Conserving dynamic theory for the electron gas

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We present a complete dynamic theory for the electron gas at high to metallic densities. The theory combines the dominant features of the shielded-interaction approximation and the T-matrix approximation within a formalism which ensures that the conservation sum rules are exactly satisfied. The theory is shown to be valid for large and small momentum transfers at high to metallic electron densities. It is argued that because conservation laws are maintained, the theory contains valid information about intermediate momentum transfers also. It is found that dynamic properties of the resulting polarization function and the dynamic structure factor cannot be adequately approximated by the well-known local-field construction, and consequently nonlocal effects are important for dynamic properties of the electron gas.

I. INTRODUCTION

This paper is the first in a series in which we present a new, comprehensive, and fully microscopic theory of the dynamics of the interacting electron gas. Brief reports of this work have already appeared.[1]

In this paper and paper II of this series we will propose a detailed and consistent explanation of recent measurements of properties of the metallic electron gas.

The present paper is divided as follows. In this Introduction we recall the striking behavior of the dynamic structure factor observed in metallic systems, and in this context we offer a critique of previous approaches to the dynamical correlation problem. Section II contains an analytical review of the general framework of Baym and Kadanoff,[2,3] which is used in Sec. III to formulate a complete microscopic model for the interacting electron gas. In Sec. IV our general model is cast in a form more suitable for practical calculation; there we base our analysis on the model's asymptotic behavior for certain ranges of particle density and momentum transfer. The concluding section V foreshadows, in addition to its imminent application to the dynamic structure factor, a series of future applications of the model to other aspects of electron-gas theory. This paper ends with an appendix outlining the derivation of the leading sum rules within the formalism.

Over the last ten years substantial experimental evidence[4–10] has been assembled, giving a strong indication that short-range correlations among the individual electrons of a metallic conduction band play a major role in the dynamics of the band. By "short-range" we mean any physical correlation mechanism other than the collective plasma oscillation, whose macroscopic Coulomb origin is well understood through the random-phase approximation (RPA).[11] These experiments, using inelastic scattering of x rays or of fast electrons off the conduction-band population, yield information on the linear-response behavior of the electron gas. The form factor extracted from the scattering data is identifiable with the dynamic structure factor $S(\vec{q},\omega)$ (Ref. 11) for the electron system, where $\vec{q}$ is the wave vector for the momentum transfer in scattering, and $\hbar\omega$ the energy lost by the probe.

For fixed values of $\vec{q}$ above the plasmon cutoff, mean-field theory and in particular RPA predicts a broad peak for $S(\vec{q},\omega)$ as a function of ω. This is in notable contrast with experimental measurements of the structure factor at large $\vec{q}$. The shape actually observed characteristically displays either a double peak or else a main peak with shoulders. In view of the persistence of these features over a range of materials [graphite, Be, Al, Li (Refs. 6–8)] differing significantly in band structure, and since the scale for the energy loss $\hbar\omega$ in most cases exceeds the typical band gaps (e.g., for Li, $\sim$20 eV as compared with $\sim$5 eV), one concludes that the deviation of the dynamic structure factor from its RPA estimate arises predominantly from Coulomb and exchange interactions among the conduction electrons.

In order to discuss in a unified way the existing approaches to this correlation problem we first recall a few elementary definitions in the dielectric-response description of the electron gas.

The macroscopic polarization function for the gas is[11]

$$\chi(\vec{q},\omega)=\frac{\chi^{sc}(\vec{q},\omega)}{1-V(\vec{q})\chi^{sc}(\vec{q},\omega)} . \quad (1)$$

Here $V(\vec{q})=4\pi e^2/q^2$ is the Fourier-transformed Coulomb potential and $\chi^{sc}(\vec{q},\omega)$ is the microscopic, or proper, polarization. In RPA, χ^{sc} is approximated by the leading term $\chi^{(0)}$ in its perturbation expansion in powers of V. The polarization function $\chi^{(0)}$ is that for the noninteracting gas.[12] It is convenient to discuss the short-range correlation part $(\chi^{sc}-\chi^{(0)})$ of the polarization function by formally defining an effective correction to $V(\vec{q})$ (the so-called local field):

$$g(\vec{q},\omega)=[V(\vec{q})]^{-1}\{[\chi^{sc}(\vec{q},\omega)]^{-1}-[\chi^{(0)}(\vec{q},\omega)]^{-1}\} . \quad (2)$$

Equation (1) can then be recast in the form

$$\chi(\vec{q},\omega)=\frac{\chi^{(0)}(\vec{q},\omega)}{1-[1-g(\vec{q},\omega)]V(\vec{q})\chi^{(0)}(\vec{q},\omega)} . \quad (3)$$

The local-field concept was an early offshoot of diagrammatic analysis; an example is Hubbard's exchange correc-

tion[13] to the large-momentum contribution in the integral for the ground-state correlation energy. Frequency-independent approximations to the local field have since been advanced by many authors, with notable success in describing static quantities (e.g., pair correlation function, ground-state energy, etc.).[14] For more comprehensive surveys of all aspects of electron-gas theory, the reader is referred to the recent literature.[14–16]

Correlation theories may be classified according to their treatment of the associated local-field correction. With some overlap, the classes are the following.

(a) Microscopic perturbation expansions.[13,17–23]

(b) Equation-of-motion schemes for density operators.[24–28]

(c) Methods assuming a model analytic structure for g or χ^{sc} as functions of ω.[29–31]

(d) Methods modifying $\chi^{(0)}$ and g (Refs. 32–34) in Eq. (3).

Since static approximations to the local field[17–19,24] only modify the static potential in the RPA, they lead to relaxation but no qualitative change in the shape of $S(\vec{q},\omega)$. We therefore now focus on existing dynamical approximations to the local field.

Among the theories of class (a), Hartree-Fock (HF) models have been intensively studied by Holas, Aravind, and Singwi[20] and by Dharma-wardana and Taylor.[21] These authors examine unscreened Coulomb correlations within a single excited particle-hole pair propagator; while the resulting local field contributes appreciably to the relaxation in $S(\vec{q},\omega)$, the shape remains RPA-like. Thus the local field here has an intrinsically weak ω dependence; this would seem to be a consequence of restricting intermediate states in χ^{sc} to one-particle plus one-hole excitations, thereby neglecting correlated multiple pairs. In contrast the recent calculation of Pajanne,[22] based on a resummation of the many-body expansion,[35] explicitly leaves out HF contributions and concentrates instead on the next-order terms, including a subset of all two-pair excitations. It is noteworthy that this parameter-free calculation of $S(\vec{q},\omega)$ shows some trend towards the experimental shape and certainly differs qualitatively from the RPA prediction, while satisfying particle conservation.

A different kind of microscopic correlation theory, the coupled-cluster expansion, has lately been applied to the electron gas by Bishop and Lührmann,[23] who formally resolve the full interacting ground-state wave function into a hierarchy of correlated clusters of particle-hole pairs. The full Schrödinger equation is replaced with a system of coupled equations for the cluster amplitudes. By truncating these equations at the two-pair level, the authors generate a model which in principle includes all possible one- and two-pair correlations, both long and short range, contributing to the ground state. The resulting calculation, while exhaustive, is necessarily limited to static properties and therefore sheds no light on dynamical effects, although it is suggested[23] that the same formalism can be generalized to describe excited states.

Among the theories of class (b), Brosens, Devreese, and Lemmens,[25] and Aravind, Holas, and Singwi,[26] also study HF correlations by solving approximate dynamical equations for the particle-hole propagator. Aravind *et al.*[26] and Utsumi and Ichimaru[27] allow for a frequency-dependent local-field factor by interpolating $g(\vec{q},\omega)$, in a sum-rule-preserving fashion, between its limits at small and large $(\vec{q},\omega)$. While these limits may be inferred from static and high-frequency sum rules,[28] the explicit form of $g(\vec{q},\omega)$ for intermediate ω remains unknown and must be guessed.[36] Apart from high-frequency tails the resulting dynamic structure factors fail to reproduce the observed peak structure.

Theories in class (c) use either the memory-function formalism (Mukhopadhyay and Sjölander,[29] and DeRaedt and DeRaedt[30]) or otherwise adopt a particular analytic continuation for $S(\vec{q},\omega)$ into the complex ω plane (Barnea[31]). Here again, a guess must eventually be made for some auxiliary function of ω whose detailed behavior cannot be established within the theory, in this case forcing the ultimate use of a parametrized fit to experiment.

Finally we discuss theories of class (d), which in turn has two subclasses. Firstly, there are phenomenological models (Gupta, Aravind, and Singwi[32]) based on the polarization-potential approach of Aldrich and Pines.[37] Secondly, there are the approximations of Mukhopadhyay, Kalia, and Singwi[33] and of Awa, Yasuhara, and Asahi,[34] which retain a static local field $g(\vec{q})$ in Eq. (3), while a quasiparticle analog χ^0 is substituted for the free electron-hole polarization $\chi^{(0)}$, with the on-shell single-particle energies modified by inclusion of self-energy terms.

The first approach is primarily tailored to studies of the collective-mode dispersion and can rigorously be related to an equation-of-motion formulation.[38] However, it shares the drawback of theories of classes (b) and (c) in having no access to the detailed behavior of $g(\vec{q},\omega)$ when $\vec{q}$ is above the plasmon cutoff.

In the second approach[33,34] the joint effect of finite quasiparticle lifetimes in χ^0 and short-ranged correlations in $g(\vec{q})$ is claimed to lead to a secondary peak in $S(\vec{q},\omega)$. We show in paper II that the secondary peak in these works arises solely from an incorrect forcing of the self-energy insertions onto the energy shell, when in fact they are off the energy shell. When the insertions are correctly placed off shell, the secondary peak is absent. The local-field correction $g(\vec{q})$, being static, cannot by itself introduce a secondary peak structure in $S(\vec{q},\omega)$. We refer the reader to paper II for a more detailed discussion of these points. The claim by Awa *et al.*[34] that sum-rule constraints (except for the f-sum rule) are not a useful guide to a reasonable dynamic theory and so need not be satisfied is unacceptable, given the intimate link with conservation principles.[11] In our judgement, approaches such as those of Mukhopadhyay *et al.*[33] or of Awa *et al.*[34] do not conclusively settle the origin of dynamical correlations in the electron gas. It is our contention that a term-by-term analysis of multipair correlations remains an essential and practicable task, despite its perceived complexity.

II. CONSERVING FORMALISM

We recall now the method of Baym and Kadanoff[2,3] (BK) to construct approximate polarization functions χ

and χ^{sc} for the strongly-correlated electron gas. The analysis is based on an expression for the ground-state energy of the interacting gas, given as a functional of the full single-particle propagator. Any approximation to this functional form, when constructed in accordance with BK, acts as a generator for both one- and two-body propagators in such a way that these are mutually consistent and satisfy the major conservation laws. A review of the sum-rule preserving properties of the related polarization functions may be found in the Appendix.

Section II A of this section defines our notation. In Sec. II B we analyze the structure of the ground-state energy functional. Section III C contains the derivation of integral equations for the polarization functions.

A. Notation

To condense the formal discussion we introduce a form of repeated-index tensor notation for coordinate- and spin-dependent functions. Repeated indices are normally summed over *except* when enclosed in parentheses. We illustrate the notation using the single-particle propagator $\underline{G}$ (see Appendix) as an example.

(i) The component $G(\vec{r}_\alpha,t_\alpha,\sigma_\alpha;\vec{r}_\beta,t_\beta,\sigma_\beta)$ of $\underline{G}$ is denoted by $G_{\alpha\beta}$, where space, time, and spin labels are symbolized as usual by $\vec{r}$, t, and σ. The free-particle propagator corresponding to $G_{\alpha\beta}$ is denoted by $G^{(0)}_{\alpha\beta}$.

(ii) The particle density $\rho(\vec{r}_\alpha,t_\alpha,\sigma_\alpha)$, which is given by $-iG(\vec{r}_\alpha,t_\alpha,\sigma_\alpha;\vec{r}_\alpha,t_\alpha^+,\sigma_\alpha)$, is written as $\rho_\alpha=-iG_{(\alpha\alpha^+)}$.

(iii) The total particle number

$$N=\sum_{\sigma_\alpha}\int dt_\alpha\,\delta(t_\alpha)\int d^3r_\alpha\,\rho_\alpha$$

is written as $N\equiv -i\delta(t_\alpha)G_{\alpha\alpha^+}$; the repeated index α implies the trace sum

$$\sum_{\sigma_\alpha}\int dt_\alpha\int d^3r_\alpha(\cdots)\,.$$

(iv) We denote the two-point unit tensor $\delta_{\sigma_\alpha\sigma_\beta}\delta^3(\vec{r}_\alpha-\vec{r}_\beta)\delta(t_\alpha-t_\beta)$ by $I_{\alpha\beta}$, so that, e.g., $I_{\alpha\beta}G_{\beta\gamma}=G_{\alpha\gamma}$.

(v) When indices are suppressed, a dot $(\cdot)$ indicates one contraction. Thus, e.g., $(\underline{A}\cdot\underline{B})_{\alpha\beta}=A_{\alpha\gamma}B_{\gamma\beta}$ and $\underline{A}:\underline{B}=A_{\alpha\gamma}B_{\gamma\alpha}$.

B. Ground-state energy functional

We turn now to the fundamental object of this discussion, the ground-state energy functional. From this we will derive the response functions for the interacting system. The usual derivation of the ground-state energy functional from the adiabatic theorem[39] results in an expression which is formally time dependent, and this makes the eventual setting up of a linear-response theory needlessly complicated. To avoid this we restore time symmetry to the energy functional by performing an additional time integration. In formal terms we suppose that the internal interaction is switched on adiabatically in the usual way with a time constant ϵ^{-1}; the internal interaction then acts at full strength over a time T, after which it is switched off adiabatically. We require that $T\gg\epsilon^{-1}\to\infty$, and this limit is implied in all the expressions to follow.

For the interacting system at equilibrium the shift in ground-state energy relative to its noninteracting value can be written in terms of the one-particle propagator $\underline{G}$ for the system[39,40]

$$E[\underline{G}]=\frac{1}{T}(\Phi[\underline{G}]-i\{\ln[(\underline{G}^{(0)})^{-1}\cdot\underline{G}]+\underline{I}-(\underline{G}^{(0)})^{-1}\cdot\underline{G}\}_{\alpha\alpha^+})\,. \tag{4}$$

Our expression for $E[\underline{G}]$ contains an extra time integral which is not included in the usual version.[39] This appears explicitly in the summation over the index α in the second contribution, and is implicit in $\Phi[\underline{G}]$. We normalize by dividing by T.

Equation (4) has the following meaning.

(a) The term $\{\ln[(\underline{G}^{(0)})^{-1}\cdot\underline{G})]\}_{\alpha\beta}$ can be interpreted as the formal matrix series

$$-\sum_{M=1}^{\infty}\{[\underline{I}-(\underline{G}^{(0)})^{-1}\cdot\underline{G}]^M\}_{\alpha\beta}/M\,,$$

or an appropriate analytic continuation of it.

(b) The functional $\Phi[\underline{G}]$ carries the information about particle correlations in the ground state, at all scales ranging from long-ranged collective modes to short-ranged Coulomb correlations and exchange; the structure of $\Phi[\underline{G}]$ is the most important element in the analysis.

The Φ functional, in which the bare Coulomb interaction $\underline{V}$ occurs explicitly, can be split into two parts. The first comprises the Hartree electrostatic contribution

$$\Phi^H[G]=\tfrac{1}{2}(\rho_\alpha-n_\alpha)V_{\alpha\beta}(\rho_\beta-n_\beta)\,, \tag{5}$$

where the matrix elements of the interaction are given by

$$V_{\alpha\beta}=\delta_{\sigma_\alpha\sigma_\beta}\delta(t_\alpha-t_\beta)\frac{e^2}{|\vec{r}_\alpha-\vec{r}_\beta|}\,, \tag{6}$$

and n_α in Eq. (5) is the number density of the rigid neutralizing background. The Hartree functional Φ^H vanishes identically for a homogeneous system at equilibrium.

The second part of Φ represents the exchange-correlation component of the ground-state energy, and we denote it by $\Phi^{sc}[\underline{G}]$. The form of this functional, which we will relate directly to the proper polarization function $\underline{\chi}^{sc}$, is

$$\Phi^{sc}[\underline{G}]=\sum_{N=1}^{\infty}\frac{i^2}{2N}G_{\alpha\beta}(\underline{\xi}_N[\underline{G}])_{\beta\beta',\alpha\alpha'}G_{\alpha'\beta'}\,, \tag{7}$$

where $\underline{\xi}_N[\underline{G}]$ is a two-body effective interaction. In terms of Feynman diagrams it consists of all irreducible skeleton graphs[39] in which N Coulomb interactions $\underline{V}$ are linked by $(2N-2)$ fully renormalized one-body propagators $\underline{G}$.

In the present context an approximate description of the electron gas is defined by choosing an approximate set of functionals $\underline{\xi}_N[\underline{G}]$. For the major conservation laws to hold, whether in the exact or in any approximate theory, the functionals $E[\underline{G}]$, $\Phi[\underline{G}]$, and $\underline{\xi}_N[\underline{G}]$ must satisfy four conditions.

(i) $\underline{\xi}_N[\underline{G}]$ must have the symmetries

$$(\xi_N[\underline{G}])_{\beta'\beta,\alpha'\alpha}=(\xi_N[\underline{G}])_{\beta\beta',\alpha\alpha'},$$

$$(\xi_N[\underline{G}^\dagger])^*_{\alpha\alpha',\beta\beta'}=(\xi_N[\underline{G}])_{\beta\beta',\alpha\alpha'}.$$

(ii) The structure of $\underline{G}:\underline{\xi}_N[\underline{G}]:\underline{G}$ must be such that removing any one of the $2N$ propagators $\underline{G}$ results in the same expression for $\underline{G}:\underline{\xi}_N[\underline{G}]$.

(iii) In the electron gas at equilibrium the ground-state functional $E[\underline{G}]$ must be a minimum when $\underline{G}$ is the solution to its equation of motion.

(iv) When an external perturbation acts on the system, $E[\underline{G}]$ becomes the expectation value of the total Hamiltonian with respect to the perturbed ground-state wave function.

In the Appendix we use these requirements on the energy functional (exact or approximate) to show how the conservation laws follow for the associated one- and two-body propagators.

There is a significant conceptual difference between the exact theory and all approximations framed in the language of BK; it lies in the interpretation of the four criteria for conservation. In the exact case, each condition is a consequence of the microscopic structure of the complete diagrammatic expansion. In the scheme of Baym and Kadanoff, these conditions serve as axioms for constructing both a functional $E[\underline{G}]$ and also the main objects, such as $\underline{G}$ and $\underline{\chi}^{sc}$, for which $E[\underline{G}]$ acts as a generator.

To see how the possible forms of these functions are constrained by properties (i)—(iv) above, we study the variation of $E[\underline{G}]$. The ground-state energy functional $E[\underline{G}]$ is approximated by choosing the exchange-correlation functional $\Phi^{sc}[\underline{G}]$ explicitly as some subset of the complete class of diagrams $\underline{G}:\underline{\xi}_N[\underline{G}]:\underline{G}$ appearing in the exact ground-state energy. Whatever the physical motivation may be for choosing this subset, one's choice must be made to satisfy (i) and (ii). In practice these rules place strong conditions on physically reasonable possibilities for Φ^{sc}, but in a purely abstract sense they are there to guarantee that the variation $\delta E[\underline{G}]$ is an exact, time-reversal invariant, differential.

The variation $\delta E[\underline{G}]$ is given by

$$\begin{aligned}\delta E[\underline{G}]&=\frac{1}{T}(\delta\Phi[\underline{G}]-i\delta\{\ln[(\underline{G}^{(0)})^{-1}\cdot\underline{G}]\\&\quad+\underline{I}-(\underline{G}^{(0)})^{-1}\cdot\underline{G}\}_{\alpha\alpha+})\\&=\frac{-i}{T}\left[i\frac{\delta\Phi}{\delta G_{\alpha\beta}}+(\underline{G}^{-1})_{\beta\alpha}-[(\underline{G}^{(0)})^{-1}]_{\beta\alpha}\right]\delta G_{\alpha\beta},\end{aligned}\tag{8}$$

where

$$\frac{\delta\Phi}{\delta G_{\alpha\beta}}=\frac{\delta\Phi^H}{\delta G_{\alpha\beta}}+\frac{\delta\Phi^{sc}}{\delta G_{\alpha\beta}}.$$

C. Correlation Functions

Now let an external perturbing potential U_α act on the system:

$$H_{ext}(t)=\delta(t-t_\alpha)U_\alpha I_{\beta\alpha+}\psi^\dagger_\beta\psi_\alpha.\tag{9}$$

From the Appendix we recall the exact equation of motion (A10) satisfied by the single-particle propagator $\underline{G}_U$ in the presence of the perturbation U and rewrite it as

$$\{[(\underline{G}^{(0)})^{-1}]_{\alpha\beta}-(\Sigma[\underline{G}_U])_{\alpha\beta}-U_{(\alpha)}I_{\beta(\alpha+)}\}(\underline{G}_U)_{\beta\gamma}=I_{\alpha\gamma}.\tag{10}$$

From (8) and the equation of motion we have, for $\underline{G}=\underline{G}_U$,

$$\delta E[\underline{G}]=-\frac{i}{T}\left[\left[i\frac{\delta\Phi}{\delta G_{\alpha\beta}}-(\Sigma[\underline{G}])_{\beta\alpha}\right]-U_\alpha I_{\beta\alpha+}\right]\delta G_{\alpha\beta}.\tag{11}$$

When $U=0$, rule (iii) demands that the term $i\delta\Phi/\delta\underline{G}-\underline{\Sigma}[\underline{G}]$ vanish identically. In the exact theory this is automatic because the self-energy $\underline{\Sigma}[\underline{G}]$ is given by the set of graphs corresponding precisely to $i\,\delta\Phi/\delta\underline{G}$. In an approximate theory, however, this identification must be built in by defining the one-particle self-energy $\underline{\Sigma}[\underline{G}]$ as just that set of diagrams given by $i\,\delta\Phi/\delta\underline{G}=-i\sum_N\underline{G}:\underline{\xi}_N$. To obtain the physical propagator $\underline{G}=\underline{G}_U$ within the approximation one must solve the equation of motion self-consistently, with a model self-energy defined from the approximate Φ. By substituting this evaluation of $\underline{G}$ in (11), we get

$$\delta E[\underline{G}_U]=\frac{i}{T}U_\alpha I_{\beta\alpha+}\delta G_{\alpha\beta}.\tag{12}$$

At this point we make contact with the linear-response polarization functions $\underline{\chi}$ and $\underline{\chi}^{sc}$, in their time-ordered guise. From Eq. (12) above there follows the weak-coupling result

$$\left.\frac{\delta E}{\delta U_\lambda}\right|_{U\to0}=-\frac{1}{T}U_\alpha\left.\frac{\delta\rho_\alpha}{\delta U_\lambda}\right|_{U\to0}=0.\tag{13}$$

We can then expand $E[\underline{G}_U]$ for small U:

$$E[\underline{G}_U]=E[\underline{G}_{U=0}]-\frac{1}{2T}U_\lambda U_\eta\chi_{\lambda\eta}+O(U^3).\tag{14}$$

This defines the susceptibility (in this case, the total polarization function) as

$$\chi_{\lambda\eta}=-T\left.\frac{\delta^2E}{\delta U_\lambda\,\delta U_\eta}\right|_{U\to0}.\tag{15}$$

For the second variation of $E[\underline{G}]$ we have on the one hand, from Eq. (8),

$$\delta^2 E[\underline{G}]=\frac{1}{T}\delta G_{\alpha'\beta'}\left[\frac{\delta^2\Phi}{\delta G_{\alpha'\beta'}\delta G_{\alpha\beta}}-i\frac{\delta(\underline{G}^{-1})_{\beta\alpha}}{\delta G_{\alpha'\beta'}}\right]\delta G_{\alpha\beta}+\frac{1}{T}\left[\frac{\delta\Phi}{\delta G_{\alpha\beta}}-i(\underline{G}^{-1})_{\beta\alpha}-[(\underline{G}^{(0)})^{-1}]_{\beta\alpha}\right]\delta^2 G_{\alpha\beta}$$

$$=\frac{1}{T}\delta G_{\alpha\beta}\{-(\Xi[\underline{G}])_{\beta\beta',\alpha\alpha'}+i(\underline{G}^{-1})_{\beta\alpha'}(\underline{G}^{-1})_{\beta'\alpha}\}\delta G_{\alpha'\beta'}+\frac{i}{T}U_\alpha I_{\beta\alpha^+}\delta^2 G_{\alpha\beta}\ , \tag{16}$$

where $\Xi[\underline{G}]=i^2\delta^2\Phi/\delta\underline{G}\,\delta\underline{G}$. The last line follows by using $\delta[(\underline{G}^{-1})\cdot\underline{G}]=\delta\underline{I}=0$ to derive $\delta(\underline{G}^{-1})_{\beta\alpha}/\delta G_{\alpha'\beta'}=-(\underline{G}^{-1})_{\beta\alpha'}(\underline{G}^{-1})_{\beta'\alpha}$, and by substituting for the coefficient of $\delta^2\underline{G}$ from Eqs. (8) and (12). On the other hand, from Eq. (12) we have

$$\delta^2 E[\underline{G}]=\frac{i}{T}\delta U_\alpha I_{\beta\alpha^+}\delta G_{\alpha\beta}+\frac{i}{T}U_\alpha I_{\beta\alpha^+}\delta^2 G_{\alpha\beta}\ . \tag{17}$$

The alternative forms (16) and (17) for $\delta^2 E[\underline{G}]$ are compatible if and only if[3]

$$[i(\underline{G}^{-1})_{\beta\alpha'}(\underline{G}^{-1})_{\beta'\alpha}-\Xi_{\beta\beta',\alpha\alpha'}]\delta G_{\alpha'\beta'}=\delta G_{\alpha'\beta'}\{i(\underline{G}^{-1})_{\beta'\alpha}(\underline{G}^{-1})_{\beta\alpha'}-\Xi_{\beta'\beta,\alpha'\alpha}\}$$
$$=i\,\delta U_{(\alpha)}I_{\beta(\alpha^+)}\ . \tag{18}$$

Taking the derivative $\delta/\delta U_\eta$, we obtain

$$i(\underline{G}^{-1})_{\beta\alpha'}(\underline{G}^{-1})_{\beta'\alpha}\frac{\delta G_{\alpha'\beta'}}{\delta U_\eta}-\Xi_{\beta\beta',\alpha\alpha'}\frac{\delta G_{\alpha'\beta'}}{\delta U_\eta}$$
$$=iI_{\alpha(\eta)}I_{\beta(\eta^+)}\ . \tag{19}$$

By contracting both sides with $-\underline{G}\underline{G}$ and carrying across the term in Ξ there follows the integral equation for the particle-hole vertex[41] defined by

$$(\Lambda[\underline{G}])_{\alpha\beta,\eta}\equiv -i\frac{\delta G_{\alpha\beta}}{\delta U_\eta}\ , \tag{20}$$

$$(\Lambda[\underline{G}])_{\alpha\beta,\eta}=(\Lambda^0[\underline{G}])_{\alpha\beta,\eta}+(-iG_{\alpha\nu}G_{\mu\beta})(\Xi[\underline{G}])_{\nu\beta',\mu\alpha'}$$
$$\times(\Lambda[\underline{G}])_{\alpha'\beta',\eta}\ , \tag{21}$$

where

$$(\Lambda^0[\underline{G}])_{\alpha\beta,\eta}=-iG_{\alpha(\eta)}G_{(\eta)\beta}\ .$$

Although Eq. (21) is valid beyond the weak-coupling limit $U\to 0$, it is this limit which determines the linear response. From Eq. (17) and the definition of the density $\rho_\alpha=-iG_{(\alpha\alpha^+)}$ we have

$$T\frac{\delta^2 E}{\delta U_\lambda\,\delta U_\eta}=-I_{\lambda\alpha}\frac{\delta\rho_\alpha}{\delta U_\eta}+O(U)\ , \tag{22}$$

i.e.,

$$-\chi_{\lambda\eta}=-\left.\frac{\delta\rho_\lambda}{\delta U_\eta}\right|_{U\to 0}\ . \tag{23}$$

This identifies $\chi_{\lambda\eta}$ of definition (15) as the time-ordered density response, whose dynamical evolution is determined by the solution to Eq. (21) for the particle-hole vertex.

Finally we apply Silin's method[39] to isolate the effects of exchange and correlation, which are intrinsically short-ranged, from the purely long-range effects associated with the Hartree contribution Φ^H to the energy functional. Introduce the screened perturbation potential $U^{\rm sc}$ through

$$U^{\rm sc}_{(\lambda)}I_{(\lambda)\mu}\equiv U_{(\lambda)}I_{(\lambda)\mu}+i\frac{\delta\Phi^H}{\delta G_{\mu\lambda}}$$
$$=I_{(\lambda)\mu}[U_{(\lambda)}+V_{\alpha(\lambda)}(\rho_\alpha-n_\alpha)]\ , \tag{24}$$

from (5).

Then

$$\frac{\delta}{\delta U_\beta}=\frac{\delta U^{\rm sc}_\lambda}{\delta U_\beta}\frac{\delta}{\delta U^{\rm sc}_\lambda}=\left[I_{\beta\lambda}+V_{\alpha\lambda}\frac{\delta\rho_\alpha}{\delta U_\beta}\right]\frac{\delta}{\delta U^{\rm sc}_\lambda}\ . \tag{25}$$

By defining the proper polarization $\underline{\chi}^{\rm sc}$ as

$$\chi^{\rm sc}_{\lambda\eta}=\left.\frac{\delta\rho_\lambda}{\delta U^{\rm sc}_\eta}\right|_{U\to 0}\ , \tag{26}$$

Eq. (25) gives the familiar relation between $\underline{\chi}$ and $\underline{\chi}^{\rm sc}$,

$$\chi_{\lambda\beta}=\chi^{\rm sc}_{\lambda\beta}+\chi^{\rm sc}_{\lambda\mu}V_{\alpha\mu}\chi_{\alpha\beta}\ . \tag{27}$$

The term $\underline{\chi}^{\rm sc}$ is the linear density response to the total potential $U^{\rm sc}$ at the microscopic level. Even when $\delta U^{\rm sc}/\delta U$ is singular, $\underline{\chi}^{\rm sc}$ remains well defined[39] since physically it is a short-ranged function which is insensitive to the long-range bulk oscillations signaled by the poles in $U^{\rm sc}$. It carries all the dynamical effects arising purely from exchange and short-range Coulomb correlations. The total polarization $\underline{\chi}$ may be obtained from Eq. (27) once $\underline{\chi}^{\rm sc}$ is known.

The proper polarization $\underline{\chi}^{\rm sc}$ can be calculated from an integral equation for the irreducible particle-hole vertex defined, in analogy with (20), as

$$(\Lambda^{\rm sc}[\underline{G}])_{\alpha\beta,\eta}\equiv -i\frac{\delta G_{\alpha\beta}}{\delta U^{\rm sc}_\eta}\ . \tag{28}$$

On adding the Hartree contribution $i^2(\delta^2\Phi^H/\delta\underline{G}\,\delta\underline{G}):\delta\underline{G}$ to both sides of Eq. (18) we obtain

$$[i(\underline{G}^{-1})_{\beta\alpha'}(\underline{G}^{-1})_{\beta'\alpha}-(\Xi^{sc}[\underline{G}])_{\beta\beta',\alpha\alpha'}]\delta G_{\alpha'\beta'}=i\delta U^{sc}_{(\alpha)}I_{\beta(\alpha)}$$
$$=\delta G_{\alpha'\beta'}\{i(\underline{G}^{-1})_{\beta'\alpha}(\underline{G}^{-1})_{\beta\alpha'}-(\Xi^{sc}[\underline{G}])_{\beta'\beta,\alpha'\alpha}\}\ . \tag{29}$$

The short-ranged interaction $\underline{\Xi}^{sc}[\underline{G}]$ is directly related to the exchange-correlation energy functional through

$$(\Xi^{sc}[\underline{G}])_{\beta\beta',\alpha\alpha'}\equiv i^2\frac{\delta^2\Phi^{sc}[\underline{G}]}{\delta G_{\alpha\beta}\delta G_{\alpha'\beta'}}\ . \tag{30}$$

In complete analogy with the derivation of Eq. (21), Eq. (29) gives

$$(\Lambda^{sc}[\underline{G}])_{\alpha\beta,\eta}=(\Lambda^0[\underline{G}])_{\alpha\beta,\eta}+(-iG_{\alpha\nu}G_{\mu\beta})(\Xi^{sc}[\underline{G}])_{\nu\beta',\mu\alpha'}(\Lambda^{sc}[\underline{G}])_{\alpha'\beta',\eta}\ . \tag{31}$$

Finally,

$$\chi^{sc}_{\lambda\eta}=-i\frac{\delta G_{(\lambda\lambda^+)}}{\delta U^{sc}_{\eta}}\bigg|_{U\to 0}$$
$$=-iG_{(\lambda\eta)}G_{(\eta\lambda)}+(\Lambda^0[\underline{G}])_{\mu\nu,\lambda}(\Xi^{sc}[\underline{G}])_{\nu\beta',\mu\alpha'}(\Lambda^{sc}[\underline{G}])_{\alpha'\beta',\eta}\ . \tag{32}$$

The structure of $\underline{\Xi}^{sc}[\underline{G}]$, the effective two-body interaction, requires comment. Consider a term $i^2(\underline{G}:\underline{\xi}_N[\underline{G}]:\underline{G})/2N$ appearing in $\Phi^{sc}[\underline{G}]$ [Eq. (7)]. Symbolically its contribution to $\underline{\Xi}^{sc}[\underline{G}]$ is

$$\frac{i^4}{2N}\frac{\delta^2(\underline{G}:\underline{\xi}_N[\underline{G}]:\underline{G})}{\delta\underline{G}\,\delta\underline{G}}=\underline{\xi}_N[\underline{G}]+\underline{G}:\frac{\delta\underline{\xi}_N}{\delta\underline{G}}\ . \tag{33}$$

Within the approximation defined by the choice of $\underline{\xi}_N$, we see that the derived two-body operator $\underline{\Xi}^{sc}$ clearly includes scattering effects beyond those directly given by the operators $\underline{\xi}_N$. If any of the terms on the right-hand side of Eq. (33) are omitted *ad hoc*, the resulting $\underline{\Xi}^{sc}$ will not in general lead to a conserving response function $\underline{\chi}^{sc}$.

We end this review of the formalism by summarizing the prescription for constructing $\underline{\chi}^{sc}$.

(a) By physical argument, select a particular subset of diagrams for the exchange-correlation energy functional $\Phi^{sc}[\underline{G}]$ so that the diagrams satisfy rules (i) and (ii) above.

(b) Use the model self-energy $(\Sigma[\underline{G}])_{\beta\alpha}=i\,\delta\Phi[\underline{G}]/\delta G_{\alpha\beta}$, obtained from $\Phi[\underline{G}]=\Phi^H[\underline{G}]+\Phi^{sc}[\underline{G}]$ by removing a single line, to solve the equation of motion Eq. (10) self-consistently for $\underline{G}$.

(c) Generate $(\Xi^{sc}[\underline{G}])_{\beta\beta',\alpha\alpha'}=i^2\,\delta^2\Phi^{sc}[\underline{G}]/\delta G_{\alpha\beta}\,\delta G_{\alpha'\beta'}$ by removing two lines $G_{\alpha\beta},G_{\alpha'\beta'}$ from the diagrams of $\Phi^{sc}[\underline{G}]$ in all possible combinations.

(d) Generate $\underline{\chi}^{sc}$ by solving the irreducible particle-hole vertex integral equation, Eq. (31), using $\underline{G}$ as defined in (b) and $\underline{\Xi}^{sc}[\underline{G}]$ as defined in (c).

III. MICROSCOPIC THEORY

We now proceed to the formulation of our own model for the electron gas. First we briefly enumerate the physical principles that we wish to incorporate.

(1) In the high-density limit the RPA is exact for all q and ω; microscopic correlations are negligible.

(2) At metallic densities and $q\gg k_F$ (k_F is the Fermi momentum), electron-electron pair correlations determine the local-field correction.[19]

(3) At metallic densities and $q\ll k_F$, residual electron-hole screening makes up the dominant correction to RPA.[41–43]

(4) At all densities and for all q and ω, it must be ensured that the conservation laws hold.

A. Model for the correlation-energy functional

The exchange-correlation-energy functional $\Phi^{sc}[\underline{G}]$ should incorporate the effects of screening from particle-hole polarization which dominate the correlations at low momentum transfer (corresponding to long range). At the other extreme, that of large momentum transfer (corresponding to short range), the functional $\Phi^{sc}[\underline{G}]$ should incorporate the effects of strong Coulomb scattering between particle pairs; the physical arguments for this are set out in Ref. 19.

Figure 1 shows the graphical structure of the simplest energy functional $\Phi^{sc}[\underline{G}]$ which correctly describes the long- and short-range behavior of the system. What is novel about our functional is that it combines the dominant features of the shielded interaction approximation[2] and the T-matrix approximation[2] within a unified scheme.

By inspection, the contributions to $\Phi^{sc}[\underline{G}]$ as defined in Fig. 1 satisfy the structural conditions (i) and (ii) outlined in Sec. II B. Consequently our model is conserving.

The shielded interaction approximation contains the principal effects of particle-hole screening which govern both the static and dynamic behavior of the electron gas at low momentum transfers. The need to fully account for screening at small wave vectors $\vec{q}$ is well documented.[41–44] Some important properties of the electron gas which are determined by the shielded interaction approximation in the high-density limit and $q\ll k_F$ include the following. In the low-frequency case: the Landau parameters and the compressibility.[41] In the dynamic case: the plasmon and quasiparticle dispersions and lifetimes,[42,43]

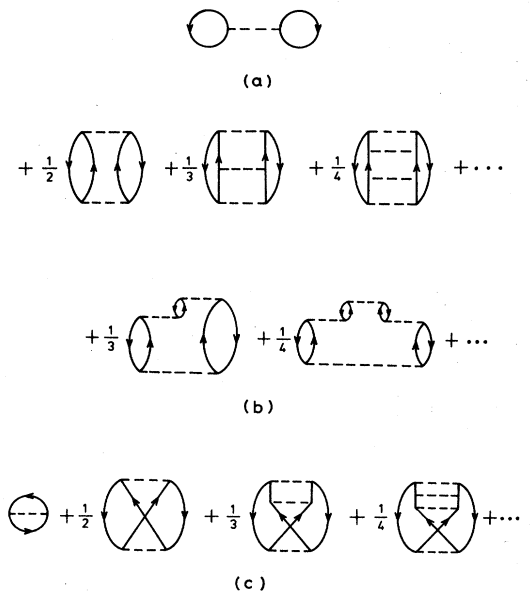

FIG. 1. Contributions to the ground-state energy functional $\Phi[\underline{G}]$ within the present model. The accompanying fractions are weighting factors. There is an implicit overall weighting factor of $\frac{1}{2}$. The solid lines indicate the self-consistent single-particle propagators $\underline{G}$ in the Feynman representation (no preferred time direction). (a) Hartree contribution. (b) Direct scattering ladder plus ring diagrams. (c) Hartree-Fock plus exchange ladder contribution.

and the high-frequency conductivity.[43]

The T-matrix approximation is formally identical to the Brueckner theory of nuclear matter.[45] For the Coulomb system the need to account for strong electron-pair scattering through the T matrix has been argued by Yasuhara[18] and Lowy and Brown[19] in the large-wave-vector limit $q \gg k_F$. The T-matrix approximation includes all pairwise correlations; it provides a physically consistent and realistic theory of the static pair correlation function at small separations[19] by accurately reproducing the relaxation of pair wave functions through short-range Coulomb repulsion, in both direct and exchange scattering. The importance of the intrinsic dynamical properties of the T-matrix approximation has only recently been demonstrated.[1]

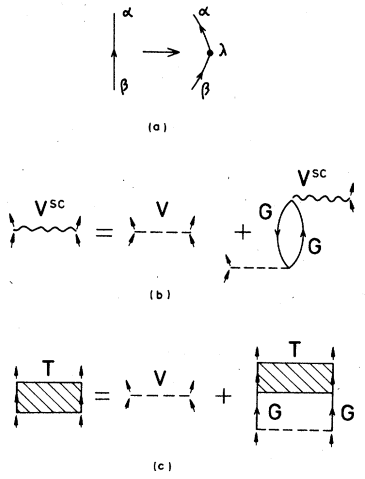

FIG. 2. (a) Insertion of an external vertex λ in the self-consistent single-particle propagator $G_{\alpha\beta}$ leads to the pair of propagators $G_{\alpha(\lambda)}G_{(\lambda)\beta}$. (b) Definition of $V^{sc}(\vec{q},\omega)$, the dynamic RPA interaction with self-consistent single-particle propagators. (c) Definition of the T matrix with self-consistent propagators. Note the pair of propagators $\underline{G}\,\underline{G}$ may be either particle-particle or hole-hole.

By combining the dominant characteristics of the shielded-interaction approximation and the T-matrix approximation, our scheme correctly recovers the physical properties of the electron gas in the two limits $q \ll k_F$ and $q \gg k_F$. Since our scheme is microscopic and strongly constrained by the conservation laws built into it, we expect to obtain some reliable information about the system's physical properties in the intermediate region of momentum transfer also.

B. Structure of χ^{sc}

Equation (32), when iterated, gives

$$\chi^{sc}_{\lambda\eta} \equiv \sum_{n=0}^{\infty} (\underline{\chi}^n)_{\lambda\eta}$$

$$= -iG_{(\lambda\eta)}G_{(\eta\lambda)} + (-iG_{\alpha(\lambda)}G_{(\lambda)\beta})(\Xi^{sc}[\underline{G}])_{\beta\beta',\alpha\alpha'}$$

$$\times(-iG_{\alpha'(\eta)}G_{(\eta)\beta'}) + \cdots , \qquad (34)$$

where we use $\underline{\chi}^n$ to denote the term of nth order in the effective two-body interaction $\underline{\Xi}^{sc}[\underline{G}]$ and where the truncated terms are of higher order in $\underline{\Xi}^{sc}$. In the second line we show the explicit forms of $\underline{\chi}^0$ and $\underline{\chi}^1$. (Note that, in a slightly different notation in Ref. 1, $\underline{\chi}^1$ is referred to as χ_2.)

We may use Eq. (32) to generate the entire set of contributions to the proper polarization $\underline{\chi}^{sc}$ once we have the full complement of diagrams for $\underline{\Xi}^{sc}$. Recalling that

$$(\Xi^{sc}[\underline{G}])_{\beta\beta',\alpha\alpha'} = i^2\delta^2\Phi^{sc}[\underline{G}]/\delta G_{\alpha\beta}\delta G_{\alpha'\beta'} ,$$

these diagrams may be generated systematically by removing two propagators $\underline{G}$ in all possible ways from the diagrams for $\Phi^{sc}[\underline{G}]$ in Figs. 1(b) and 1(c).

To construct the leading-order term in Eq. (34) we simply attach two pairs of lines $G_{\alpha(\lambda)}G_{(\lambda)\beta}$ and $G_{\alpha'(\eta)}G_{(\eta)\beta'}$ [Fig. 2(a)] to the free vertices in $(\Xi^{sc}[\underline{G}])_{\beta\beta',\alpha\alpha'}$. With appropriate definitions for the dynamic screened interaction $\underline{V}^{sc}$ and the T matrix $\underline{T}$ [see Figs. 2(b) and 2(c)], we represent the result schematically in Figs. 3 and 4, where Fig. 3 shows $(\chi^0)_{\lambda\eta}$ and Fig. 4 shows the contributions to $(\chi^1)_{\lambda\eta}$, grouped according to structural type. The form of $\underline{\Xi}^{sc}$ is implicitly shown by displaying $\underline{\chi}^1$.

IV. CALCULABILITY OF THE MODEL

We now discuss the practical evaluation of Eq. (32) for the proper polarization function $\underline{\chi}^{sc}$ within the model of the interacting electron gas. In Sec. IV A we study the

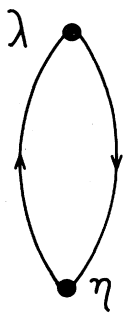

FIG. 3. The contribution $(\chi^0)_{\lambda\eta}$ to the proper polarization $(\chi^{sc})_{\lambda\eta}$. Note the single-particle propagators here are fully self-consistent, so that $(\chi^0)_{\lambda\eta}$ differs from the Lindhard function.

asymptotic behavior of $\underline{\chi}^{sc}$. In Sec. IV B we examine more closely the contributions to $\underline{\chi}^{sc}$ in the large-momentum limit and then introduce a general method for resolving $\underline{\chi}^{sc}$ into local and nonlocal contributions. The discussion ends with Sec. IV C, in which we propose a tractable approximation to Eq. (32) which can be applied for all momentum transfers at metallic densities.

A. Limiting behavior of $\underline{\chi}^{sc}$

For a uniform system it is appropriate to consider the space-time Fourier transform of $\underline{\chi}^{sc}$, $\chi^{sc}(\vec{q},\omega)$. We will study $\chi^{sc}(\vec{q},\omega)$ in three ranges of the parameters r_s and q. The separation parameter r_s is defined from the mean particle density n and the Bohr radius a_0 by $r_s=(4\pi n/3)^{-1/3}a_0^{-1}$. The Fermi energy for the interacting system is denoted by E_F. We adopt units such that $\hbar=m=1$, with momentum expressed as an inverse length and energies in units of momentum squared. Thus, for example, the free-particle Fermi energy is given as $E_F^{(0)}=k_F^2/2$ and the Coulomb coupling constant becomes $e^2=a_0^{-1}$.

1. High-density limit, $r_s \ll 1$

For all q in this limit, both the one-body self-energy $\underline{\Sigma}[\underline{G}]$ and the two-body effective interaction $\underline{\Xi}^{sc}[\underline{G}]$ are rapidly convergent series in powers of r_s. Their leading terms, linear in r_s, are, respectively, the HF self-energy and the HF particle-hole correlation. In this region, the truncation of Eq. (32) to second order in $\underline{\Xi}^{sc}[\underline{G}]$ retains all the contributions to $\underline{\chi}^{sc}$ to order r_s^2. We can therefore write

$$\chi^{sc}(\vec{q},\omega)=\chi^0(\vec{q},\omega)+\chi^1(\vec{q},\omega)+\chi^2(\vec{q},\omega)+O(r_s^3)\ , \qquad (35)$$

where χ^0, χ^1, and χ^2 are as defined in Eq. (34).

We note that for q much smaller than the plasmon cutoff wave vector q_c ($q_c\approx\sqrt{r_s}k_F/2$ for $r_s\ll 1$), the three terms on the right side of Eq. (35) to order r_s^2 are exactly equivalent to the high-density theory of DuBois.[46]

2. Small momenta

As indicated in the Appendix, our complete model contains a microscopic Landau quasiparticle description of the electron gas in the low-lying excitation region ($q\ll k_F$, $0<\omega\ll E_F$). Some standard manipulations[47] lead to a resummation of Eq. (32), enabling $\chi^{sc}(\vec{q},\omega)$ to be expressed in terms of the quasiparticle propagator $\tilde{G}$ corresponding to the one-body propagator $\underline{G}$. In the Landau limit Eq. (34) for $\chi^{sc}(\vec{q},\omega)$ becomes[47]

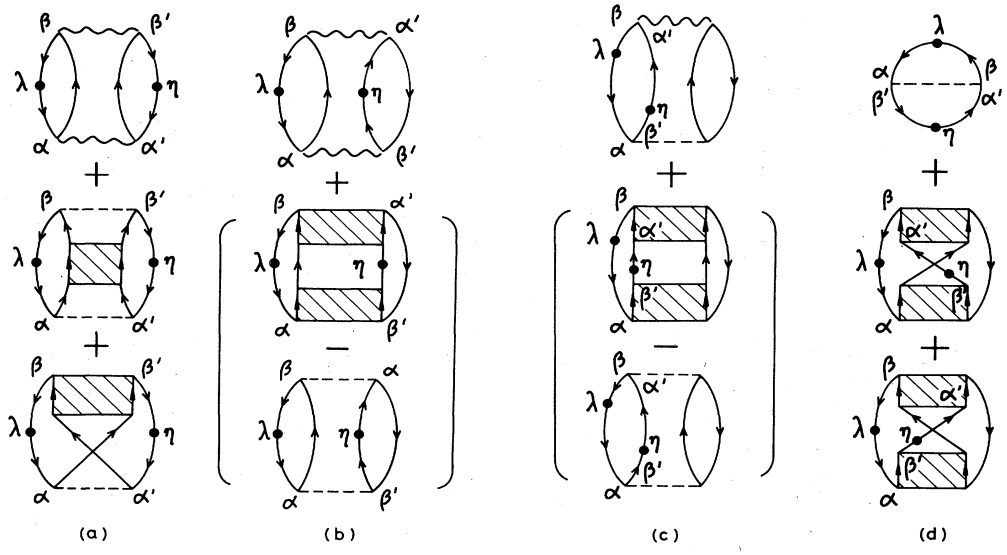

FIG. 4. The contributions $(\chi^1)_{\lambda\eta}$ to the proper polarization $(\chi^{sc})_{\lambda\eta}$ [see Eq. (34)]. (a) Contributions arising from particle-particle or hole-hole scattering. The wavy horizontal line denotes the dynamic screened interaction $\underline{V}^{sc}$, and the shaded block denotes the T-matrix $\underline{T}$, both of which are defined in Fig. 2. (b) Contributions to $(\chi^1)_{\lambda\eta}$ from particle-hole or hole-particle scattering. (c) Particle-hole one-pair contributions to $(\chi^1)_{\lambda\eta}$. (d) Hartree-Fock plus particle-hole one-pair exchange contributions to $(\chi^1)_{\lambda\eta}$.

$$\chi^{sc}(\vec{q},\omega)=Z_F^{-2}\sum_{n=0}^{\infty}\tilde{\chi}^n(\vec{q},\omega)\ , \tag{36}$$

where Z_F is the quasiparticle renormalization constant at the Fermi surface and each term $\tilde{\chi}^n(\vec{q},\omega)$ is structurally identical to $\chi^n(\vec{q},\omega)$ with the quasiparticle-quasihole propagator $(-i\tilde{G}\tilde{G})$ replacing $(-i\underline{G}\underline{G})$ between successive interactions Ξ^{sc}.

In the static limit $\omega=0$, $\chi^{sc}(\vec{q},\omega)$ in Eq. (36) is completely determined by the first two terms $\tilde{\chi}^0$ and $\tilde{\chi}^1$. Specifically, we have

$$\lim_{q\to 0}\chi^{sc}(\vec{q},0)=Z_F^{-2}\lim_{q\to 0}\frac{[\tilde{\chi}^0(\vec{q},0)]^2}{\tilde{\chi}^0(\vec{q},0)-\tilde{\chi}^1(\vec{q},0)}$$

$$\equiv\frac{\kappa}{\kappa^{(0)}}\chi^{(0)}(\vec{0},0)\ , \tag{37}$$

where the compressibilities κ and $\kappa^{(0)}$ are defined in the Appendix in connection with the compressibility sum rule (A3).

In the dynamic regime $qk_F\ll\omega\ll k_F^2$, the proper polarization is given to order $(qk_F/\omega)^4$ by

$$\chi^{sc}(\vec{q},\omega)=Z_F^{-2}\sum_{n=0}^{3}\tilde{\chi}^n(\vec{q},\omega)\ . \tag{38}$$

The coupling of successive quasiparticle-quasihole propagators by an interaction Ξ^{sc} occurs only through the inner product taken between quasihole momenta at the Fermi level. For this reason the calculation of Eq. (38), although tedious, needs no additional knowledge of $\underline{\Sigma}$ and $\underline{\Xi}$ at the Fermi level beyond that which is already available from a microscopic calculation of $\tilde{\chi}^0$ and $\tilde{\chi}^1$. The same consideration also applies at lower values of ω. On the other hand, terms higher than $\tilde{\chi}^3$ in Eq. (36) become increasingly important on approaching the quasiparticle excitation region $\omega\lesssim qk_F\ll k_F^2$.

3. Large momenta

When $q\gg k_F$, the most interesting behavior of $\chi^{sc}(q,\omega)$ as a function of ω occurs in the single-particle excitation region $q^2/2-qk_F\lesssim\omega\lesssim q^2/2+qk_F$. We can systematically expand $\chi^{sc}(\vec{q},\omega)$ in this region as a series in the small parameter (k_F/q). This can be shown by writing any particle-hole propagator $(-i\underline{G}\underline{G})$ appearing in $\chi^{sc}(\vec{q},\omega)$ as [Eq. (A34)]

$$P(\vec{k};\vec{q},\omega)=\int_{-\infty}^{E_F}d\omega'\int_{E_F}^{\infty}d\omega''\frac{A_{\vec{k}}(\omega')A_{\vec{q}+\vec{k}}(\omega'')}{\omega+\omega'-\omega''+i\eta}$$

$$+O\left[\frac{1}{\omega+\frac{1}{2}q^2}\right]\ . \tag{39}$$

The one-particle spectral density $A_{\vec{q}+\vec{k}}(\omega'')$ [Eq. (A33)] at large q behaves as $\delta(\omega''-\epsilon^{(0)}_{\vec{q}+\vec{k}})$, since the self-energy $\Sigma(\vec{q}+\vec{k},\omega'')$ for a fast particle becomes small compared to E_F as the scattering amplitude vanishes for $q\to\infty$. Hence in this limit

$$P(\vec{k};\vec{q},\omega)=\Theta^{>}_{\vec{q}+\vec{k}}\int_{-\infty}^{E_F}\frac{A_{\vec{k}}(\omega')}{\omega-\epsilon^{(0)}_{\vec{q}+\vec{k}}+\omega'+i\eta}d\omega'$$

$$=\Theta^{>}_{\vec{q}+\vec{k}}\left[\frac{n_{\vec{k}}}{\omega-\epsilon^{(0)}_{\vec{q}+\vec{k}}+\epsilon_{\vec{k}}+i\eta}+\int_{-\infty}^{E_F}A_{\vec{k}}(\omega')\left[\frac{1}{\omega-\epsilon^{(0)}_{\vec{q}+\vec{k}}+\omega'+i\eta}\right.\right.$$

$$\left.\left.-\frac{1}{\omega-\epsilon^{(0)}_{\vec{q}+\vec{k}}+\epsilon_{\vec{k}}+i\eta}\right]d\omega'\right]\ , \tag{40}$$

where we have introduced the usual Pauli protection operators $\Theta^{>}$, $\Theta^{<}$, the state occupation number[48] $n_{\vec{k}}\equiv\int_{-\infty}^{E_F}d\omega' A_{\vec{k}}(\omega')$, and the quasihole energy[48] $\epsilon_{\vec{k}}\equiv\epsilon^{(0)}_{\vec{k}}+\mathrm{Re}\Sigma(\vec{k},\epsilon_{\vec{k}})$. The leading term in Eq. (40) scales as $(1/qk_F)$ for energies ω in the range $|\omega-q^2/2|\lesssim qk_F$. The remainder, which includes incoherent as well as quasihole residual contributions, is of order $E_F/q^2k_F^2$.

see that to order k_F/q the dominant term of the proper polarization function is simply its leading term in Eq. (34):

$$\chi^{sc}(\vec{q},\omega)\to\chi^0(\vec{q},\omega)\to\sum_{\vec{k}}\frac{\Theta^{>}_{\vec{q}+\vec{k}}n_{\vec{k}}}{\omega-\epsilon^{(0)}_{\vec{q}+\vec{k}}+\epsilon_{\vec{k}}+i\eta}\ . \tag{41}$$

The nth-order iterate $\chi^n(\vec{q},\omega)$ of Eq. (34) for $\chi^{sc}(\vec{q},\omega)$ contains $n+1$ particle-hole propagators with the same structure as P in Eq. (40), and consequently $\chi^n(\vec{q},\omega)$ can at most scale as $(k_F/q)^{n+1}$ for energies in the single-particle excitation region, since $\Xi^{sc}[\underline{G}]$ is bounded for large q.

We conclude that to order $(k_F/q)^5$ one may approximate $\chi^{sc}(\vec{q},\omega)$ by

$$\chi^{sc}(\vec{q},\omega)\approx\sum_{n=0}^{4}\chi^n(\vec{q},\omega)\ . \tag{42}$$

B. Local and nonlocal effects in χ^{sc}

The form of Eq. (42) does not bring out the contrasting roles played by different contributions to $\Xi^{sc}[\underline{G}]$. The

two-body effective interaction is known to include multipair scattering components which sensitively depend on the value of the energy transfer ω, and other quasistatic components which may dominate the broad-scale relaxation effects in ω but do not have a fine-scale dependence on ω. As an important example, in Sec. I we cited the HF correlations which lead to significant but only broad-scale relaxation.

The quasistatic contributions can be approximated for large values of q by a local average over the momenta of the internal hole lines attached to $\underline{\Xi}^{\rm sc}[\underline{G}]$.[19] In contrast, it is straightforward to show that the contributions leading to the fine-scale dependence on ω in, for example, the response function $\chi^{\rm sc}(\vec{q},\omega)$, are not well approximated by a local average. Furthermore, such an average smooths out most of the interesting fine ω dependence.

The magnitude of the slowly-varying quasistatic components can be significantly larger than the fine-scale nonlocal contributions, and we are faced with a situation where in Eq. (42) there are local contributions in $\chi^4(\vec{q},\omega)$ which are of the same order as the interesting first nonlocal effects contained in $\chi^1(\vec{q},\omega)$.

We may unravel the fine-scale effects from the broad-scale effects by splitting $\underline{\Xi}^{\rm sc}[\underline{G}]$ into two parts,

$$\underline{\Xi}^{\rm sc}[\underline{G}]\equiv\underline{\Xi}^{\rm loc}[\underline{G}]+\underline{\Xi}^{\rm nl}[\underline{G}]\ , \tag{43}$$

in such a way that $\underline{\Xi}^{\rm loc}[\underline{G}]$ does not deviate much from its average over the internal hole states, $\langle\underline{\Xi}^{\rm loc}\rangle_{\rm loc}$, throughout the full range of the external energy ω. The remainder $\underline{\Xi}^{\rm nl}$ then contains the "nonlocal" part of $\underline{\Xi}^{\rm sc}$.

We can develop a simple measure of "nonlocality" as follows. Taking a particular term $\underline{\Gamma}[\underline{G}]$ in the interaction $\underline{\Xi}^{\rm sc}[\underline{G}]$, we can compare the contribution $(\underline{\Lambda}^0{:}\underline{\Gamma}{:}\underline{\Lambda}^0)$ to the first-order term $\underline{\chi}^1$ of the proper polarization with its localized approximation $(\underline{\chi}^0\langle\underline{\Gamma}\rangle_{\rm loc}\underline{\chi}^0)$. The deviation functional defined by

$$\sigma[\underline{\Gamma}]^2\equiv\int_0^\infty d\omega\frac{1}{qk_F}\left[\left|\frac{(\underline{\Lambda}^0{:}\underline{\Gamma}{:}\underline{\Lambda}^0)(\vec{q},\omega)}{\chi^0(\vec{q},\omega)^2\langle\underline{\Gamma}\rangle_{\rm loc}(\vec{q},\omega)}\right|-1\right]^2\ , \tag{44}$$

measures the deviation of $(\underline{\Lambda}^0{:}\underline{\Gamma}{:}\underline{\Lambda}^0)$ from locality, i.e., $\sigma[\underline{\Gamma}]$ is small if $\underline{\Gamma}$ is approximately local, and large if $\underline{\Gamma}$ is significantly nonlocal for some values of ω. The two terms $\underline{\Xi}^{\rm loc}$ and $\underline{\Xi}^{\rm nl}$ may be chosen to maximize the difference $\sigma[\underline{\Xi}^{\rm nl}]-\sigma[\underline{\Xi}^{\rm loc}]$.

It should be noted that $\underline{\Xi}^{\rm loc}$ itself is in general not a local function. The label "loc" here merely indicates that it is possible to approximate $\underline{\Xi}^{\rm loc}$ by a local average, $\underline{\Xi}^{\rm loc}\approx\langle\underline{\Xi}^{\rm loc}\rangle_{\rm loc}$.

A further condition on $\underline{\Xi}^{\rm nl}[\underline{G}]$ and $\underline{\Xi}^{\rm loc}[\underline{G}]$ is that they must have the same symmetry properties as the complete $\underline{\Xi}^{\rm sc}[\underline{G}]$. (This is automatic if $\underline{\Xi}^{\rm nl}[\underline{G}]$ is derivable from a subset—itself compatible with the Baym-Kadanoff prescription—of the ground-state diagrams for $\Phi^{\rm sc}[\underline{G}]$.) With this constraint it becomes possible to recast Eq. (32) for $\underline{\chi}^{\rm sc}$ into the form of an integral equation in which the dynamical interaction $\underline{\Xi}^{\rm nl}$ appears explicitly. First reexpress Eq. (29) in the form

$$\begin{aligned}[i(G^{-1})_{\beta\alpha'}(G^{-1})_{\beta'\alpha}-\Xi^{\rm sc}_{\beta\beta',\alpha\alpha'}]\Lambda^{\rm sc}_{\alpha'\beta',\eta}&=I_{\alpha(\eta)}I_{(\eta)\beta}\\&=\Lambda^{\rm sc}_{\alpha'\beta',\lambda}\{i(G^{-1})_{\beta'\alpha}(G^{-1})_{\beta\alpha'}-\Xi^{\rm sc}_{\beta'\beta,\alpha'\alpha}\}\ .\end{aligned} \tag{45}$$

Now define a new particle-hole vertex $\underline{\Lambda}^{\rm loc}[\underline{G}]$ as the solution to the symmetrical equation

$$\begin{aligned}[i(G^{-1})_{\beta\alpha'}(G^{-1})_{\beta'\alpha}-\Xi^{\rm loc}_{\beta\beta',\alpha\alpha'}]\Lambda^{\rm loc}_{\alpha'\beta',\eta}&=I_{\alpha(\eta)}I_{(\eta)\beta}\\&=\Lambda^{\rm loc}_{\alpha'\beta',\eta}\{i(G^{-1})_{\beta'\alpha}(G^{-1})_{\beta\alpha'}-\Xi^{\rm loc}_{\beta'\beta,\alpha'\alpha}\}\ .\end{aligned} \tag{46}$$

Subtracting Eq. (46) from Eq. (45) we obtain

$$[i(G^{-1})_{\beta\alpha'}(G^{-1})_{\beta'\alpha}-\Xi^{\rm loc}_{\beta\beta',\alpha\alpha'}](\Lambda^{\rm sc}-\Lambda^{\rm loc})_{\alpha'\beta',\eta}-\Xi^{\rm nl}_{\beta\beta',\alpha\alpha'}\Lambda^{\rm sc}_{\alpha'\beta',\eta}=0\ . \tag{47}$$

Multiplication on the left by $\Lambda^{\rm loc}_{\alpha\beta,\lambda}$ and use of the symmetry of Eq. (46) together transform Eq. (47) into

$$I_{\alpha'(\lambda)}I_{(\lambda)\beta'}(\Lambda^{\rm sc}-\Lambda^{\rm loc})_{\alpha'\beta',\eta}=\Lambda^{\rm loc}_{\alpha\beta,\lambda}\Xi^{\rm nl}_{\beta\beta',\alpha\alpha}\Lambda^{\rm sc}_{\alpha'\beta',\eta}\ , \tag{48}$$

and, on simplifying the left-hand side, we arrive at

$$\chi^{\rm sc}_{\lambda\eta}=\chi^{\rm loc}_{\lambda\eta}+\Lambda^{\rm loc}_{\alpha\beta,\lambda}(\Xi^{\rm nl}[\underline{G}])_{\beta\beta',\alpha\alpha'}\Lambda^{\rm sc}_{\alpha'\beta',\eta}\ . \tag{49}$$

The auxiliary polarization function $\underline{\chi}^{\rm loc}$ is itself determined explicitly by $\underline{\Xi}^{\rm loc}$ [Eq. (46)]:

$$\chi^{\rm loc}_{\lambda\eta}=\chi^0_{\lambda\eta}+\Lambda^0_{\alpha\beta,\lambda}(\Xi^{\rm loc}[\underline{G}])_{\beta\beta',\alpha\alpha'}\Lambda^{\rm loc}_{\alpha'\beta',\eta}\ . \tag{50}$$

Note that $\underline{\chi}^{\rm loc}$, which represents only a partial summation of correlation contributions, is not in general conserving because its one-body propagators still retain the full self-energy $\underline{\Sigma}[\underline{G}]$, and are therefore consistent with the full $\underline{\Xi}^{\rm sc}[\underline{G}]$ and $\underline{\chi}^{\rm sc}$ rather than with $\underline{\Xi}^{\rm loc}[\underline{G}]$ and $\underline{\chi}^{\rm loc}$.

At this stage we have formally separated the broad relaxation effects associated with $\underline{\Xi}^{\rm loc}$ from the fine-scale dynamical correlations contained in $\underline{\Xi}^{\rm nl}$. When $\underline{\Xi}^{\rm nl}$ is numerically small compared with $\underline{\Xi}^{\rm loc}$, Eq. (49) can be truncated to lowest order in $\underline{\Xi}^{\rm nl}$:

$$\chi^{\rm sc}_{\lambda\eta}\approx\chi^{\rm loc}_{\lambda\eta}+\Lambda^{\rm loc}_{\alpha\beta,\lambda}\Xi^{\rm nl}_{\beta\beta',\alpha\alpha'}\Lambda^{\rm loc}_{\alpha'\beta',\eta}\ . \tag{51}$$

In the high-density limit this truncation is valid at all momentum transfers; here $\underline{\Xi}^{\rm loc}$ is dominated by the HF exchange correlation, of order r_s, while the dynamical correlations are at most of order r_s^2.[46] Equation (51) therefore retains the first effects of dynamical correlations

as we take the system down from its high-density limit.

When q is large, $\chi^{sc}(\vec{q},\omega)$ as obtained through Eq. (49) can be expanded in powers of k_F/q to regain the approximation in Eq. (42). If, however, one similarly expands Eq. (51) in powers of (k_F/q), a simpler form of Eq. (42) results in which Ξ^{nl} appears only linearly. Performing the expansion of Eq. (51) we obtain

$$\underline{\chi}\approx\underline{\chi}^0+\underline{\chi}^{loc1}+\underline{\chi}^{loc2}+\underline{\chi}^{loc3}+\underline{\chi}^{loc4}+[\underline{\Delta}^0+\underline{\Delta}^0:\underline{\Xi}^{loc}:(-i\underline{G}\underline{G})]:\underline{\Xi}^{nl}:[\underline{\Delta}^0+(-i\underline{G}\underline{G}):\underline{\Xi}^{loc}:\underline{\Delta}^0]\ , \tag{52}$$

where $\underline{\chi}^{loc1}$ is the quasistatic part of $\underline{\chi}^1$, etc. This equation retains the effects of relaxation to order $(k_F/q)^5$ from iterating $\underline{\Delta}^{loc}$ in powers of $\underline{\Xi}^{loc}$, as well as the lowest-order dynamical effects resulting from pair-pair scattering in $\underline{\Xi}^{nl}$.

When q is small, the resolution of $\underline{\Xi}^{loc}[\underline{G}\,]$ into $\underline{\Xi}^{nl}[\underline{G}\,]$ and $\underline{\Xi}^{loc}[\underline{G}\,]$ becomes less clearcut. This is because *all* parts of the effective two-body interaction couple in similar fashion to their attached particle-hole propagators through the angular variable $\hat{k}_1\cdot\hat{k}_2$ (the hole momenta $\vec{k}_1$ and $\vec{k}_2$ are at the Fermi level). Hence $\sigma[\underline{\Xi}^{nl}]$ and $\sigma[\underline{\Xi}^{loc}]$ would be comparable for almost any choice of $\underline{\Xi}^{nl}$. In this case the appropriate analysis of $\underline{\chi}^{sc}$ is to be found in the Landau Fermi-liquid theory.

C. Calculation of χ^{sc} at metallic densities

When the momentum is comparable to k_F, the propagator $(-i\underline{G}\underline{G})$ is of order unity, and the expansion of Eq. (52) in powers of k_F/q is no longer valid. However at *high density* $\underline{\Xi}^{nl}$ is small compared with $\underline{\Xi}^{loc}$. We recall, for example, that the HF exchange correlation is of order r_s, while multiple pair correlations which include the nonlocal contributions are of order r_s^2 or smaller. In this case Eq. (51) is still valid to order $|\underline{\Xi}^{nl}[\underline{G}\,]/\underline{\Xi}^{loc}[\underline{G}\,]|$ even for $q\sim k_F$.

At *metallic densities* $\underline{\Xi}^{nl}$ will still be smaller than $\underline{\Xi}^{loc}$, so we may continue to approximate $\chi^{sc}(\vec{q},\omega)$ by Eq. (51) for all momenta $q\gtrsim k_F$. Since the starting point for these approximations is Eq. (32), which by construction obeys the sum rules exactly, we can determine the accuracy of our approximation for some particular density and momentum q by checking the f sum rule and the conductivity sum rule at the end of the calculation. To the extent that these sum rules remain approximately valid we may infer that Eq. (51) is a good approximation for Eq. (32).

For $q\lesssim k_F$ in the same density range we may use Eq. (38) for $\chi^{sc}(\vec{q},\omega)$ in the Landau limit. Note that at high densities Eqs. (38) and (51) have overlapping regions of validity since to order r_s^2 the two diagrammatic expansions in powers of $\underline{G}^{(0)}$ and $\underline{V}$ can be shown to be identical. Hence at moderate densities Eq. (38) can be expected to go smoothly over into Eq. (51) as the momentum q is increased.

The use of Eq. (51) permits us to separately calculate the slowly-varying quantities $\underline{\Delta}^{loc}$ and $\underline{\chi}^{loc}$ and then convolute them with the dynamical interaction $\underline{\Xi}^{nl}$. The problem of approximating the slowly-varying quantities and the problem of approximating intrinsically dynamical quantities such as $\underline{\Xi}^{nl}$ can be neatly separated, making our approach particularly flexible for practical applications.

V. CONCLUSION

In constructing this theory our primary purpose was to incorporate, as simply as possible, the dominant correlation mechanisms at large and small electron separations into a unified and microscopic theory, and to carry this out in such a way that conservation laws are satisfied even under dynamic conditions. The importance of maintaining the conservation laws has occasionally been overlooked in the literature, perhaps because they are almost automatically maintained provided one confines one's study to static electron-gas properties and then adopts one of the local-field-type or effective-interaction-type approaches. This task becomes much more formidable once one attempts to treat dynamic effects. As we have seen, dynamic and nonlocal effects cannot be overlooked under these conditions, and conservation laws are only satisfied because of subtle cancellations between terms which appear to be quite different.

We shall report elsewhere on some practical applications of our theory which include the following.[49]

(1) Calculation of the dynamic structure factor $S(q,\omega)$ at metallic densities and large momentum transfers, $q\gtrsim 1.5k_F$.

(2) Construction of a Landau Fermi-liquid theory at metallic densities for small q, and the calculation of quasiparticle dispersion and lifetimes, effective scattering parameters, compressibility, and plasmon dispersion and lifetimes.

(3) Calculation of the plasmon dispersion at intermediate $q\sim k_F$, and examination of the mixing of collective and two-particle modes by studying the crossover between large- and small-q effects in our theory.

(4) Calculation of transport properties in two-dimensional electron systems (e.g., silicon inversion layers), where electron-electron scattering significantly affects dynamical behavior at the low densities which can be attained in such systems.

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APPENDIX: CONSERVATION LAWS AND SUM RULES

In this appendix we have a twofold objective: firstly, to establish that our own model strictly maintains the lead-

ing sum rules; secondly, to bring together for easy reference some useful concepts which are needed for constructing any conserving microscopic theory but which are at present somewhat scattered through the literature.

We now trace the derivation of the leading sum rules in model theories of the Baym-Kadanoff (BK) type.[2,3] For the uniform electron gas, these sum rules are as follows: f sum,

$$-\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega\,\mathrm{Im}[\epsilon^{-1}(\vec{q},\omega)-1]=\omega_p^2\ , \tag{A1}$$

conductivity,

$$\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega\,\mathrm{Im}[\epsilon(\vec{q},\omega)-1]=\omega_p^2\ , \tag{A2}$$

compressibility,

$$\lim_{q\to 0}\left[q^2\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{1}{\omega}\mathrm{Im}[\epsilon(\vec{q},\omega)-1]\right]=\frac{\kappa}{\kappa(0)}q_{\mathrm{TF}}^2\ , \tag{A3}$$

and perfect screening,

$$\lim_{q\to 0}\left[-\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{1}{\omega}\mathrm{Im}[\epsilon^{-1}(\vec{q},\omega)-1]\right]=1\ . \tag{A4}$$

Here $\epsilon(\vec{q},\omega)$ is the retarded dielectric function for the uniform gas. The plasma energy ω_p is given by $\omega_p^2=4\pi e^2 n$, and the Thomas-Fermi screening wave vector q_{TF} is given by $q_{\mathrm{TF}}^2=3\omega_p^2/k_F^2$. We also introduce the static compressibility $\kappa=(n^2 dE_F/dn)^{-1}$ for the model interacting system, and its RPA counterpart $\kappa^{(0)}=(nk_F^2/3)^{-1}$.

In theories constructed according to the BK prescription (just as in the exact theory) the particle density, total energy, and momentum, and total angular momentum are strictly conserved. Since the BK formalism works directly with expectation values and does not require explicit knowledge of the ground-state wave function, all these observables are defined directly as functionals of the one-particle propagator $\underline{G}$ [see, e.g., Eq. (A5) below]. In the formalism the propagator $\underline{G}$ is obtained as the self-consistent solution to the one-particle equation of motion and its adjoint. The form of the collision term in both equations is determined from the energy functional $\Phi[\underline{G}]$ for the model.

We will concentrate on the law of conservation of particles, from which follow the sum rules (A1)–(A4). The remaining conservation laws can be derived in a similar way to particle conservation. Our first objective is to obtain, within the BK framework, the equation of continuity which relates the particle density ρ_λ and current $\vec{J}_\lambda$. For the model density-current four vector $(\rho,\vec{J})_\lambda$ we adopt the natural definition, in terms of the model single-particle propagator $\underline{G}$ at equilibrium:

$$(\rho_\lambda,\vec{J}_\lambda)\equiv\left[-iG_{(\lambda\lambda+)},\ \frac{\vec{\nabla}_{(\lambda)}-\vec{\nabla}_{(\mu)}}{2i}(-iG_{(\lambda\mu)})_{\mu\to\lambda+}\right], \tag{A5}$$

where $\vec{\nabla}_\alpha$ denotes the gradient operator $\partial/\partial\vec{r}_\alpha$.

In the exact theory the equation of motion for $\underline{G}$ and its adjoint take their form from the evolution equations of the field operators $\psi(\vec{r},t;\sigma)$ and $\psi^\dagger(\vec{r},t;\sigma)$. The system Hamiltonian is

$$H(t)=\delta(t-t_\alpha)[\psi_\alpha^\dagger\epsilon_\alpha\psi_\alpha+\tfrac{1}{2}V_{\alpha\beta}(\psi_\beta^\dagger\psi_\alpha^\dagger\psi_\alpha\psi_\beta-2n_\beta\psi_\alpha^\dagger\psi_\alpha+n_\alpha n_\beta)]\ , \tag{A6}$$

where ϵ_α is the single-particle energy, consisting of the kinetic term $-\frac{1}{2}\nabla_\alpha^2$ plus a static external one-body potential $\mathscr{V}(\vec{r}_\alpha)$; $V_{\alpha\beta}$ is the two-particle interaction as defined, for example, in Eq. (6), and n_α is the neutralizing background density introduced in Eq. (5). For a uniform system $\mathscr{V}(\vec{r}_\alpha)$ is equal to zero and n_α is the mean particle density n. The perturbation Hamiltonian is

$$H_{\mathrm{ext}}(t)=\delta(t-t_\alpha)I_{\alpha\beta}\left[\phi_\alpha+\vec{A}_\alpha\cdot\frac{\vec{\nabla}_\alpha-\vec{\nabla}_\beta}{2i}\right]\psi_\beta^\dagger\psi_\alpha$$

$$\equiv\delta(t-t_\alpha)I_{\alpha\beta}U_{\alpha\beta}\psi_\beta^\dagger\psi_\alpha\ , \tag{A7}$$

where $(\phi_\alpha,\vec{A}_\alpha)\equiv(\phi(\vec{r}_\alpha,t_\alpha),\ \vec{A}(\vec{r}_\alpha,t_\alpha))$ is a real four-vector potential. We differ here from Sec. II in employing a slightly more general nonlocal perturbation potential $U_{\alpha\beta}$. This affects the variational derivative $\delta/\delta\underline{U}$ but not $\delta/\delta\underline{G}$, and it therefore leaves unchanged the internal structural relationships among the functionals $\Phi[\underline{G}]$, $\underline{\Sigma}[\underline{G}]$, and $\underline{\Xi}[\underline{G}]$. Note that $U_{\alpha\beta}$ is an operator function of its space-time labels, and that care must be taken with the relative ordering of these labels.

The resulting evolution equations for the field operators are (more details can be found in Ref. 48):

$$i\frac{\partial}{\partial t_{(\lambda)}}\psi_{(\lambda)}=(\epsilon_{(\lambda)}-V_{(\lambda)\beta}n_\beta+V_{(\lambda)\beta}\psi_\beta^\dagger\psi_\beta)\psi_{(\lambda)}$$

$$+I_{\alpha\beta}U_{\alpha\beta}I_{\lambda\beta}\psi_\alpha\ , \tag{A8}$$

$$-i\frac{\partial}{\partial t_{(\mu)}}\psi_{(\mu)}^\dagger=(\epsilon_{(\mu)}-V_{\beta(\mu)}n_\beta+V_{\beta(\mu)}\psi_\beta^\dagger\psi_\beta)\psi_{(\mu)}^\dagger$$

$$+I_{\alpha\beta}U_{\alpha\beta}I_{\alpha\mu}\psi_\beta^\dagger\ . \tag{A9}$$

Using Eqs. (A8) and (A9) one can obtain the one-particle equation of motion and its adjoint for the exact Green's function:

$$\left[i\frac{\partial}{\partial t_{(\lambda)}}-\epsilon_{(\lambda)}\right](G_U)_{(\lambda)\mu}=I_{\lambda\mu}+(\Sigma[\underline{G}_U])_{\lambda\beta}(\underline{G}_U)_{\beta\mu}+I_{\alpha\beta}U_{\alpha\beta}I_{\lambda\beta}(\underline{G}_U)_{\alpha\mu}\ , \tag{A10}$$

$$\left[-i\frac{\partial}{\partial t_{(\mu)}}-\epsilon_{(\mu)}\right](G_U)_{\lambda(\mu)}=I_{\lambda\mu}+(G_U)_{\lambda\beta}(\Sigma[\underline{G}_U])_{\beta\mu}+I_{\alpha\beta}U_{\alpha\beta}I_{\alpha\mu}(G_U)_{\lambda\beta}\ . \tag{A11}$$

The exact $\underline{G}_U$ is defined as $(G_U)_{\lambda\mu} \equiv -i\langle T[\psi_\lambda \psi_\mu^\dagger]\rangle_U$, where T is the fermion time-ordering operator and the expectation $\langle \cdots \rangle_U$ is taken with respect to the perturbed exact ground state. The exact self-energy acting on $\underline{G}_U$ in Eqs. (A10) and (A11) is defined as

$$(\Sigma[\underline{G}_U])_{\alpha\beta} \equiv -\left\{(V_{(\alpha)\gamma} n_\gamma)(G_U)_{(\alpha)\eta} + iV_{(\alpha)\gamma}\langle T[\psi_\gamma^\dagger \psi_\gamma \psi_{(\alpha)} \psi_\eta^\dagger]\rangle_U\right\}(G_U^{-1})_{\eta\beta} . \tag{A12}$$

For convenience, we may split $\underline{\Sigma}[\underline{G}_U]$ into its Hartree and exchange-correlation parts:

$$(\Sigma^H[\underline{G}_U])_{\alpha\beta} \equiv \{V_{(\alpha)\gamma}[-i(G_U)_{\gamma\gamma^+} - n_\gamma](G_U)_{(\alpha)\eta}\}(G_U^{-1})_{\eta\beta},$$

$$(\Sigma^{sc}[\underline{G}_U])_{\alpha\beta} \equiv -i\{V_{(\alpha)\gamma}[\langle T[\psi_\gamma^\dagger \psi_\gamma \psi_{(\alpha)} \psi_\eta^\dagger]\rangle_U - (G_U)_{\gamma\gamma^+}(G_U)_{(\alpha)\eta}]\}(G_U^{-1})_{\eta\beta} .$$

At this point we recall the symmetry conditions (i) and (ii) for $\underline{\xi}_N[\underline{G}]$ from Sec. II B. These determine a functional form

$$\underline{\Sigma}[\underline{G}] = \underline{\Sigma}^H[\underline{G}] - i\sum_{N=1}^{\infty}(\underline{G}; \underline{\xi}_N[\underline{G}])$$

with the same space-time symmetry as the exact form (A12). When we replace the exact self-energy with its model counterpart in Eqs. (A10) and (A11), this symmetry ensures that the equation of motion and its adjoint both generate one and the same solution for the model propagator $\underline{G}_U$.

We may derive the equation of continuity within the model as follows. Subtract (A11) from (A10). Taking the limit $(\vec{r}_\mu, t_\mu; \sigma_\mu) \to (\vec{r}_\lambda, t_\lambda^+, \sigma_\lambda)$ the left-hand side becomes

$$\left[i\left[\frac{\partial}{\partial t_{(\lambda)}} + \frac{\partial}{\partial t_{(\mu)}}\right] - (\epsilon_{(\lambda)} - \epsilon_{(\mu)})\right](G_U)_{(\lambda\mu)}\Big|_{\mu\to\lambda^+} \to i\left[\frac{\partial}{\partial t_{(\lambda)}} + \frac{1}{i}\vec{\nabla}_{(\lambda)}\cdot\left[\frac{\vec{\nabla}(\lambda) - \vec{\nabla}(\mu)}{2}\right]\right](G_U)_{(\lambda\mu)}\Big|_{\mu\to\lambda^+} . \tag{A13}$$

Taking the same limit on the right-hand side, we get

$$[\Sigma_{(\lambda)\beta}(G_U)_{\beta(\lambda^+)} - (G_U)_{(\lambda)\beta}\Sigma_{\beta(\lambda^+)}] + I_{\alpha\beta}U_{\alpha\beta}[I_{(\lambda)\beta}(G_U)_{\alpha(\lambda^+)} - (G_U)_{(\lambda)\beta}I_{\alpha(\lambda^+)}]$$
$$\to \phi_\alpha[I_{(\lambda)\alpha}(G_U)_{\alpha(\lambda^+)} - (G_U)_{(\lambda)\alpha}I_{\alpha(\lambda^+)}] + I_{\alpha\beta}\vec{A}_\alpha\cdot\frac{\vec{\nabla}_\alpha - \vec{\nabla}_\beta}{2i}[I_{(\lambda)\beta}(G_U)_{\alpha(\lambda^+)} - (G_U)_{(\lambda)\beta}I_{\alpha(\lambda^+)}] . \tag{A14}$$

The collision term $(\underline{\Sigma}\cdot\underline{G}_U - \underline{G}_U\cdot\underline{\Sigma})_{(\lambda\lambda^+)}$ vanishes identically because of the symmetry of $\underline{\Sigma}$ and the uniqueness of $\underline{G}_U$.

Using the delta-function identities for any function $f(\beta)$,

$$I_{\alpha(\beta)}\vec{\nabla}_{(\beta)}f(\beta) = -f(\alpha)\vec{\nabla}_{(\beta)}I_{\alpha(\beta)}$$

and

$$\vec{\nabla}_{(\beta)}I_{\alpha(\beta)} = -\vec{\nabla}_{(\alpha)}I_{(\alpha)\beta} ,$$

we can reduce (A14) to the form

$$[\phi_{(\lambda)}(G_U)_{(\lambda\lambda^+)} - (G_U)_{(\lambda\lambda^+)}\phi_{(\lambda^+)}] - i\vec{\nabla}_{(\lambda)}\cdot[(G_U)_{(\lambda\lambda^+)}\vec{A}_\alpha I_{\alpha(\alpha)}] . \tag{A15}$$

The local term involving ϕ_λ vanishes.

Finally, equating the expressions (A13) and (A15), we obtain

$$\frac{\partial}{\partial t_{(\lambda)}}(G_U)_{(\lambda\lambda^+)} + \vec{\nabla}_{(\lambda)}\cdot\frac{\vec{\nabla}(\lambda) - \vec{\nabla}(\mu)}{2i}(G_U)_{(\lambda\mu)}\Big|_{\mu\to\lambda^+} = -\vec{\nabla}_{(\lambda)}\cdot[(G_U)_{(\lambda\lambda^+)}\vec{A}_\alpha I_{(\lambda\alpha)}] . \tag{A16}$$

Equation (A16), which is a direct consequence of choosing a model self-energy consistent with BK, forms the basis of all sum-rule derivations connected with particle conservation. In the weak-coupling limit $U \to 0$, the right-hand side of (A16) goes to zero, and using Eq. (A5) we obtain the equation of continuity within the model:

$$\frac{\partial \rho_{(\lambda)}}{\partial t_{(\lambda)}} + \vec{\nabla}_{(\lambda)}\cdot\vec{J}_{(\lambda)} = 0 . \tag{A17}$$

By taking the variation of both sides of Eq. (A16), we establish the conserving character of the time-ordered response functions. In Sec. II we saw that for the density response $\chi_{\lambda\eta} = (-i\delta G_{(\lambda\lambda^+)}/\delta U_\eta)_{U\to 0}$ [Eq. (23)]—where the $\underline{U}$ there was local. To study the current response we need the nonlocal functional derivative $-i\delta G_{\lambda\mu}/\delta U_{\alpha\beta}$. Two important properties of the nonlocal $\delta\underline{G}/\delta\underline{U}$ are[3]

$$\frac{\delta G_{\lambda\mu}}{\delta U_{\alpha\beta}}=\frac{\delta G_{\alpha\beta}}{\delta U_{\lambda\mu}} \tag{A18}$$

and

$$\chi_{\lambda\eta}=\lim_{\mu\to\lambda^+}\lim_{\alpha\to\eta^+}\left[-i\frac{\delta G_{\lambda\mu}}{\delta U_{\eta\alpha}}\right]\Bigg|_{U\to 0} . \tag{A19}$$

Similar results hold for the generalization of $\delta\underline{G}/\delta\underline{U}^{\rm sc}$ which leads to the proper polarization function [compare Eqs. (24) and (25) for the local $\underline{U}^{\rm sc}$ and $\delta/\delta\underline{U}^{\rm sc}$].

We introduce two sets of time-ordered response functions, or correlation functions:

(a) *density-density and current-density correlations,*

$$(\chi_{\rho\rho},\vec{\chi}_{J\rho})_{\lambda\eta}\equiv\frac{\delta U_{\alpha\beta}}{\delta\phi_\eta}\left[-i\frac{\delta G_{(\lambda\lambda^+)}}{\delta U_{\alpha\beta}}\ ,\ \frac{\vec{\nabla}_{(\lambda)}-\vec{\nabla}_{(\mu)}}{2i}\left[-i\frac{\delta G_{(\lambda\mu)}}{\delta U_{\alpha\beta}}\right]_{\mu\to\lambda^+}\right]_{U\to 0} , \tag{A20a}$$

and (b) *density-current and current-current correlations,*

$$(\vec{\chi}_{\rho J},\overleftrightarrow{\chi}_{JJ})_{\lambda\eta}\equiv\frac{\delta U_{\alpha\beta}}{\delta\vec{\mathrm{A}}_\eta}\left[-i\frac{\delta G_{(\lambda\lambda^+)}}{\delta U_{\alpha\beta}}\ ,\ \frac{\vec{\nabla}_{(\lambda)}-\vec{\nabla}_{(\mu)}}{2i}\left[-i\frac{\delta G_{(\lambda\mu)}}{\delta U_{\alpha\beta}}\right]_{\mu\to\lambda^+}\right]_{U\to 0} . \tag{A20b}$$

For the proper correlation functions there are identical definitions in which the differentials $\delta\underline{U}^{\rm sc}[\underline{I}\,\underline{U}^{\rm sc}\equiv\underline{I}\,\underline{U}+\underline{\Sigma}^H]$ and $\delta\phi^{\rm sc}[\phi^{\rm sc}\equiv\phi+\underline{V}\cdot(\underline{\rho}-\underline{n})]$ replace $\delta\underline{U}$ and $\delta\phi$ in Eqs. (A20). Since $\delta\underline{U}^{\rm sc}/\delta\vec{\mathrm{A}}=\delta\underline{U}/\delta\vec{\mathrm{A}}$, by varying Eq. (A16) independently with respect to ϕ, $\phi^{\rm sc}$, and $\vec{\mathrm{A}}$ we obtain two sets of exact relations for the correlations $\underline{\chi}$ and $\underline{\chi}^{\rm sc}$:

$$-\frac{\partial}{\partial t_{(\lambda)}}(\chi_{\rho\rho})_{(\lambda)\eta}+\vec{\nabla}_{(\lambda)}\cdot(\vec{\chi}_{J\rho})_{(\lambda)\eta}=0 , \tag{A21a}$$

$$\frac{\partial}{\partial t_{(\lambda)}}(\vec{\chi}_{\rho J})_{(\lambda)\eta}+\vec{\nabla}_{(\lambda)}\cdot(\overleftrightarrow{\chi}_{JJ})_{(\lambda)\eta}=-\rho_{(\lambda)}\vec{\nabla}_{(\lambda)}I_{(\lambda)\eta} , \tag{A21b}$$

and

$$\frac{\partial}{\partial t_{(\lambda)}}(\chi^{\rm sc}_{\rho\rho})_{(\lambda)\eta}+\vec{\nabla}_{(\lambda)}\cdot(\vec{\chi}^{\rm sc}_{J\rho})_{(\lambda\eta}=0 , \tag{A22a}$$

$$\frac{\partial}{\partial t_{(\lambda)}}(\vec{\chi}^{\rm sc}_{\rho J})_{(\lambda)\eta}+\vec{\nabla}_{(\lambda)}\cdot(\overleftrightarrow{\chi}^{\rm sc}_{JJ})_{(\lambda)\eta}=-\rho_{(\lambda)}\vec{\nabla}_{(\lambda)}I_{(\lambda)\eta} . \tag{A22b}$$

The equations (a) and (b) within each of these pairs are linked through the symmetries of the correlation functions which follow from (A18) and (A19). For example,

$$\{\chi_{\rho\rho},\ \vec{\chi}_{J\rho},\overleftrightarrow{\chi}_{JJ}\}_{\lambda\eta}=\{\chi_{\rho\rho},\vec{\chi}_{\rho J},\overleftrightarrow{\chi}_{JJ}\}_{\eta\lambda} . \tag{A23}$$

In the case of a homogeneous system the Fourier transforms of these functions reduce to a set of scalar functions of momentum q and energy ω. Thus the correlation functions become

$$\chi_{\rho\rho}(\vec{\mathrm{q}},\omega)=\chi_{\rho\rho}(-\vec{\mathrm{q}},-\omega)\equiv\chi(q,\omega) , \tag{A24}$$

$$\vec{\chi}_{J\rho}(\vec{\mathrm{q}},\omega)=\vec{\chi}_{\rho J}(-\vec{\mathrm{q}},-\omega)\equiv -i\vec{\mathrm{q}}\frac{1}{e^2}\sigma_{\rm ext}(q,\omega) , \tag{A25}$$

$$\overleftrightarrow{\chi}_{JJ}(\vec{\mathrm{q}},\omega)=\overleftrightarrow{\chi}_{JJ}(-\vec{\mathrm{q}},-\omega)\equiv\hat{q}\,\hat{q}\chi_L(q,\omega)+(\overleftrightarrow{I}-\hat{q}\,\hat{q})\chi_T(q,\omega) . \tag{A26}$$

We recognize the *density-density correlation function* $\chi(q,\omega)$, the *longitudinal conductivity* $\sigma_{\rm ext}(q,\omega)$ in response to the external electric field, and the longitudinal and transverse components of the *current-current correlation tensor,* $\chi_L(q,\omega)$ and $\chi_T(q,\omega)$ respectively. Similar definitions apply to the proper correlations.

We can now combine Eqs. (A21a) and (A21b) in Fourier space by using Eqs. (A24)—(A26) to obtain

$$\chi(q,\omega)=\frac{q^2}{\omega^2}\left[\frac{\omega_p^2}{4\pi e^2}+\chi_L(q,\omega)\right] . \tag{A27}$$

Similarly using Eqs. (A22a) and (A22b), we can link the proper correlation functions $\chi^{\rm sc}$ and $\chi^{\rm sc}_L$:

$$\chi^{\rm sc}(q,\omega)=\frac{q^2}{\omega^2}\left[\frac{\omega_p^2}{4\pi e^2}+\chi^{\rm sc}_L(q,\omega)\right] . \tag{A28}$$

The f sum and conductivity sum rules (A1) and (A2) require knowledge of the large ω limits of Eqs. (A27) and (A28). We show, by following the same general argument that applies to the exact theory, that for $|\omega|\to\infty$, $\chi^{\rm sc}_L(q,\omega)\sim\omega^{-2}$. A similar analysis applies to $\chi_L(q,\omega)$.

We first examine the lowest-order term χ^0_L in the expansion of $\chi^{\rm sc}_L$ in powers of the two-body effective interaction $\underline{\Xi}^{\rm sc}$. The term χ^0_L has the form[39]

$$\chi^0_L(q,\omega)=2\sum_{\vec{\mathrm{k}}}(\hat{q}\cdot\vec{\mathrm{k}}+\tfrac{1}{2}q)^2P(\vec{\mathrm{k}};\vec{\mathrm{q}},\omega) , \tag{A29}$$

where

$$P(\vec{\mathrm{k}};\vec{\mathrm{q}},\omega)\equiv\int_{-\infty}^{\infty}\frac{dk^0}{2\pi i}G(\vec{\mathrm{k}},k^0)G(\vec{\mathrm{q}}+\vec{\mathrm{k}},\omega+k^0) . \tag{A30}$$

$G(\vec{\mathrm{p}},p^0)$ is the solution of Eq. (A10), in Fourier space, for the unperturbed system:

$$[p^0-\epsilon_p^{(0)}-\Sigma^{\rm sc}(\vec{\mathrm{p}},p^0)]G(\vec{\mathrm{p}},p^0)=1\quad(\epsilon_p^{(0)}=\tfrac{1}{2}p^2) . \tag{A31}$$

Since $\underline{\Sigma}^{\rm sc}[\underline{G}\,]$ (and $\underline{\Xi}^{\rm sc}[\underline{G}\,]$) have been constructed to represent short-ranged exchange and correlation effects in

the electron gas, their Fourier coefficients are bounded in the limit of large energy and momentum transfers; if this were not the case then the model, although conserving, would not describe a normal Fermi system.

To perform the frequency integration in $P(\vec{k};\vec{q},\omega)$ we use the spectral representation[48] for $G(\vec{p},p^0)$,

$$G(\vec{p},p^0)=\int_{-\infty}^{E_F}d\omega'\frac{A_{\vec{p}}(\omega')}{p^0-\omega'-i\eta}+\int_{E_F}^{\infty}d\omega'\frac{A_{\vec{p}}(\omega')}{p^0-\omega'+i\eta}\quad(\eta=0^+),$$

where

$$A_{\vec{p}}(\omega')\equiv\frac{1}{\pi}|\,\mathrm{Im}G(\vec{p},\omega')\,|=\frac{1}{\pi}|\,G(\vec{p},\omega')\,|^2\,|\,\mathrm{Im}\Sigma(\vec{p},\omega')\,|\ . \tag{A33}$$

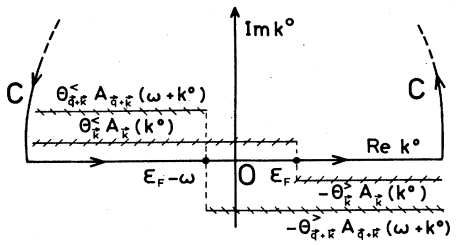

FIG. 5. The branch cut structure of the propagators G in the integrand for $P(\vec{k};\vec{q},\omega)$; see Eq. (A30).

The branch-cut structure of the propagators G in P is shown in Fig. 5. The integrand of P vanishes as $|k^0|^{-2}$ on the asymptotic circuit C, as do the discontinuities proportional to $A_{\vec{k}}(k^0)$ and $A_{\vec{q}+\vec{k}}(\omega+k^0)$ across the branch cuts. We need only include in P those contributions in which $G(\vec{k},k^0)$ and $G(\vec{q}+\vec{k},\omega+k^0)$ have branch cuts on opposite sides of the real k^0 axis. For the two possible contributions (particle-hole propagation) we obtain, using Eq. (A32),

$$P(\vec{k};\vec{q},\omega)=\int\frac{dk^0}{2\pi i}\left[\int_{-\infty}^{E_F}\frac{d\omega' A_{\vec{k}}(\omega')}{k^0-\omega'-i\eta}\int_{E_F}^{\infty}\frac{d\omega'' A_{\vec{q}+\vec{k}}(\omega'')}{k^0+\omega-\omega''+i\eta}+\int_{E_F}^{\infty}\frac{d\omega' A_{\vec{k}}(\omega')}{k^0-\omega'+i\eta}\int_{-\infty}^{E_F}\frac{d\omega'' A_{\vec{q}+\vec{k}}(\omega'')}{k^0+\omega-\omega'-i\eta}\right]$$

$$=\int_{-\infty}^{E_F}d\omega' A_{\vec{k}}(\omega')\int_{E_F}^{\infty}\frac{d\omega'' A_{\vec{q}+\vec{k}}(\omega'')}{\omega-\omega''+\omega'+i\eta}+\int_{-\infty}^{E_F}d\omega'' A_{\vec{q}+\vec{k}}(\omega'')\int_{E_F}^{\infty}\frac{d\omega' A_{\vec{k}}(\omega')}{-\omega+\omega''-\omega'+i\eta}\ . \tag{A34}$$

With the transformation $(\vec{k},\omega')\leftrightarrows(-\vec{q}-\vec{k},\omega'')$ in the second term of P in Eq. (A29), the function χ_L^0 becomes

$$\chi_L^0(q,\omega)=\sum_{\vec{k}}(\hat{q}\cdot\vec{k}+\tfrac{1}{2}q)^2\int_{-\infty}^{E_F}d\omega' A_{\vec{k}}(\omega')\int_{E_F}^{\infty}d\omega'' A_{\vec{q}+\vec{k}}(\omega'')\frac{2(\omega''-\omega')}{\omega^2-(\omega''-\omega'-i\eta)^2}\ . \tag{A35}$$

For fixed q and $|\omega|\to\infty$ we see that $\chi_L^0(q,\omega)$ vanishes as (ω^{-2}). Generalizing to terms $\chi_L^n(q,\omega)$ of higher order in the effective interaction Ξ^{sc}, it is easy to show that each P-like propagator linking successive interactions makes $\chi_L^n(q,\omega)$ vanish at least as ω^{-n-1}. It follows from Eq. (A28) that

$$\chi^{sc}(q,\omega)=\frac{q^2}{4\pi e^2}\frac{\omega_p^2}{\omega^2}+O(q^2\omega^{-4})\to\frac{1}{V(\vec{q})}\frac{\omega_p^2}{\omega^2}\quad\text{as}\ |\omega|\to\infty\ . \tag{A36}$$

To obtain the sum rule (A2) we now apply (a) the fluctuation-dissipation theorem[11] relating the retarded response functions to their time-ordered counterparts, and (b) the Kramers-Krönig causality relations[11,50] relating real and imaginary parts of the retarded response. In particular the fluctuation-dissipation theorem gives

$$\epsilon(\vec{q},\omega)-1=-V(\vec{q})[\Theta(\omega)\chi^{sc}(q,\omega)+\Theta(-\omega)\chi^{sc}(q,\omega)^*]\ , \tag{A37}$$

where $\Theta(\omega)$ is the step function. The Kramers-Kronig causality relations give ($\mathscr{P}$ denotes a principal-value integral):

$$\mathrm{Re}[\epsilon(\vec{q},\omega)-1]=-\mathscr{P}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\mathrm{Im}[\epsilon(\vec{q},\omega')-1]}{\omega-\omega'}\ . \tag{A38}$$

Equations (A36) and (A37) together determine the familiar high-frequency form of $\epsilon(q,\omega)$:

$$\epsilon(\vec{q},\omega)\to1-\frac{\omega_p^2}{\omega^2}\quad\text{as}\ |\omega|\to\infty\ . \tag{A39}$$

Expansion of the right-hand side of Eq. (38) in inverse powers of ω immediately yields the conductivity sum rule, Eq. (A2). The f sum rule, Eq. (A1), is obtained from a

similar analysis of the quantities χ_L, χ, and $\epsilon^{-1}(\vec{q},\omega)$ (since the long-ranged interaction $\underline{\Xi}[\underline{G}]=\underline{\Xi}^{sc}[\underline{G}]+\underline{IVI}$ is a bounded function of ω for finite values of $\vec{q}$).

We end this Appendix with the static sum rules (A3) and (A4). These results follow from the existence of a Landau quasiparticle description in the small $(\vec{q},\omega)$ limit for models of the BK type. A close analysis of this limit in such models can be found in the work of Geldart and Vosko.[41] Here we outline the main ideas.

In the small $(\vec{q},\omega)$ limit the dominant one-body excitations are quasiparticles and quasiholes near the Fermi surface. These modes are described by the poles of $\underline{G}$, as determined by $\underline{\Sigma}^{sc}[\underline{G}]$ near the Fermi level. The same one-body modes participate in the polarization excitations described by the two-body propagators $\underline{\Lambda}^{sc}$ and $\underline{\chi}^{sc}$, as determined by the two-body interaction $\underline{\Xi}^{sc}[\underline{G}]$ [Eqs. (27) and (28)]. Both excitations are linked by the fundamental relation $i\delta\underline{\Sigma}^{sc}[\underline{G}]/\delta\underline{G}\equiv\underline{\Xi}^{sc}[\underline{G}]$. When expressed through the Ward identities[39] at small $(\vec{q},\omega)$, this relation quantitatively connects quasiparticle parameters such as the Fermi energy E_F on the one hand, and polarization parameters such as the static dielectric function $\epsilon(\vec{q},0)$ on the other. We again stress the fact that the relation between $\underline{\Sigma}^{sc}$ and $\underline{\Xi}^{sc}$ is a theorem in the exact description while it serves as the prescription for constructing $\underline{\Xi}^{sc}$ in BK schemes. The automatic incorporation of the Ward identities is a hallmark the construction of Baym and Kadanoff.

The Ward identities imply the result

$$\chi^{sc}(\vec{q},0)\rightarrow\left[\frac{\frac{1}{3}k_F^2}{n\,dE_F/dn}\right]\chi^{(0)}(\vec{q},0)\ ,\quad \text{as } q\rightarrow 0 \qquad \text{(A40)}$$

so that

$$\epsilon(\vec{q},0)-1=-V(\vec{q})\chi^{sc}(\vec{q},0)$$
$$\rightarrow\frac{\kappa}{\kappa(0)}\frac{q_{TF}^2}{q^2},\quad \text{as } q\rightarrow 0\ . \qquad \text{(A41)}$$

The compressibility sum rule (A3) follows by using Eq. (A41) with the Kramers-Krönig relation (A38) when $\omega=0$.

From Eq. (A41) we also have that $\epsilon^{-1}(\vec{q},0)\sim q^2$ as $q\rightarrow 0$, and therefore

$$1-\epsilon^{-1}(\vec{q},0)\rightarrow 1,\quad \text{as } q\rightarrow 0\ . \qquad \text{(A42)}$$

The perfect screening sum rule (A4) follows from Eq. (A42) again by application of the Kramers-Krönig relation for $\epsilon^{-1}(\vec{q},\omega)-1$ at $\omega=0$.

This completes the discussion of the sum rules (A1)—(A4) for Baym-Kadanoff models in general, and our own model in particular. We hope that the techniques and results assembled in this appendix might encourage the even more widespread application of this powerful formalism.

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