'_{ph,h'p'} \\ X'_{hp,p'h'} & X'_{hp,h'p'} \end{bmatrix} \ . \tag{2.23}$$

Again, it is worth stressing that Eq. (2.22) is not to be solved by constructing the inverse of $(1 + \frac{1}{2}C)$. Rather, X' is generated from W by *omitting* certain diagrams.

At this juncture, we can also draw the connection to the Landau definition of the quasiparticle interaction. This is generated by functional variation of the energy expectation value with respect to the quasiparticle occupation number,

$$f(\vec{k}, \vec{k}') = \delta^2 H_{00} / \delta n(k) \delta n(k') \ . \tag{2.24}$$

Since the occupation number $n(k)$ enters the energy expectation value only through the exchange line $l(rk_F)$ [Eq. (2.11)], the variation (2.24) may be performed explicitly by variation with respect to the exchange function $l(rk_F)$ as

$$f(\vec{k}, \vec{k}') = A^{-2} \int [\delta^2 H_{00} / \delta l(r_{ij} k_F) \delta l(r_{kl} k_F)] \exp[i(\vec{k} \cdot \vec{r}_{ij} + \vec{k}' \cdot \vec{r}_{kl})] d^3 r_i d^3 r_j d^3 r_k d^3 r_l \ . \tag{2.25}$$

Here, and throughout the paper, we suppress spin labels for ease of writing. Fermi sea orbitals will be referred to as by their associated momenta. In Eq. (2.5) we allow for $i=j$, in which case the variation with respect to the exchange function reduces to a density derivative.

It has been pointed out in various places (see, e.g., Ref. 15) that the procedure (2.25), if carried out order by order in a diagrammatical expansion of the energy expectation value H_{00}, produces all matrix elements of $\mathscr{W}(12)$ which survive in the Landau limit (2.13). The construction (2.22) eliminates all those diagrams that vanish in the Landau limit. Consequently, we have also

$$\lim_{q\to 0} X'_{\vec{\mathrm{k}}'+\vec{\mathrm{q}},\vec{\mathrm{k}};\vec{\mathrm{k}}',\vec{\mathrm{k}}+\vec{\mathrm{q}}} = f(\vec{\mathrm{k}},\vec{\mathrm{k}}') \ . \tag{2.26}$$

To conclude this section, we emphasize that the Landau limit alone is insufficient to characterize the portions of the effective interaction that should be kept in a finite-momentum extension of the quasiparticle interaction. We will identify below a further class of contributions, arising from the kinetic-energy operator, that vanish for zero momentum transfer.

III. CORRELATED RPA, LINEAR RESPONSE, AND THE SELF-ENERGY

The formal analog of the RPA equation was derived recently[1-3] by embedding the small-amplitude limit of the time-dependent Hartree-Fock theory in the CBF context. The most satisfactory derivation is based on a least-action principle, which is applied to a class of time-dependent correlated states

$$|\psi(t)\rangle = F|\phi(t)\rangle / \langle\phi(t)|F^\dagger F|\phi(t)\rangle^{1/2} \ . \tag{3.1}$$

The time-dependent model state $|\phi(t)\rangle$ is taken to be a Slater determinant of particle-hole states:

$$|\phi(t)\rangle = \exp(-iH_{00}t/\hbar) \times \exp\left[\sum_{ph} c_{ph}(t) a_p^\dagger a_h\right] |\phi_0\rangle \ . \tag{3.2}$$

Studying small-amplitude oscillations about the (assumed) stationary state leads by a derivation invoking the least-action principle

$$\delta \int \langle\psi(t)|H - i\hbar\partial/\partial t|\psi(t)\rangle dt = 0 \tag{3.3}$$

to the CBF analog of the RPA equations. Details of the algebraic manipulations may be found in Refs. 1–3. The CRPA equations are expressed in terms of the CBF single-particle energies and effective interactions: Introducing the usual Fourier decomposition of $c_{ph}(t)$ in the form

$$c_{ph}(t) = z_{ph}[x_{ph}(t)e^{-i\omega t} + y^*_{ph}(t)e^{i\omega t}] \ , \tag{3.4}$$

one finds a set of RPA-type equations of the form

$$\begin{bmatrix} A & B \\ B^* & A^* \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix} = \hbar\omega \begin{bmatrix} M & 0 \\ 0 & -M^* \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix} , \tag{3.5}$$

where

$$\begin{aligned} A &= (A_{ph,p'h'}) = [e(p) - e(h)]\delta_{pp'}\delta_{hh'} \\ &\qquad + \langle ph'|\mathscr{V}(12)|hp'\rangle_a \ , \\ B &= (B_{ph,h'p'}) = \langle pp'|\mathscr{V}(12)|hh'\rangle_a \ , \\ M &= (M_{ph,p'h'}) = \delta_{pp'}\delta_{hh'} + \langle ph'|\mathscr{N}(12)|hp'\rangle_a \ . \end{aligned} \tag{3.6}$$

Note that we have, in contrast to Ref. 2, absorbed the normalization constants z_{ph} in the amplitudes $X=(X_{ph})$ and $Y=(Y_{ph})$. This is necessary to guarantee the appearance of the unit matrix as the leading, diagonal contribution to M, and the proper definition of the CBF single-particle energies in A. We note that the nonorthogonality corrections appearing in the nontrivial part of the "metric matrix[1]" M may also be understood as an energy dependence of the particle-hole interaction. The elements of the amplitude vector (X_{ph}) should not be confused with the irreducible normalization matrix X introduced in Eq. (2.18).

The procedure for constructing the dynamic structure factor and the response function from the amplitude vectors X and Y may be found in Refs. 2 and 3. Here, we wish to go a step further and utilize the CRPA equations (3.5) and (3.6) to generate the ring diagrams in CBF theory. Owing to the intimate relation[16] between the particle-hole propagator and the response function, and in view of the applications of the last section, we must briefly review the derivations of Ref. 2.

As usual, the system is subjected to an external time-dependent perturbation

$$H'(t) = P(\omega)(e^{i\omega t} + e^{-i\omega t}) \ . \tag{3.7}$$

To be definite, we may think of a periodic density fluctuation. Assuming that the time-dependent state $|\psi(t)\rangle$ may be faithfully expressed as a superposition of the correlated $1p$-$1h$ states $|\psi_{ph}\rangle$, and linearizing in the amplitude of the perturbation, one finds that in analogy to Eq. (3.4) the new amplitudes X', Y' are determined by solving

$$\begin{bmatrix} A & B \\ B^* & A^* \end{bmatrix}\begin{bmatrix} X' \\ Y' \end{bmatrix} = \hbar\omega \begin{bmatrix} M & 0 \\ 0 & -M^* \end{bmatrix}\begin{bmatrix} X' \\ Y' \end{bmatrix} - \begin{bmatrix} P \\ P^* \end{bmatrix} . \tag{3.8}$$

Here, $P = (P_{ph})$ are the matrix elements of the external perturbation $P(\omega)$,

$$P_{ph} = \langle \psi_{ph} \mid P \mid \psi_0 \rangle, \quad P_{hp} = P_{ph}^* . \tag{3.9}$$

By applying formal analogy arguments, the matrix

$$G^{\mathrm{CRPA}}(\omega) = \begin{bmatrix} A - \hbar\omega M - i\eta & B \\ B^* & A^* + \hbar\omega M^* + i\eta \end{bmatrix}^{-1} \tag{3.10}$$

is identified as the particle-hole approximation for the Green's function. From this we may, for example, calculate, as described in Ref. 2, the density-density response function

$$\Pi(q,\omega) = -\sum_{i,j} \rho_i(q) G_{i,j}^{\mathrm{CRPA}}(\omega) \rho_j(q) ,$$
$$\rho_{ph}(q) = \langle \psi_{ph} \mid \rho_q \mid \psi_0 \rangle , \tag{3.11}$$

where the subscripts i and j stand for particle-hole pairs (ph) and (hp).

We have constructed the object $G^{\mathrm{CRPA}}(\omega)$ here simply by taking over equations from conventional RPA (see, e.g., Ref. 17). It must be stressed that the formal identity of our definition does not also justify carrying over the physical interpretation or uncritically using working formulas from conventional many-body theory: The Green's function (3.10) should be understood as a correction to the full particle-hole propagator. An explicit example in which the blind application of standard many-body techniques with CBF quantities fails is the self-energy, which we will discuss later.

Appealing to our study of the effective CBF interactions, we now transform Eq. (3.10) to a new equation in terms of the irreducible vertex functions (2.18) and (2.23). To this end, we define

$$\Omega = \begin{bmatrix} e(p) - e(h) - \hbar\omega - i\eta & 0 \\ 0 & e(p) - e(h) + \hbar\omega + i\eta \end{bmatrix} \tag{3.12}$$

and observe that (3.5) can be written in the form

$$(\Omega + W + \tfrac{1}{2}\,\Omega C + \tfrac{1}{2}\,C\Omega) G^{\mathrm{CRPA}}(\omega) = I , \tag{3.13}$$

where I is the unit matrix. The CBF diagrams contributing to the particle-hole propagator may be obtained as usual[17] by iterating Eq. (3.13) starting with the bare propagator $G_0^{\mathrm{CRPA}}(\omega) = \Omega^{-1}$. The presence of the energy numerator terms in Eq. (3.13) [c.f. also Eq. (2.8)] means, however, that the resulting expansion is no longer ordered strictly according to the number of energy denominators. Rather, successive cancellations between energy-denominator and energy-numerator terms result in a series in which the nth-order contribution to $G^{\mathrm{CRPA}}(\omega)$ contains diagrams with $1,2,\ldots,n$ energy denominators. We will now show that a rearrangement of this series according to the number of energy denominators is, in essence, equivalent to a reformulation of the CRPA equations in terms of the irreducible vertex functions X' and X introduced in the last section. Defining

$$G(\omega) = (1 + \tfrac{1}{2}C) G^{\mathrm{CRPA}}(\omega)(1 + \tfrac{1}{2}C) , \tag{3.14}$$

we can rewrite (3.13) in the form

$$[\Omega + U(\omega)] G(\omega) = I , \tag{3.15}$$

with $U(\omega)$ again being a supermatrix, expressible entirely in terms of the irreducible quantities X and X' defined in Sec. II:

$$U(\omega) = X' - \tfrac{1}{4} X\Omega X . \tag{3.16}$$

Let us study the structure of the energy-dependent term in $U(\omega)$ a bit more closely. Denoting by i and j a pair (ph) or (hp), the second term in Eq. (3.16) has the form

$$(X\Omega X)_{ij} = \sum_{p,h} \{ (X_{i,ph} X_{ph,j} + X_{i,hp} X_{hp,j})[e(p) - e(h)] - \hbar\omega (X_{i,ph} X_{ph,j} - X_{i,hp} X_{hp,j}) \} . \tag{3.17}$$

The last term in Eq. (3.17) is the only remaining energy-dependent term in the effective interaction. We note that this term vanishes for a local X, i.e., if X is just a function of the momentum transfer $q = |\vec{p} - \vec{h}|$. In fact, the symmetries of the operator $\mathcal{N}(12)$ may be used to prove that only combinations of exchange matrix elements give nonzero contributions to the energy dependence of the irreducible operator $U(\omega)$, and all of them vanish in the Landau limit $q \to 0$. It also turns out that the local approximations discussed in the preceding section will cause the energy dependence to disappear entirely. We expect therefore that the energy dependence of $U(\omega)$ is of relatively little importance. It is also worth noting that the nonvanishing contributions to the energy-dependent term in $U(\omega)$ are of fairly complicated structure (mostly "elementary" in the language of variational theory[4,5]). To be consistent, they should be included only together with contributions of corresponding structure occurring in the energy-independent terms. Actually, the energy dependence may be entirely eliminated by an additional transformation of the CRPA equations similar to the one performed above. We will refrain from such a transformation since it leads to additional complications without producing any further physical insight. It is of relevance only in cases when also elementary diagrams are included in the energy-*independent* parts. From now on, we will neglect the energy dependence, we also drop corresponding terms in the investigations of the next section. In this approximation, we will refer to the supermatrix $U_{ij}(\omega=0)$ simply as U_{ij}.

By the transformation (3.14) we have arrived at a formulation of the CRPA that is formally and conceptually identical to conventional RPA. In addition, precise prescriptions can be given for obtaining the particle-hole interaction from the underlying microscopic force. Our derivations also provide a tool for investigating the justifiability of the *ad hoc* use of "screened" interactions.[18] Finally, by using local approximations, one readily makes contact with pseudopotential[11] or static screening theories.[12]

Let us now turn to the study of the self-energy of a single particle. Relying on the formal correspondence between the CBF perturbation expansion and ordinary Goldstone perturbation theory, we try to write the self-energy in the form[17]

$$\Sigma(k,E)=u_v(k)+i\int\frac{d\omega}{2\pi}\sum_{p,i,j,m,n}G^0(p,E-\hbar\omega)\langle ki\,|\,\mathscr{V}(\omega)\,|\,pj\rangle_a G^{\mathrm{CRPA}}_{ij,mn}(\omega)\langle pm\,|\,\mathscr{V}(\omega)\,|\,kn\rangle_a\;. \tag{3.18}$$

Here, $G^0(p,E)$ is the free one-particle Green's function. The energy-dependent effective interaction is of the form

$$\langle ki\,|\,\mathscr{V}(E)\,|\,pj\rangle_a=\langle ki\,|\,\mathscr{W}(12)\,|\,pj\rangle_a\pm\tfrac{1}{2}[e(i)-e(j)-E]\langle ki\,|\,\mathscr{N}(12)\,|\,pj\rangle_a\;. \tag{3.19}$$

The labels (ij) and (mn) refer to particle-hole pairs (ph) or (hp), the positive sign applies if (ij) is a pair (ph). The energy-dependence of (3.19) might seem somewhat *ad hoc,* it is built after the CBF self-energy diagrams in second and third order.[15,19] We see immediately that the uncritical application of Eq. (3.18) leads to problems. The reason for this is that the (linear) energy dependence of the interaction $\mathscr{V}(E)$ generates diverging contributions to the frequency integral. Actually, by inserting the first-order approximation $G_0^{\mathrm{CRPA}}(\omega)=\Omega^{-1}$, we find that (3.18) misses even a part of the second-order CBF approximation for the self-energy. The missing terms, which might be understood as Hartree-Fock-type contributions (we will confirm this interpretation later), have to be singled out and treated separately.

In order to make the frequency integration in (3.18) work as desired, we have to eliminate the contributions containing energy numerators. We have already pointed out that the energy dependence of the effective interaction generates contributions to $G^{\mathrm{CRPA}}(\omega)$ which go as ω^{-1} in all orders. To rearrange the CBF series, we transform the integrand of Eq. (3.18) to the irreducible representation. A few algebraic manipulations show that

$$\sum_{i,j,m,n}\langle ki\,|\,\mathscr{V}(\omega)\,|\,pj\rangle_a G^{\mathrm{CRPA}}_{ij,mn}(\omega)\langle pm\,|\,\mathscr{V}(\omega)\,|\,kn\rangle_a =\sum_{i,j,m,n}[U_{kp,ij}(\omega)G_{ij,mn}(\omega)U_{mn,kp}(\omega)-U_{kp,pk}(\omega)+W_{kp,pk}]\;, \tag{3.20}$$

where (ij) and (mn) refer to pairs (ph) and (hp), respectively. To the extent that we can neglect the frequency dependence of $U(\omega)$ we have singled out the "catastrophic" terms in the frequency integral (3.18). One expects therefore that the full self-energy can be expressed in the form of a Hartree-Fock-type term $u(k)$ and a subtracted frequency integral[20] involving only $U_{ij,mn}$:

$$\Sigma(k,E)=u(k)+i\int\frac{d\omega}{2\pi}\sum_{p,i,j,m,n}G^0(p,E-\hbar\omega)U_{kp,ij}\times G_{ij,mn}(\omega)U_{mn,pk}\;. \tag{3.21}$$

The leading, Hartree-Fock-type term consists of the CBF average field $u_v(k)$, *plus* correction terms originating from all those CBF diagrams in which the energy-numerator and the energy-denominator terms completely cancel. We have already pointed out that these terms are not identical with the frequency-independent term W-U in Eq. (3.20). They cannot be obtained from the analysis of the CRPA equations, but call for a separate determination which we will pursue in the next section. An expression similar to (3.21) may be derived for the CRPA correction to the ground-state energy by closing the remaining particle-hole loop and performing the familiar integration over a ficticious coupling constant.[16,21]

IV. CBF RING DIAGRAMS

We have demonstrated in Sec. III that the simple iteration of the interaction, using the particle-hole approximation for the two-particle Green's function and the subsequent frequency integration does not generate all ring diagrams of CBF theory. We therefore go back to the CBF expansion of the ground-state energy and identify, to a satisfactorily high order, CBF diagrams with those generated by the iteration of the RPA equations. Most important, we have to isolate all terms in which the energy numerators of the effective interaction (2.8) cancel all energy denominators. At the same time, we confirm that the CBF expansion may in fact be reformulated entirely in terms of the irreducible vertex U.

Following the analysis for the ground-state energy, we obtain the self-energy by functional variation with respect to the particle occupation number. This seems like a detour, but actually leads to considerable simplifications. The reason is that the leading term $u(k)$ of Eq. (3.21) also contains contributions arising from the variation of the vertex functions (2.18) and (2.22) with respect to the particle number. (Recall that these involve summations over particle-hole loops.) This leads to a profusion of diagrams, which makes the identification of the distinct terms complex and opaque.

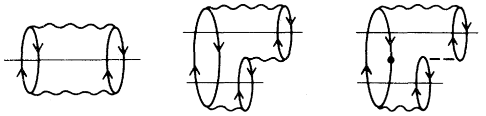

FIG. 2. Diagrammatical representation of second- and third-order CBF ring diagrams. The wavy line represents an effective interaction $\mathscr{V}(12)$, the dashed line a nonorthogonality correction $\mathscr{N}(12)$. Particle and hole lines are drawn as up- and down-going arrows, respectively. The horizontal bar indicates an energy denominator, a closed circle on a particle-hole loop an energy numerator $e(p)-e(h)$.

The Goldstone-type diagrams of CBF perturbation theory may be obtained either by a step-by-step evaluation[22] or by the generating equations of the correlated-coupled-cluster theory.[6] The result is a perturbation expansion that is structurally very similar to an ordinary Goldstone expansion. The essential differences may be understood to be due to the fact that we always deal with many-body wave functions. This is reflected in the appearance of effective three-, four- , . . . , n-body interactions and in the energy dependence which we have already encountered above. This energy dependence is determined by the simple rule that each (say, two-body) interaction $\langle ij \,|\, \mathscr{V}(12) \,|\, kl \rangle$ has to be supplemented by a term $E\langle ij \,|\, \mathscr{N}(12) \,|\, kl \rangle$, where E is the energy carried by all particle lines *minus* the energy carried by all hole lines at the same time.

Let us now turn to the explicit construction of the leading CBF ring diagrams. The construction is straightforward in second and third order; the diagrams are shown in Fig. 2. The diagrammatical conventions used in there and in Fig. 3 are as follows: particle and hole lines are drawn as up- and down-going arrows; antisymmetrized matrix elements of the two-body operators $\mathscr{V}(12)$ and $\mathscr{N}(12)$ are drawn as a wavy and a dashed line, respectively. Energy denominators are drawn as horizontal bars, and a heavy dot on a particle or a hole line represents an energy numerator $e(p)-e(h)$ associated with this particle-hole bubble.

In fourth order,[23] an awkward feature of the CBF perturbation expansion appears: The four-body

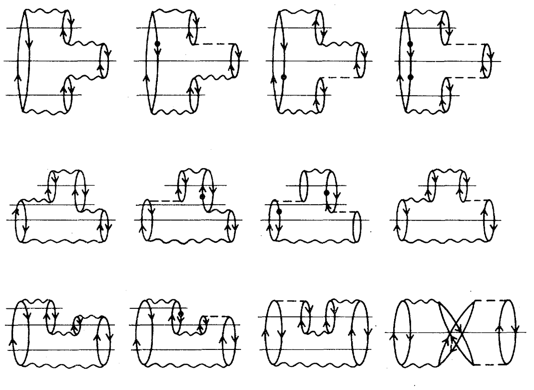

FIG. 3. Fourth-order CBF ring diagrams. See Fig. 2 for further explanations.

operators $\mathcal{N}(1234)$ and $\mathcal{W}(1234)$ contain unlinked contributions, e.g.,

$$\mathcal{N}(1234)=\mathcal{N}(12)\mathcal{N}(34)+\mathcal{N}(13)\mathcal{N}(24)+\mathcal{N}(14)\mathcal{N}(23)+\mathcal{N}_c(1234)\ . \quad (4.1)$$

[$\mathcal{N}_c$ stands for the connected part of $\mathcal{N}(1234)$, which vanishes whenever any particle or any pair of particles is moved far away from the others.] These diagrams lead to a catastrophic dependence of the CBF perturbation series on the particle number unless special truncation prescriptions are employed to cancel the unlinked diagrams in different orders of the CBF expansion. For example, the unlinked diagram arising in the second-order CBF correction from the four-body interaction is canceled against a fourth-order diagram containing only two-body operators.

While the unlinked diagrams can be canceled systematically by an appropriate classification of the CBF expansion, they leave remainders which are of a structure similar to the ordinary Goldstone-type diagrams of the CBF series. Examples are shown in Fig. 3. Diagrams 1–7, 9, and 10 represent fourth-order ring diagrams in terms of $\mathcal{V}(12)$ and some correction terms arising from the energy dependence of the effective interaction. Diagrams 8 and 11 are third-order diagrams including the reducible part of one four-body interaction. Finally, diagram 12 is the linked remainder of the second-order $4p$-$4h$ contribution. Clearly all of these diagrams must be considered of equal importance. In fact, some algebraic manipulations exhibit substantial cancellations, including, among others, the exact cancellation of all diagrams of the types shown as the last three in Fig. 3. It is important to notice that the energy dependence of the *pp-hh* and the *hh-pp* matrix elements has been eliminated entirely. This cancellation between the reducible parts of the four-body interaction and some of the energy dependence of the two-body interaction will actually make it possible to use the (C)RPA equations to sum CBF ring diagrams. Of course, we have to assume that the cancellations observed here will also occur in higher orders of the CBF expansion.

In order to construct the connection between the CBF diagrams and those generated by the (C)RPA equations we have to isolate and cancel all energy numerator and denominator terms. Formally, we start from the series

$$E=\sum_{n=2}^{\infty}(\delta E)_n \quad (4.2)$$

of all CBF ring diagrams in terms of the effective interaction $\mathcal{V}(12)$, where the index counts the number of energy denominators. We seek a rearrangement of series (4.2)

$$E=\sum_{n=0}^{\infty}(\Delta E)_n\ , \quad (4.3)$$

obtained by cancellation of all energy numerator terms and subsequent rearrangement according to the number of remaining energy denominators. This procedure has the two purposes already posed above: first, to determine all those contributions to the energy which do not have energy denominators and therefore cannot be determined by the frequency integration (3.18). Owing to the absence of energy denominators, all hole lines reduce in this case to exchange functions $l(rk_F)$, and all particle lines to a δ function *minus* an exchange function. Consequently, the diagrammatical elements to describe the resulting expansion for $(\Delta E)_0$ are identical to those used in the variational estimate H_{00} of the ground-state energy.

It must be stressed, however, that the procedure of separating interaction and energy-numerator terms is only valid if all diagrams of the same topological structure are retained. This is so because the small quantities $\langle ij\,|\,\mathcal{V}(12)\,|\,kl\rangle$ are effectively split into large pieces $\langle ij\,|\,\mathcal{W}(12)\,|\,kl\rangle$ and $E\langle ij\,|\,\mathcal{N}(12)\,|\,kl\rangle$.

The second task of analyzing the CBF ring diagrams is to verify that the sum of all of the remaining ring diagrams (i.e., all those containing proper energy denominators) is correctly given by the subtracted frequency integration (3.21). The reader is reminded that the original derivation of the (C)RPA is based on one- and two-body matrix elements alone. There is no *a priori* reason to assume that the reducible four-, six- , . . . , $2n$-body diagrams are also correctly treated. If, on the other hand, the interpretation of the Fermi hypernetted chain (FHNC) diagrams as ring diagrams with a simplified (local) propagator is valid, the identification should be exact.

The cancellation between the energy-denominator and the energy-numerator terms of the CBF ring diagrams is a tedious task, one in which we have persevered through all fourth-order ring diagrams. The essentially new aspects arising in fourth order were already discussed; for a demonstration of the general calculational procedure it is sufficient to consider second- and third-order terms. For ease of writing we introduce the abbreviation

$$e_{ph}=e(p)-e(h)\ . \tag{4.4}$$

Since the frequency integrals [(3.18) and (3.21)] overcount the second-order diagram by a factor of 2, we also include this term with this artificial factor. Using the notation of Eqs. (2.17), (2.21), and (4.4), we find

$$(\delta E)_2=-\tfrac{1}{2}\sum_{p,h,p',h'}\left[W_{ph,h'p'}\frac{1}{e_{ph}+e_{p'h'}}W_{hp,p'h'}+\tfrac{1}{2}(C_{ph,h'p'}W_{hp,p'h'}+W_{ph,h'p'}C_{hp,p'h'})+\tfrac{1}{2}e_{ph}C_{ph,h'p'}C_{hp,p'h'}\right], \tag{4.5}$$

and the identification of the three distinct contributions to $(\Delta E)_0$ and $(\Delta E)_1$ is obvious. In third order we obtain

$$\begin{aligned}(\Delta E)_3=\sum_{\substack{p,p',p''\\ h,h',h''}}\Bigg[&W_{ph,p'h'}\frac{1}{e_{ph}+e_{p'h'}}W_{p'h',p''h''}\frac{1}{e_{ph}+e_{p''h''}}W_{hp,p''h''}\\ &+\tfrac{1}{2}W_{ph,h'p'}\frac{1}{e_{ph}+e_{p'h'}}(W_{p'h',p''h''}C_{hp,p''h''}+C_{p'h',p''h''}W_{hp,p''h})\\ &+\tfrac{1}{2}(W_{ph,h'p'}C_{p'h',p''h''}+C_{ph,h'p}W_{p'h',p''h''})\frac{1}{e_{ph}+e_{p''h''}}W_{hp,p''h''}\\ &+\tfrac{1}{4}\left[W_{ph,h'p'}\frac{e_{ph}+e_{p''h''}}{e_{ph}+e_{p'h'}}C_{p'h',p''h''}C_{hp,p''h''}+C_{ph,h'p'}C_{p'h',p''h''}\frac{e_{ph}+e_{p'h'}}{e_{ph}+e_{p''h''}}W_{hp,p''h''}\right]\\ &+\tfrac{1}{4}(W_{ph,h'p'}C_{p'h',p''h''}C_{hp,p''h''}+C_{ph,h'p'}W_{p'h',p''h''}C_{hp,p''h''}+C_{ph,h'p'}C_{p'h',p''h''}W_{hp,p''h''})\\ &+\tfrac{1}{8}(2e_{ph}+e_{p'h'}+e_{p''h''})C_{ph,h'p'}C_{p'h',p''h''}C_{hp,p''h''}\Bigg]\ ,\end{aligned} \tag{4.6}$$

where we sum over all particle and hole labels p, p', p'', h, h', and h''. The terms in Eq. (4.6) containing a ratio of single-particle energies call for additional rearrangement. The representative first term is written as

$$\begin{aligned}\sum W_{ph,h'p'}\frac{e_{ph}}{e_{ph}+e_{p'h'}}C_{p'h',p''h''}C_{hp,p''h''}=\tfrac{1}{4}\sum\Bigg[&W_{ph,h'p'}(C_{p'h',p''h''}C_{hp,p''h''}+C_{ph,p''h''}C_{h'p',p''h''})\\ &+W_{ph,h'p'}\frac{e_{ph}-e_{p'h'}}{e_{ph}+e_{p'h'}}(C_{p'h',p''h''}C_{hp,p''h''}-C_{ph,p''h''}C_{h'p',p''h''}\Bigg]\ .\end{aligned} \tag{4.7}$$

We are now ready to identify the third-order contributions to $(\Delta E)_0$, $(\Delta E)_1$, and $(\Delta E)_2$. In the terms with one remaining energy denominator we discover the supplementation of W with kinetic-energy terms in the combination

$$\begin{aligned}W_{ph,h'p'}-\tfrac{1}{4}\sum_{p'',h''}&e_{p''h''}(C_{p'h',p''h''}C_{hp,p''h''}+C_{ph,p''h''}C_{h'p',p''h''})\\ &-\tfrac{1}{8}\sum_{p'',h''}(e_{ph}-e_{p'h'})(C_{p'h',p''h''}C_{hp,p''h''}-C_{ph,p''h''}C_{h'p',p''h''})\ ,\end{aligned} \tag{4.8}$$

which we found already in our reformulation of the CRPA equations (3.15) and (3.16). The last term of (4.8) obviously originates from the remaining energy dependence. The second and the third term of Eq.

(4.6) display, moreover, the rearrangement of interaction and correlation terms corresponding to the reduction (2.22) of $W_{ph,h'p'}$ to its irreducible part. Thus we find first evidence that the series of CBF ring diagrams may in fact be rearranged and formulated in terms of the irreducible vertex function $U(\omega)$ driving the CRPA equations.

These findings are confirmed by extending the rearrangement to the fourth-order ring diagrams of Fig. 3, which also gives sufficient information to identify the leading term $(\Delta E)_0$ of the expansion (4.3). Without engaging in further details of the tedious algebraic manipulations, we display the end result:

$$(\Delta E)_0 = -\frac{1}{4}\sum_{p,h,p',h'} \big(e_{ph}X_{ph,h'p'}X_{hp,p'h'} + X'_{ph,h'p'}C_{hp,p'h'} + C_{ph,h'p'}X'_{hp,p'h'} \big) \,. \tag{4.9}$$

In (4.9) we have dropped, in keeping with the approximation discussed above, some of the nonlocal terms introduced by the energy dependence of the irreducible vertex function $U(\omega)$. Equation (4.9) is exact for the direct terms of the RPA summation and also for the local approximations introduced in the next section.

The "no-energy-denominator" term (4.9) has a fairly obvious interpretation in terms of the variational energy expectation value: The first term *plus* the kinetic-energy terms in X' subtracts from the variational energy the chain contributions to the kinetic-energy operator. The potential terms cancel all chain diagrams involving the Jackson-Feenberg interaction, starting at second order. Remaining are Hartree-Fock-type terms, obtained from, say, the FHNC approximation for H_{00} by omitting all chain diagrams.

Thereby, we have established a direct correspondence between the ring diagrams summed by the RPA equations and the chain diagrams of the variational description of the ground-state wave function. The degree to which the correspondence can be exploited depends, of course, on the technology available to produce the ingredients of the theory. To some extent the task of computing nonlocal contributions has been simplified, since many of these terms are not present in the irreducible vertex function U.

The computation of energy corrections due to the inclusion of the (C)RPA diagrams is presumably the least demanding problem to be attacked by the CRPA formalism, since the success of variational methods indicates that the approximations on the propagator do not have serious consequences in this case. The situation is significantly different in situations where one concentrates on effects close to the Fermi surface. Examples are the self-energy, Fermi-liquid parameters, and the pairing interaction. In all of these cases, CBF corrections to the variational estimates were found to be large, if not overwhelming.[24,15,19]

To study the self-energy, we must calculate the variation of the variational ground-state energy *plus* its (C)RPA correction with respect to the particle number. This leads us to a representation of the form (3.21), in which we can identify in a symbolic notation,

$$u(k) = u_v(k) + \frac{\delta[(\Delta E)_0]}{\delta n(k)} + \frac{\delta E^{\mathrm{RPA}}}{\delta U}\frac{\delta U}{\delta n(k)} \,. \tag{4.10}$$

By E^{RPA} we mean the sum of all ring diagrams in terms of the irreducible vertex U, i.e., the sum (4.3) starting at $n=1$. It is worth noting here again that the second term in Eq. (4.10) subtracts pieces contained in $u_v(k)$. Since the Hartree-Fock-type terms are usually smoothly varying functions which depend only little on the approximation used, one can obtain the combination

$$u_v(k) + \delta[(\Delta E)_0]/\delta n(k)$$

with satisfactory accuracy from the CBF single-particle energies[4] by taking out the chain diagrams. A similar argument applies to the last term in Eq. (4.10): The irreducible vertex U is a more "highly connected" quantity than, for example, the operators $\mathscr{W}(12)$ or $\mathscr{N}(12)$ entering the original CBF self-energy. The variation of U with respect to the occupation number generates genuine three-body terms, whereas the variation of $\mathscr{W}(12)$ and $\mathscr{N}(12)$ can also generate products of two-body operators. It is also worth noting that all contributions to $u(k)$ are real. Unless these terms are singled out and treated individually, the real part of the self-energy cannot be obtained from the imaginary part using a Kramers-Kronig relation. The argument applies quite generally to CBF calculations of the self-energy, irrespective of whether RPA summations were performed or not. Currently[19] physically most interesting effects are, of course, expected from the complex portions of the self-energy which may, using the irreducible vertex function U, be computed with conventional methods.[25]

V. IRREDUCIBLE VERTEX FUNCTION

Our last task is to provide explicit expressions for the irreducible vertex function $U_{ij,kl}$. Here of course, we have to specify the correlation operator. We restrict ourselves to the Jastrow choice (2.2), but expect structurally similar results for state-dependent correlations.

The construction of the configuration-space representation of the energy-independent part of U [cf. Eqs. (3.16) and (3.17)] amounts, in essence, to the repetition of the analysis of Ref. 4. We shall refrain here from such a general construction as it involves the study of the elementary structures and a fairly tedious and unrewarding diagrammatical analysis. Rather, we will restrict ourselves to making the general result plausible using a simplified model in which all calculations can be carried out analytically. Also, we will only present the relevant working formulas to an order which has been found to be tractable, but also indispensable, for most applications in nuclear systems[15] and in liquid ^{3}He.[14] At this level of accuracy, the exchange terms of X' and X are identical to the exchange terms of $\mathscr{W}$ and $\mathscr{N}$.

Concerning our notation and the definition of the relevant quantities, we rely on Ref. 5 and our recent work on the optimized variational description of the many-fermion ground state.[14] The reader may find it necessary to consult these references for notational and technical matters. Following the notations introduced there, we denote the diagrams used in the FHNC summation technique with X_{ij} and N_{ij}, where X refers to "non-nodal" and N refers to "nodal" (or chain) diagrams. The subscripts (ij) [equal to (dd), (de), (ee), and (cc)] characterize the exchange structure at the external points.

The solution of the FHNC equations is sufficient[4] for the construction of the two-body operator $\mathscr{N}(12)$. For the calculation of $\mathscr{W}(12)$ we have to solve another set of linear integral equations, the so-called FHNC′ equations, which are constructed from the FHNC equations by linearization and which use the Jackson-Feenberg interaction (2.20) as the driving term. The solution of these equations is required anyway if the Jastrow function is determined by minimization of the energy expectation value.

Owing to their close resemblance to our approximations for the effective interactions in the next section, we display here the FHNC′ equations. The dimensionless three-dimensional Fourier transform is denoted by a tilde as

$$\tilde{f}(\vec{k})=\rho\int d^3r\, f(\vec{r})\exp(k\vec{k}\cdot\vec{r}) \,. \tag{5.1}$$

Let ν denote the degeneracy of the single-particle levels. It is helpful to introduce the quantities

$$L(r)=l(r,k_F)-\nu N_{cc}(r)\,, \tag{5.2}$$

$$\Gamma_{dd}(r)=X_{dd}(r)+N_{dd}(r)\,,$$
$$\Gamma'_{dd}(r)=X'_{dd}(r)+N'_{dd}(r)\,, \tag{5.3}$$

$$S_d(k)=\frac{\{1+[1+\tilde{X}_{ee}(k)]\tilde{\Gamma}_{dd}(k)\}}{[1+\tilde{X}_{de}(k)]}\,, \tag{5.4}$$

and the representation of the static structure function

$$S(k)=\frac{[1+\tilde{X}_{ee}(k)]S_d(k)}{[1+\tilde{X}_{de}(k)]} \tag{5.5}$$

in terms of the basic ingredients of FHNC theory. The FHNC′ equations may now be obtained by linearization of the FHNC equations, i.e.,

$$\hat{N}_{ij}(k)=\sum_{r,s}[\delta\hat{N}_{ij}(k)/\delta\hat{X}_{rs}(k)]\tilde{X}'_{rs}(k)\,, \tag{5.6}$$

where the driving terms are determined by diagrammatical analysis.[4] One obtains two sets of four linear equations, one being algebraic in momentum space, the other one in coordinate space. While the momentum-space equations are exact, the coordinate-space equations require the specification of "elementary" diagrams $E'_{ij}(r)$, which are set to zero in the simplest version of the FHNC′ equations. However, a minimum estimate of elementary exchange diagrams is required[14] to include "Pauli-blocking" effects which are necessary for some of the applications discussed below.

The coordinate-space equations are

$$X'_{dd}(r)=[1+\Gamma_{dd}(r)][v_{\mathrm{JF}}(r)+E'_{dd}(r)]+\Gamma_{dd}(r)N'_{dd}(r)\,, \tag{5.7}$$

$$X'_{de}(r)=\Gamma'_{dd}(r)[N_{de}(r)+E_{de}(r)]+[1+\Gamma_{dd}(r)]E'_{de}(r)+\Gamma_{dd}(r)N'_{dd}(r)\,, \tag{5.8}$$

$$\begin{aligned}X'_{ee}(r)=\;&\Gamma'_{dd}(r)\{-L^2(r)/\nu+[N_{de}(r)+E_{de}(r)]^2+N_{ee}(r)+E_{ee}(r)\}+\Gamma_{dd}(r)N'_{ee}(r)\\&+2[1+\Gamma_{dd}(r)]\{L(r)[N'_{cc}(r)+E'_{cc}(r)]+[N_{de}(r)+E_{de}(r)][N'_{de}(r)+E'_{de}(r)]\}\\&+[1+\Gamma_{dd}(r)]E'_{dd}(r)-(\hbar^2/2m\nu)[1+\Gamma_{dd}(r)]\{L(r)\nabla^2 l(rk_F)+[\nabla l(rk_F)]^2\}\,,\end{aligned} \tag{5.9}$$

$$X'_{cc}(r)=-\Gamma'_{dd}(r)L(r)/\nu+[1+\Gamma_{dd}(r)]E'_{cc}(r)+\Gamma_{dd}(r)N'_{cc}(r)-(\hbar^2/4m\nu)\Gamma_{dd}(r)\nabla^2 l(rk_F)\ . \tag{5.10}$$

[In Eq. (5.9) we correct a misprint of Eq. (A14) in Ref. 14.] The momentum-space equations (or, the equations for the nodal diagrams) read

$$\tilde{N}'_{dd}(k)=[S_d^2(k)-1]\tilde{X}'_{dd}(k)+2\tilde{\Gamma}_{dd}(k)S_d(k)\tilde{X}'_{de}(k)+\tilde{\Gamma}^2_{dd}(k)\tilde{X}'_{ee}(k)\ , \tag{5.11}$$

$$\begin{aligned}\tilde{N}'_{de}(k)= {} & S_d(k)[S(k)-S_d(k)]\tilde{X}'_{dd}(k)+\{\tilde{\Gamma}_{dd}(k)[S(k)-S_d(k)]+S_d(k)[S_d(k)-\tilde{\Gamma}_{dd}(k)]\}\tilde{X}'_{de}(k)\\ & +\tilde{\Gamma}_{dd}(k)[S_d(k)-\tilde{\Gamma}_{dd}(k)]\tilde{X}'_{ee}(k)\ ,\end{aligned} \tag{5.12}$$

$$\begin{aligned}\tilde{N}'_{ee}(k)= {} & [S(k)-S_d(k)]^2\tilde{X}'_{dd}(k)+2[S(k)-S_d(k)][S_d(k)-\tilde{\Gamma}_{dd}(k)]\tilde{X}'_{de}(k)\\ & +\{[S_d(k)-\tilde{\Gamma}_{dd}(k)]^2-1\}\tilde{X}'_{ee}(k)\ ,\end{aligned} \tag{5.13}$$

$$\tilde{N}'_{cc}(k)=\{[1-\tilde{l}(k)/\nu]/[1-\tilde{X}_{cc}(k)]^2-1\}\tilde{X}'_{cc}(k)\ . \tag{5.14}$$

Finally, it is useful to introduce the quantity

$$\begin{aligned}S'(k)&=\sum_{i,j}[\delta S(k)/\delta\tilde{X}_{ij}(k)]\tilde{X}'_{ij}(k)\\ &=S^2(k)\tilde{X}'_{dd}(k)+2S(k)S_d(k)\tilde{X}'_{de}(k)\\ &\quad+S_d^2(k)\tilde{X}'_{ee}(k)\ .\end{aligned} \tag{5.15}$$

The quantities $\tilde{X}_{ee}(k)$ and $\tilde{X}'_{ee}(k)$ have leading terms which are present even in the absence of correlations:

$$\tilde{X}_{ee}(k)=S_F(k)-1+O(f^2-1)\ , \tag{5.16}$$

$$\tilde{X}'_{ee}(k)=-(\hbar^2k^2/4m)[S_F(k)-1]+O(f^2-1)\ . \tag{5.17}$$

In terms of the structure function $S(k)$ and the generalized structure factor $S'(k)$, the optimization condition for the two-body correlation function

$$[\delta H_{00}(f)/\delta\ln f](r)=0 \tag{5.18}$$

reads, in Fourier space,[13]

$$\Omega(k)=S'(k)+(\hbar^2k^2/4m)[S(k)-1]=0\ . \tag{5.19}$$

The form (5.19) of the optimization condition for the two-body correlations would be unaffected by an additional three-body correlation factor, which can be absorbed in the elementary quantities $E'_{ij}(r)$ appearing in Eqs. (5.7)–(5.10).

The FHNC quantities introduced above are the basic building blocks for the variational single-particle energies[4,14] and the two-body operators $\mathcal{N}(12)$ and $\mathcal{W}(12)$. For example, the "local" approximation for $\mathcal{N}(12)$ is

$$\langle ij\,|\,\mathcal{N}_{\rm loc}(12)\,|\,kl\rangle=D^{-1}\langle ij\,|\,\Gamma_{dd}(r)\,|\,kl\rangle\ , \tag{5.20}$$

with

$$\begin{aligned}D=\{&[1-\tilde{X}_{cc}(p_i)][1-\tilde{X}_{cc}(p_j)]\\ &\times[1-\tilde{X}_{cc}(p_k)][1-\tilde{X}_{cc}(p_l)]\}^{1/2}\ .\end{aligned} \tag{5.21}$$

For the two-body operator $\mathcal{W}(12)$ one finds similarly

$$\begin{aligned}&\langle ij\,|\,\mathcal{W}_{\rm loc}(12)\,|\,kl\rangle\\ &\quad=D^{-1}\langle ij\,|\,\Gamma'_{dd}(r)+(\hbar^2/4m)\nabla^2\Gamma_{dd}(r)\,|\,kl\rangle\ .\end{aligned} \tag{5.22}$$

A complete discussion and explicit expressions for more complicated contributions to $\mathcal{W}(12)$ and $\mathcal{N}(12)$ may be found in Ref. 14.

Following the construction of the particle-hole correlation matrix X in Sec. 2, and using the basic building blocks of the FHNC quantities introduced here, we find, e.g.,

$$X_{ph,p'h'}=\tilde{X}_{dd}(q)/A-\langle ph'\,|\,\mathcal{N}(12)\,|\,p'h\rangle\ . \tag{5.23}$$

[Note that the direct term $\tilde{X}_{dd}(q)$ in (5.23) is normalized with the particle number A, not with the volume. This is due to the fact that the Fourier transform contains a density factor.] Again, $q=|\vec{p}-\vec{h}|$ is the momentum transfer in the direct channel.

From (5.23) it is straightforward to obtain the portion of the corresponding matrix element of X' originating from the Jackson-Feenberg interaction by "diagrammatical differentiation." The kinetic-energy terms require some additional attention. Here we have to combine the term $(\hbar^2/4m)\nabla^2\Gamma_{dd}(r)$

in Eq. (5.22) with the kinetic-energy terms of (3.16) and (3.17),

$$(X(t_p-t_h)X)_{ij}=\sum_{p,h}(\hbar^2p^2/2m-\hbar^2h^2/2m)\times(X_{i,ph}X_{ph,j}+X_{i,hp}X_{hp,j})\ . \tag{5.24}$$

The calculation may be performed by an order-by-order expansion starting from the definitions (2.18), (2.22), and (3.16). Special cases can also be verified analytically in all orders, for example, if we neglect all exchange terms, and use the chain approximations for the FHNC equations. Since this calculation is very similar to the one given in the next section, we display here only the end result.

The direct terms of the irreducible vertex function are given in terms of the FHNC quantities introduced above as

$$AU^{\rm dir}(q)=\widetilde{X}'_{dd}(q)-(\hbar^2q^2/4m)\widetilde{X}_{dd}(q)\times\{1-[1-m/m^*(q)]\widetilde{X}_{dd}(q)\}\ , \tag{5.25}$$

where $m^*(q)$ is an average momentum-dependent effective mass defined by

$$\hbar^2q^2/2m^*(q)=A^{-1}\sum_h n(h)[1-n(|\vec{\rm h}+\vec{\rm q}|)]\times[e(|\vec{\rm h}+\vec{\rm q}|)-e(h)]\ . \tag{5.26}$$

It is possible, of course, to go beyond the simplest approximation (5.25) for $U(q)$ by, for example, including terms where the single-particle potential $u_v(k)$ couples direct and exchange diagrams in the quadratic terms (3.15) and (3.16). However, much care is needed in such a case since it will generally be necessary to include elementary diagrams in order to guarantee the correct Landau limit. Past experience[14] has shown that it is much more important to keep the correct *combination* of diagrams to CBF quantities than to calculate a part of them, which happens to have a simpler analytical structure. We anticipate that the expression (5.25) will, when supplemented with the exchange term of $\mathscr{W}(12)$, be a satisfactory starting point for numerical applications.

VI. LOCAL APPROXIMATIONS

In principle, the (C)RPA equations formulated in the original work[1–3] or in the irreducible form presented here may be solved numerically on a suitable mesh. They contain all the information needed to study the single-particle spectrum and collective modes. In fact, the brute-force diagonalization appears to be the most promising treatment in finite nuclei, and is also feasible for infinitely extended nuclear systems.[26] However, such studies remain limited to the computation of the spectrum and to the study of collective modes. To study the coupling of excited states to the particle-hole and collective modes of the medium, for example, requires additional manipulations.[25] Substantial simplifications are possible if reliable approximations for the solutions of the CRPA equations are available in closed form. Moreover, theoretical understanding is usually promoted by formal studies and analytically solvable models. It will also provide contact with, for example, the pseudopotential model of Aldrich and Pines,[11] or to "local-field corrections."[12] We turn in this section to the study of solvable models of the (C)RPA equations.

To motivate the choice of our local approximations, let us turn to a simplified description of collective excitations within the variational framework. Such a study depends to some extent on the explicit form of the correlation operator F. To be definite, we assume for the ground-state correlation operator F the Feenberg form

$$F=\exp\left[\sum_{i<j}u(r_{ij})+\sum_{i<j<k}u(\vec{\rm r}_i,\vec{\rm r}_j,\vec{\rm r}_k)+\cdots\right]\ . \tag{6.1}$$

For the study of collective density fluctuations, a symmetrized operator product or an exponential involving spin, isospin, and tensor correlations may also be used. We include "backflow"[27] correlations only to the extent that these can be rewritten in terms of multiparticle correlation functions. This can always be done in a boson system. For a Fermion system, this amounts to neglecting the action of the backflow correlation operator on the Slater function. To include these type of correlations, a separate study of the optimization of the backflow correlation operator is required, which is presently not available and beyond the scope of this paper.

The variational nature of the wave function (2.2) suggests that it is also well suited to the description of coherently excited states, in which all particles are equally involved. In fact, we will see that the spectrum of collective modes is already built into the variational wave function.

On the other hand, one expects that additional considerations are required to correctly describe single-particle excitations. Already the work of Tan and Feenberg[24] indicated that substantial corrections to the single-particle spectrum are to be expected from going beyond the variational, static description of the wave function. These findings were recently substantiated and broadened,[15,19] using present technology for the computation of the relevant CBF quantities.

In a collective mode, the particle-hole amplitudes $c_{ph}(t)$ describe a coherent state, i.e., they are to a good approximation functions of the momentum transfer $q=|\vec{p}-\vec{h}|$ alone. The trial wave function (3.2) may in this case be written in the simplified form

$$|\phi_{\rm coll}(t)\rangle=\exp\left[-iH_{00}t/\hbar+\sum_q c_q(t)\rho_q\right]|\phi_0\rangle \ , \tag{6.2}$$

where ρ_q is the density operator

$$\rho_q=\sum_{\vec{k}} a^\dagger_{\vec{k}+\vec{q}}\,a_{\vec{k}} \ .$$

With this wave function, we carry out manipulations like those leading to the CRPA equations. However, we can now perform all summations over hole states explicitly. The matrices A, B, and M are replaced by their hole-state averages which depend only on the wave vector q of the collective mode. They may be written in the form

$$B(q)=I_{00}^{-1}\langle\phi_0|F^\dagger(H-H_{00})F\rho_q^\dagger\rho_q|\phi_0\rangle \ , \tag{6.3}$$

$$\begin{aligned}A(q)&=I_{00}^{-1}\langle\phi_0|\rho_q^\dagger F^\dagger(H-H_{00})F\rho_q|\phi_0\rangle\\&=B(q)+\hbar^2q^2/2m \ ,\end{aligned} \tag{6.4}$$

$$M(q)=I_{00}^{-1}\langle\phi_0|F^\dagger F\rho_q^\dagger\rho_q|\phi_0\rangle=S(q) \ . \tag{6.5}$$

Equations (6.4) and (6.5) require the abovementioned locality of the correlation operator F (more generally the commutation property $[\rho_q,F]=0$).

The simplifications (6.3)–(6.5) turn the CRPA equations into a set of algebraic equations with the solution

$$\begin{aligned}\hbar\omega(q)=&\,[\hbar^2q^2/2mS(q)]\\&\times[1+(4m/\hbar^2q^2)B(q)]^{1/2} \ .\end{aligned} \tag{6.6}$$

We note also that, if we have chosen to determine the central (Jastrow) part of the correlation operator $f(r)$ by the variational principle (5.18), we find[14]

$$B(f_{\rm opt})(q)=\Omega(q)=0 \ , \tag{6.7}$$

which leads us immediately to the well-known Bijl-Feynman dispersion relation for the zero-sound mode

$$\hbar\omega(q)=\hbar^2q^2/[2mS(q)] \ . \tag{6.8}$$

Note that the $S(q)$ in Eq. (6.8) is the static structure function *obtained from the variational wave function.* The result that optimal variational wave functions lead to this dispersion relation is not new[28] and was already implicit in Feenberg's work.[13] In essence, it shows again that the RPA is, in a collective sense, already built into the variational theory of the ground state. This is consistent with the fact that the summation of the chain diagrams is a minimum requirement to obtain a physically meaningful solution of the variational problem (5.18). In essence, the collective model amounts to the contraction of the cut in the Lindhard function[29] to a single pole describing a collective mode; it is exact in Boson systems. We do not see much point at present in a numerical application for the helium liquids, since the Bijl-Feynman dispersion relation gives a poor description of the experimental situation. This is, however, a fault of the linearized treatment of the excitations within the RPA, and not a shortcoming of the Jastrow wave function.

The collective model (6.2) is implicit in recent studies of the response function in the electron gas and in liquid ^{3}He.[30] Embedding the theory of Refs. 30 in the more general framework of the correlated RPA is therefore not only of pedagogical value, it also allows one to relax systematically some of the underlying approximations and to study dynamical effects and the influence of single-pair excitations. Relying on the general analysis of the dynamic response function in Sec. IV, and in Refs. 2 and 3, we find, in the collective model,

$$\begin{aligned}G_{\rm coll}(q,\omega)=&\,(\hbar^2q^2/m)\\&\times\{[\hbar^2q^2/2m+\Omega(q)]^2\\&\quad-\Omega^2(q)-\hbar^2\omega^2S^2(q)\}^{-1} \ ,\end{aligned} \tag{6.9}$$

and the density-density response function

$$\begin{aligned}\Pi(q,\omega)=&\,-[\hbar^2q^2S^2(q)/m]\\&\times\{[\hbar^2q^2/2m+\Omega(q)]^2\\&\quad-\Omega^2(q)-\hbar^2\omega^2S^2(q)\}^{-1} \ .\end{aligned} \tag{6.10}$$

In the case of optimal correlations, (6.10) simplifies to

$$\Pi(q,\omega) = -(\hbar^2 q^2/m) \times \{ [\hbar^2 q^2/2mS(q)]^2 - \hbar^2\omega^2 \}^{-1} . \qquad (6.11)$$

One does not expect that the response function in the collective model contains as a leading term the Lindhard function, since the present approach amounts to the approximation

$$\frac{\sum_k n(k)[1-n(|\vec{k}+\vec{q}|)]/[e(|\vec{k}+\vec{q}|)-e(k)-\hbar\omega]}{\sum_k n(k)[1-n(|\vec{k}+\vec{q}|)]} \approx \frac{\sum_k n(k)[1-n(|\vec{k}+\vec{q}|)]}{\sum_k \{n(k)[1-n(|\vec{k}+\vec{q}|)][e(|\vec{k}+\vec{q}|)-e(k)-\hbar\omega]\}} \qquad (6.12)$$

The above example substantiates our argument that the collective modes are naturally built into the variational description of the ground state. It also motivates our suggestion that the hole-state average involved in Eqs. (6.3)–(6.5) is an approximation that is sympathetic with the use of correlated wave functions. Let us therefore go beyond the collective model (6.3)–(6.5) and consider, in concert with our studies of Sec. III, the single-particle spectrum and the energy-numerator terms individually. In principle, any approximation for the matrix elements of $\mathcal{N}(12)$ and $\mathcal{W}(12)$ or of the irreducible vertex U, which is a function of momentum transfer alone, will generate a closed-form solution of the (C)RPA equations. However, some care must be exercised in order to preserve the accuracy of the HNC calculation of the ground-state properties. To see this, we write the static structure function as

$$\begin{aligned} S(q) &= A^{-1}\sum_{kk'} \langle \phi_0 | F^\dagger F a^\dagger_{\vec{k}'-\vec{q}} a_{\vec{k}'} a^\dagger_{\vec{k}+\vec{q}} a_{\vec{k}} | \phi_0 \rangle / I_{00} \\ &= S_F(q) + A^{-1}\sum_{k,k'} z_{\vec{k}+\vec{q},\vec{k}} z_{\vec{k}'-\vec{q},\vec{k}'} \langle \vec{k},\vec{k}' | \mathcal{N}(12) | \vec{k}+\vec{q},\vec{k}-\vec{q} \rangle_a , \end{aligned} \qquad (6.13)$$

where the sums over k and k' are restricted to $k \langle k_F$ and $|\vec{k}+\vec{q}| \rangle k_F$. The most general configuration space contributions to $\mathcal{N}(12)$ are four-point functions, the computation of $\mathcal{N}(12)$ remains therefore practically limited to the leading, local terms. The computation of $S(q)$ from $\mathcal{N}(12)$ via Eq. (6.13) will consequently be less accurate than the direct computation of $S(q)$ by means of the FHNC equations. If we envision the calculation of an improved structure function via the CBF and/or RPA equations, we must take care that we do not lose much of the calculational accuracy due to approximations dictated by the complicated structure of $\mathcal{N}(12)$. In other words, we have to devise a systematic approximation scheme for the matrix elements of $\mathcal{N}(12)$ which preserves the relation (6.13) order by order. Relying on this argument, the adequate local approximation will be

$$z_{ph} z_{p'h'} \langle hh' | \mathcal{N}(12) | pp' \rangle \approx A^{-1} N(|\vec{p}-\vec{h}|)\delta(\vec{p}+\vec{p}'-\vec{h}-\vec{h}'), \quad N(q) = [S(q)-S_F(q)]/S_F^2(q) . \qquad (6.14)$$

Similar considerations are required for the interaction matrix elements. Here, the preservation of the optimization condition (5.19) and (6.7) provides the necessary guidance. Local approximations for the second particle-hole channel may be derived correspondingly. However, if we wish to have the same local approximation for both particle-hole channels of $\mathcal{W}(12)$ and $\mathcal{N}(12)$ (and, hence, for the irreducible vertex U), the relation (6.4) forces us to absorb the variational average field $u_v(k)$ (2.6) seen by a single particle in the local approximations for the matrix elements of $\mathcal{W}(12)$. Thus we arrive at

$$\begin{aligned} A_{ph,p'h'} \approx{} & (\hbar^2/2m)(\vec{p}^2-\vec{h}^2)\delta(\vec{p}-\vec{p}')\delta(\vec{h}-\vec{h}') \\ & + A^{-1}[W(|\vec{p}-\vec{h}|) + (\hbar^2/4m) \\ & \times (p^2+p'^2-h^2-h'^2) N(|\vec{p}-\vec{h}|)] \\ & \times \delta(\vec{p}+\vec{p}'-\vec{h}-\vec{h}') , \end{aligned} \qquad (6.15)$$

$$B_{ph,h'p'} \approx A^{-1}[\,W(|\vec{p}-\vec{h}\,|)+(\hbar^2/4m)\times(p^2+p'^2-h^2-h'^2)N(|\vec{p}-\vec{h}\,|)\,]\times\delta(\vec{p}+\vec{p}\,'-\vec{h}-\vec{h}\,')\,, \tag{6.16}$$

and

$$M_{ph,p'h'} \approx \delta(\vec{p}-\vec{p}\,')\delta(\vec{h}-\vec{h}\,')+A^{-1}N(|\vec{p}-\vec{h}\,|)\delta(\vec{p}+\vec{p}\,'-\vec{h}-\vec{h}\,')\,, \tag{6.17}$$

where

$$W(q)=[\Omega(q)-\hbar^2q^2S_F(q)N(q)/2m]/S_F^2(q)\,. \tag{6.18}$$

We note that the full single-particle spectrum may also be retained, this leads still to a closed-form, but less transparent representation of the Green's function. These studies will be necessary for actual numerical applications in nuclear many-body systems, where the variational single-particle energies give most of the effective mass. In ^{3}He, most of the effective mass is due to the CBF perturbation corrections.[19] Here, the variational single-particle energies are close to the noninteracting spectrum, and the neglect of the average field is a reasonable first approximation.

Owing to our averaging, the correlation matrix becomes local, and can be inverted explicitly. After some algebraic manipulations, we find

$$\begin{aligned} U_{ij}&=A^{-1}U(q)\,,\\ U(q)&=\frac{[W(q)-(\hbar^2q^2/4m)N^2(q)]}{[1+N(q)S_F(q)]^2}\\ &=\Omega(q)/S^2(q)\\ &\quad+(\hbar^2q^2/4m)[1/S^2(q)-1/S_F^2(q)]\,. \end{aligned} \tag{6.19}$$

We note that the manipulations are identical to the ones performed for the chain approximation, but here we included exchange effects in an average way. Equation (6.19) becomes particularly simple for the optimal $f(r)$. Then the $\Omega(q)$ term vanishes, and the averaged irreducible vertex may be determined from the structure function alone:

$$U_{\text{opt}}(q)=(\hbar^2q^2/4m)[1/S^2(q)-1/S_F^2(q)]\,. \tag{6.20}$$

The assumption of optimal correlation functions closes the circle: We have reconstructed a very familiar result, namely, the RPA connection between a weak, local interaction and the structure function $S(q)$ in the fluid-dynamic approximation[9,10] (or in the "uniform limit"[13]). However, the meaning of Eq. (6.20) is totally different. While (6.20) is usually employed to derive the static structure function from a weak, local vertex function, we have shown here that we can use, in turn, the structure function obtained in a preceding variational calculation to determine weak, local interaction.

It is clear that our identification (6.20) offers a wide field of applications of results obtained by variational ground-state calculations without having to derive a new, "variational" theory of the physical observable under considerations. For example, we may use this local interaction to calculate the density-response function, which assumes in this approximation the familiar form

$$\Pi^{-1}(q,\omega)=\Pi_0^{-1}(q,\omega)-U(q)\,, \tag{6.21}$$

or to calculate the self-energy,

$$\Sigma(k,E)=u(k)+i\int\frac{d^3q\,d\omega}{(2\pi)^4}G^0(\vec{k}-\vec{q},E-\hbar\omega)\times U^2(q)\Pi(q,\omega)\,. \tag{6.22}$$

$\Pi_0(q,\omega)$ is the Lindhard function.

The connection to the collective model discussed earlier is readily made through the additional approximation (6.12) for the Lindhard function, which reproduces Eq. (6.10). While (6.12) is exact for large frequencies, one does not expect that low-frequency excitations are adequately treated by the simple collective model (6.12).

A further application is the determination of CBF corrections to the (variational) static structure function, which may be calculated from the density-response function (6.21) via the dynamic structure factor

$$S(q,\omega)=\text{Im}\Pi(q,\omega)/\pi\,.$$

In the "fluid-dynamic" approximation we obtain

$$S_{\text{RPA}}^{-2}(q)=S^{-2}(q)+4m\Omega(q)/(\hbar^2q^2)\,. \tag{6.23}$$

As expected, the RPA does not give rise to a correction to the variational $S(q)$ in the case that the two-body correlations were optimized. At this juncture it is worth recalling the argument that the local approximations should be chosen such that the relations between the matrix elements of $\mathscr{N}(12)$, $\mathscr{W}(12)$, the (variational) static structure function and the optimization condition are preserved. Otherwise, it would not be clear if additional approximations for the relevant two-body operators introduce larger uncertainties in the variational $S(q)$ than what is gained by the improvement for the propagator through the RPA.

The local approximation discussed here is, in some respect, oversimplified in comparison with the usual sophistication of variational CBF calculations. It leaves out some dynamic screening effects[31] which appear to be important in the electron gas at metallic densities. Presumably, it will also not be adequate to study the *momentum dependence*[19] of the self-energy (and, hence, the effective mass) in liquid ^{3}He. On the other hand, it provides a straightforward microscopic foundation of theories of comparable structure.

Among these, the polarization potential model[11] for liquid ^{3}He appears to be one of the most successful ones. Clearly, $U(q)$ should be identified with f_q^s given by Aldrich and Pines. The comparison is shown in Fig. 4; the "theoretical" curve was obtained from an optimized variational calculation[19] for the HFDHE2 potential[32] at experimental equilibrium density. The agreement with the results of Aldrich and Pines is quite satisfactory. The reader is reminded that the calculated equilibrium density in a Jastrow variational calculation is approximately 25% below the experimental one. This has the effect that one is actually considering the system at finite pressure, which causes $U(q)$ to be pushed up at small values of q.

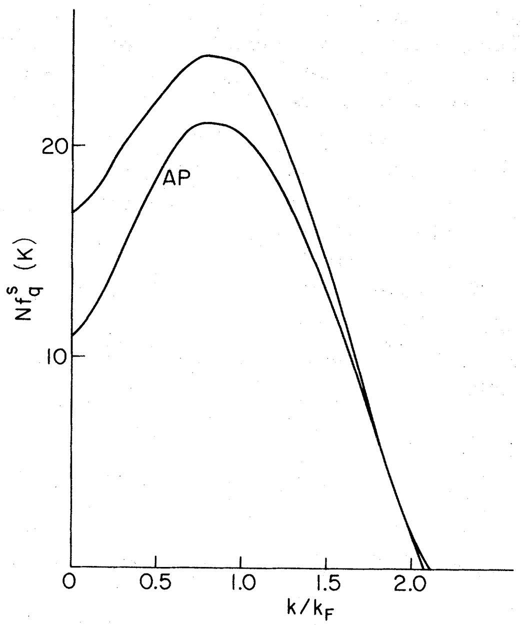

FIG. 4. Polarization potential Nf_q^s of Aldrich and Pines (AP) (Ref. 11) (curve labeled with AP) is compared with the variational result from Eq. (6.20) (unlabeled curve). The underlying variational $S(q)$ is taken from a ground-state calculation with the HFDHE2 potential of Aziz *et al.* (Ref. 32) at experimental equilibrium density.

Another case of interest is the determination of a local screening function[12] in the electron gas, which was recently[30] treated within the collective model. Unfortunately, the relations (6.18) and (6.19) are extremely sensitive functionals of $S(q)$, so that inconsistencies of a few percent result in substantial variations in $U(q)$. The direct evaluation of a local screening function from the irreducible vertex, without relying on the optimization condition, may provide a more robust algorithm, although the structure of the theory becomes somewhat obscured. One may also envision making a local approximation directly for the irreducible vertex $U(q)$. The present studies present only the general theory and the simplest applications. Future studies and numerical applications will have to solve some of the technical aspects.

VII. DISCUSSION

A number of formal and practical consequences of our investigations need to be mentioned. Our considerations have pointed out a way for the microscopic determination of the basic ingredients of the RPA and linear response theory and, because of their resemblance to phenomenological theories, offer a wide field of applications. In general terms, the road between the microscopic description of many-body systems and their macroscopic properties has been broadened.

It occurs to us that this road should be used in both directions. Coming from a microscopic theory for the irreducible vertex function, we are able to determine the general structure and estimate the type and relevance of nonlocalities. We may also use the theory to give microscopic foundation for more phenomenological approaches like the polarization potential model and to extend their field of application. An immediate application would be to use the pseudopotentials of Aldrich and Pines in Eq. (6.21) to determine the mass operator in ^{3}He.

Incidentally, our considerations also offer a way to attack problems occurring in the microscopic description of the most interesting terrestrial quantum liquids, liquid ^{3}He at zero temperature and the electron gas. In these systems, the convergence of cluster expansions for the relevant CBF quantities is usually poor, due to either the high density of the system or the long range of the correlations. The evaluation of four-point functions $\mathscr{N}(12)$ and $\mathscr{W}(12)$ remains limited naturally to the simplest, leading terms. The "separable" approximation used in Ref. 14 appears to be optimal within practical numerical effort. To confirm a sufficiently accurate treatment of the nonlocal contributions to the effective interaction, estimates for their size are called for.

Similarly, it is hard to confirm the convergence of the CBF perturbation expansion by numerically exhausting the array of tractable perturbation corrections. Again, solvable models will provide estimates for higher-order CBF perturbation corrections. We anticipate that the local approximations discussed in the preceding section can be used as a tool to attack both of the above-mentioned convergence problems: They give estimates for higher-order CBF corrections that are inaccessible to direct numerical evaluation. They may also be used as a starting point for perturbative expansions in terms of the nonlocality of the effective interactions. A number of formal and conceptual consequences of our analysis are worth pointing out at the end.

(1) Our result, that optimized Jastrow correlations lead to the Bijl-Feynman dispersion relation, is independent of the possible additional presence of discretely state-dependent or multiparticle correlations. These affect the result only because a better approximation for the ground-state wave function leads to a better static structure factor.

(2) We have encountered an example where the use of optimized Jastrow correlations actually leads to appreciable changes in the results. With the use of, e.g., Schiff-Verlet correlation functions, for liquid ^{3}He, the factor

$$[1+(4m/\hbar^2q^2)\Omega(q)]^{1/2}$$

causes maximum corrections of as much as 15% to the Bijl-Feynman dispersion relation, even though the optimization does not lead to a significant lowering of the energy expectation value nor to significant changes in $S(q)$ except at low momenta. In fact, after the influence of the optimization condition has been identified, it is a better approximation to the dispersion relation always to assume an optimized correlation function, even if the actual calculation has not been carried through.

(3) We have again encountered the significance of the "average-zero" condition for the effective interaction, which led to the Bijl-Feynman dispersion relation for the density mode. More generally, it allows in the local approximation of the effective interaction to be expressed in terms of the static structure function. One would like to carry the same analysis through for different (iso)spin channels. Unfortunately, none of the presently available state-dependent correlation operators leads to a generalization of (6.3) and (6.7) with an operator-weighted-average-zero property.

(4) We have discovered the intimate relationship between the effective interactions in CBF theory and the variational calculation of ground-state properties. The cancellation of the chain diagrams described in Sec. IV works correctly, of course, only if the chain diagrams are originally built into the effective interaction $\mathscr{W}(12)$. It goes without saying that the same argument applies in any finite order of the CBF expansion. Our investigations also show a way how to overcome this problem: Carrying out the RPA summations studied here, and using the irreducible vertex function, should largely eliminate the need to sum chain diagrams with state-dependent correlation operators.

(5) Our investigations seem to be only the beginning of a wide array of further explorations in the field of microscopic theories of quantum systems. Previous studies have considered either the variational wave functions or the CBF perturbation expansion independently. The present study of ring diagrams has revealed the first example of the intimate relationship between both. One expects that similar studies will be feasible for other familiar diagrammatical substructures of perturbation theory, like ladder diagrams or hole-line insertions.

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[1] J. W. Clark, The Many Body Problem, Jastrow Correlations Versus Breuckner Theory, Vol. 138 of *Lecture Notes in Physics,* edited by R. Guardiola and J. Ros (Springer, New York, 1981), p. 184. D. G. Sandler, N.-H. Kwong, J. W. Clark, and E. Krotscheck, Recent Progress in Many-Body Theories, Vol. 142 of *Lecture Notes in Physics,* edited by J. G. Zabolitzky, M. de Llano, M. Fortes and J. W. Clark (Springer, New York, 1981), p. 228.

[2] J. M. C. Chen, J. W. Clark, and D. G. Sandler, Z. Phys. A 305, 223 (1982).

[3] D. G. Sandler, E. Krotscheck, and J. W. Clark (unpublished).

[4] E. Krotscheck and J. W. Clark, Nucl. Phys. A328, 73 (1979).

[5] J. W. Clark, in *Progress in Particle and Nuclear Physics,* edited by D. H. Wilkinson (Pergamon, Oxford, 1979), Vol. 2.

[6] E. Krotscheck, H. Kümmel, and J. G. Zabolitzky, Phys. Rev. A 22, 1343 (1980).

[7] K. H. Sim, C.-W. Woo, and J. R. Buchler, Phys. Rev. A 2, 2024 (1970).

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

[9] G. Bertsch, Nucl. Phys. A249, 253 (1979).

[10] F. Lado, J. Chem. Phys. 47, 5369 (1967).

[11] C. H. Aldrich III and D. Pines, J. Low Temp. Phys. 32, 689 (1978).

[12] J. Hubbard, Proc. R. Soc. London, Ser. A 243, 336 (1957).

[13] E. Feenberg, *Theory of Quantum Fluids* (Academic, New York, 1969).

[14] E. Krotscheck, R. A. Smith, J. W. Clark, and R. M. Panoff, Phys. Rev. B 24, 6383 (1981).

[15] A. D. Jackson, E. Krotscheck, D. E. Meltzer, and R. A. Smith, Nucl. Phys. A386, 125 (1982).

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

[17] G. E. Brown, *Many Body Problems* (North-Holland, Amsterdam, 1969).

[18] M. R. Anastasio and G. E. Brown, Nucl. Phys. A285, 516 (1977).

[19] E. Krotscheck, R. A. Smith, and A. D. Jackson, Phys. Lett. 104B, 421 (1981); E. Krotscheck and R. A. Smith (unpublished).

[20] J. P. Jeukenne, A. Lejeune, and C. Mahaux, Phys. Rep. 25C, 83 (1976).

[21] B. L. Friman and E. M. Nyman, Nucl. Phys. A302, 365 (1978).

[22] J. W. Clark, L. Mead, E. Krotscheck, K. E. Kürten, and L. M. Ristig, Nucl. Phys. A328, 45 (1979).

[23] C.-W. Woo, Phys. Rev. 151, 138 (1966).

[24] H.-T. Tan and E. Feenberg, Phys. Rev. 176, 360 (1968).

[25] J. P. Blaizot and B. L. Friman, Nucl. Phys. A372, 69 (1981).

[26] N.-H. Kwong, Ph.D. thesis, California Institute of Technology, 1982 (unpublished).

[27] R. P. Feynman and M. Cohen, Phys. Rev. 102, 1189 (1956).

[28] C. E. Campbell, *Progress in Liquid Physics,* edited by C. A. Croxton (Wiley, New York, 1978), Chap. 6.

[29] J. Lindhard, K. Dan. Vidensk. Selsk. Mat.-Fys. Medd. 28, No. 8 (1954).

[30] L. J. Lantto, P. Pietilainen, and A. Kallio, Phys. Rev. B (in press); A. Kallio, V. Halonen, and P. Pietilainen (unpublished).

[31] F. Green, D. N. Lowy, and J. Szymanski, Phys. Rev. Lett. 48, 638 (1982).

[32] R. A. Aziz, V. P. S. Nain, J. C. Carley, W. L. Taylor, and G. T. McConville, J. Chem. Phys. 70, 4330 (1979).