Response functions for multicomponent plasmas. II. Velocity-average approximation and dynamical mean-field theory for strong coupling

Hong Zhang and G. Kalman
Department of Physics, Boston College, Chestnut Hill, Massachusetts 02167
(Received 11 March 1991)

We establish the multispecies generalization of the velocity-average formalism for the calculation of plasma response functions at arbitrary values of the coupling. We use a set of pseudopotentials rather than the bare Coulomb potential to represent the interaction between the particles in order to describe quantum effects due to the formation of bound states, diffraction, inner-shell-electron exchange, etc. The result is a self-consistent integral equation for the partial response functions. In the weak-coupling limit the calculation can be carried out and the outcome compared with the result of the exact perturbation-theoretical calculations: in the long-wavelength $k=0$ limit they are in total agreement.

PACS number(s): 52.25.Dg, 51.10.+y, 52.25.Mq, 05.20.Dd

I. INTRODUCTION

The determination of the frequency and wave-number-dependent dielectric-response function $\epsilon(\mathbf{k}\omega)$ has been one of the central problems of the physics of correlated Coulomb systems. The strength of the correlations can be characterized by the coupling parameter which for one-component plasma is $\Gamma=\beta Z^2e^2/a$ or $\gamma=\kappa^3/4\pi n$, where $\beta=(k_BT)^{-1}$, d is the interparticle distance $(4\pi/3)a^3n=1$, κ is Debye wave number, $\kappa=(4\pi Z^2e^2n\beta)^{1/2}$; the former is appropriate for strong, the latter for weak coupling; for a multicomponent plasma there is no unique definition, but a similar definition can be adopted with appropriate average $\overline{Z^2},\bar{n}$ values. For weak coupling ($\gamma<1$) perturbation theory is applicable and the preceding paper [1] (to be referred to as paper I) discusses the result of the systematic expansion of the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy to obtain the $O(\gamma)$ contribution to $\epsilon(\mathbf{k}\omega)$. This paper concerns itself with the strong-coupling ($\Gamma>1$) situation. In approaching this problem, where perturbation theory obviously does not apply, one has to observe the guiding principle that the correct treatment of the dynamical, frequency-dependent character of the correlations is crucially important in generating an $\epsilon(\mathbf{k}\omega)$ that can provide reasonably reliable information on collective mode dispersion, damping, mode-mode interaction, etc. A dynamical mean-field theory (DMFT) for the calculation of $\epsilon(\mathbf{k}\omega)$ for a binary value of the coupling was proposed by Golden, Kalman, and Silevitch [2] and worked out in detail by Golden and Kalman [2] for the one-component plasma (OCP). More recent developments of the theory are due to Tao and Kalman [3] and Kalman and Tao [4]. The major ingredients of the approach are the velocity-average approximation (VAA) and the application of the nonlinear (or quadratic) fluctuation-dissipation theorem (NLFDT) [5]. The role of the VAA is to reduce the dielectric function to become a functional of the quadratic response function. This result can be regarded either as a convenient jumping board for perturbation calculation when the coupling is weak, or as an intermediate stage, when the coupling is strong. This latter case requires a further approximation in order to obtain the quadratic response function as a functional of $\epsilon(\mathbf{k}\omega)$, generating in this way a self-consistency requirement, applicable without the use of perturbation technique. The original work of Golden and Kalman [2] and the more recent work of Tao and Kalman [3] deviate from each other in the way this second stage of the calculation is structured.

The DMFT based on the VAA scheme has a number of attractive features: it is exact in the static limit, it satisfies the high-frequency sum rule, and it is amenable to the application of a number of additional approximation techniques. In the cases of the OCP [6,7], successful work has been done in applying this theory for the analysis of the dielectric function and of the plasmon dispersion relation. The calculated dispersion relation is in good agreement with the exact result in the weak-coupling limit and for intermediate and strong coupling it reproduces the numerical simulation results of Hansen, McDonald, and Pollock [8]. The VAA formalism has been generalized for the case of two-component systems, the binary ionic mixture (BIM) (two ion species immersed in an inert neutralizing background) in particular, in the important and impressive work of Golden, Green, and Neilsen (GGN) [9]. GGN have derived a general formalism (about which more will be said below) and worked out applications to the plasmon dispersion both in the weak- and the strong-coupling limits.

The primary purpose of the present paper is to further generalize and develop the VAA formalism to multispecies plasmas and to reconsider its application to two component both electron-ion and ion-ion BIM systems [10]. The generalization and development of the theory incorporates four different elements. The first is the adoption of a set of generalized pseudopotentials [11–13], rather than the bare Coulomb potential, to represent the interaction between the particles. Pseudopotentials, in general, are introduced either to phenomenologically describe short-range quantum-mechanical effects within the classical formalism, or because the interacting "particles"

have a structure [13] that causes the short-range potential to deviate from its Coulomb form. A detailed discussion on the choice of pseudopotentials is given in paper I. However, the adoption of pseudopotentials gains more importance in the strong-coupling situation. This is due to the fact that a classical electron-ion plasma does not constitute a thermodynamically stable system. This lack of stability manifests itself, as is well known, in the divergence of the partition function and of the correlation functions, and in the possible unstable softening of the collective modes. Even though these problems do not show up either in the random-phase approximation (RPA), or in the $O(\gamma)$ perturbation calculation, they are expected to fatally affect calculations for strong coupling. Thus it is essential that a strong-coupling approximation be equipped with the correctly formulated pseudopotential formalism. The second line of development in the present paper consists of the adoption of the partial response function formalism as developed by Kalman and Golden [14]. This formalism has also been introduced in paper I, where its development is presented. The special importance of the partial response formalism [14,15] in the context of the VAA is that with its help the analysis of the multispecies problem can be brought into a one-to-one correspondence with that of a simple OCP. This is not a trivial simplification. Indeed, in the work of GGN [9], where this method was not followed, the complexity of the formalism becomes a major obstacle and a deterrent in any attempt to translate the formal results into a useful calculational algorithm. It is also a serious impediment to transparency and to the visualization of the physical implications of the formal steps. We believe that by espousing the method described we have successfully circumvented these problems. An additional benefit of the formalism is that the results are not restricted to binary systems, but hold for systems of an arbitrary number of components.

The third new element in our development is based upon the new results obtained in the analysis of the NLFDT [3,4]. By introducing the "response function of the second kind" [3,4,16–18], which relates perturbed two-point density correlations to the perturbing field, the derivation of the DMFT can be presented in a much more compact and physically meaningful way than before.

Finally, in this paper in deriving the self-consistency requirement from the VAA result we follow the recently formulated method of Tao and Kalman [3,6,17], rather than the dynamical superposition approximation employed in the earlier approaches both to the OCP [2,6] and to the BIM [9] problems. The method, briefly, consists of representing the quadratic response function in a universal mean-field-theory (UMFT) -like structure, where the screening function is postulated to be the product of the *linear* screening functions. We have discussed elsewhere [4] why we believe that this method is in many ways superior to the dynamical superposition approximation. Although the arguments of Ref. [4] have been directed at the OCP problem, they hold *a fortiori* for the multicomponent case. Indeed, as demonstrated by the work of GGN [9], the implementation of the dynamical superposition approximation for the BIM becomes a task much more involved, with outcomes more difficult to interpret, than the same procedure in the case of the OCP. Thus, the simplification brought about by the new approximation method is an additional major advantage in the multicomponent situation. A word of caution, however, is in order: a conclusive verdict on the relative merits (or demerits) of the new approach can be reached only on the basis of concrete calculations based on, but going beyond, the formal results; such calculations have to be contemplated as a major new undertaking and are not available at the present time.

The development of the ideas discussed so far is the subject of the first three sections of this paper. Section II contains the development of the VAA: the NLFDT enters as a relationship between the "response function of the second kind" [3,4,16–18] and the quadratic response function. As a result, the (linear) dielectric-response function appears as a functional of the quadratic response: this is the main result of the VAA and it constitutes the first stage of the derivation. Section III is devoted to the establishment of the self-consistency requirement by expressing the quadratic response function in terms of the linear one: the final product is a coupled set of integral equations that determines the dielectric-response function. The derivation is, of course, independent of the value of the coupling parameter, and therefore the result is valid for arbitrary coupling; in particular, it is expected to provide a good calculational algorithm for $\epsilon(\mathbf{k}\omega)$ in the case of strong coupling. The result at this point is formal in the sense that even though it provides a complete formalism, more work is needed to develop it into concrete numerical values for given physical systems.

The remainder of the paper is not concerned with either the results or the limitations of Sec. III. We return to the VAA formula of Sec. II and use it as a calculational tool to determine $\epsilon(\mathbf{k}\omega)$ for the weakly coupled ($\gamma \ll 1$) situation. In contrast to the strong-coupling problem, this can be done without any additional approximation. We establish a general formula for the partial response functions and $\epsilon(\mathbf{k}\omega)$, valid to first order in the coupling and for arbitrary $\mathbf{k}$ and ω values. Specializing to the two-component situation [electron-ion or ion-ion (BIM) plasmas], we can compare the result with the product of exact perturbation calculation to first order in the coupling of paper I (for earlier work see the work of Coste [19]). The comparison, whose details are given in the Appendices, shows both the structural difference between the VAA and the exact expressions and the relative simplicity of the former.

Further specializing to the important long-wavelength ($k=0$) properties of $\epsilon(\mathbf{k}\omega)$ that determine the dc conductivity and the plasmon frequency shift, we derive a compact formula that upon comparison with the corresponding $k=0$ exact perturbation expression of paper I exhibits a complete identity with the latter. Thus, with some hindsight, we can argue that in the uniform ($k=0$) system velocity correlations vanish and the VAA is exact, at least in the weak-coupling limit.

In view of the identity of the two results, we do not

pursue any further the analysis of $\epsilon(\mathbf{k}=0\omega)$: this is done in detail in the Refs. [10] and [20], which address the technique and results of the perturbation approach.

II. VAA APPROXIMATION

The theory of the partial response functions [14] is a central tool in the formalism of this paper. Section I in paper I summarizes it and the related definitions.

The velocity-average approximation is the major assumption in the dynamical mean-field theory of Golden and Kalman [2]. Under this approximation, the velocity correlations in the nonequilibrium two-body function are averaged out and replaced by the product of the one-particle velocity distributions. Since this approximation still preserves the dominant dynamic properties of the pair correlations, it is in several respects superior to the earlier static mean-field approximations [21,22]. The approximation satisfies the ω^{-4} (third frequency moment) sum-rule requirement [2,9,23] and in the static ($\omega=0$) limit, where the correlations between particles in velocity space vanish, the VAA is formally exact [2,19,24].

Our derivation starts from the first kinetic equation in the BBGKY hierarchy, which is given as

$$\left[\frac{\partial}{\partial t}+\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{x}}-\frac{1}{m_A}\frac{\partial\hat{\Phi}_A}{\partial \mathbf{x}}\cdot\frac{\partial}{\partial \mathbf{v}}\right]F_A(\mathbf{x},\mathbf{v};\mathbf{t}) =\frac{1}{m_A}\frac{\partial}{\partial \mathbf{v}}\cdot\int d^3v'd^3x'\frac{\partial\psi_{AC}(|\mathbf{x}-\mathbf{x}'|)}{\partial \mathbf{x}} \times G_{CA}(\mathbf{x}',\mathbf{v}';\mathbf{x},\mathbf{v};t)\ , \quad (1)$$

where $\psi_{AC}(|\mathbf{x}-\mathbf{x}'|)$ is the effective pair interaction potential between the particles of species A and C, F_A is the one-particle distribution function, G_{CA} is the two-particle distribution function, and $\hat{\Phi}_A$ is the perturbing external field (for notational convention, see paper I).

The VAA is introduced by setting

$$G_{CA}(\mathbf{x}',\mathbf{v}';\mathbf{x},\mathbf{v};t)\Longrightarrow f_C(\mathbf{x}',\mathbf{v};t)f_A(\mathbf{x},\mathbf{v};t) \times\int d^3v'd^3vG_{CA}(\mathbf{x}',\mathbf{v}';\mathbf{x},\mathbf{v};t)\ , \quad (2)$$

where

$$f_A(\mathbf{x},\mathbf{v};\mathbf{t})=F_A(\mathbf{x},\mathbf{v};\mathbf{t})/\langle n_A(\mathbf{x}t)\rangle\ . \quad (3)$$

$\langle\ \rangle$ stands for the ensemble average appropriate for the perturbed systems.

In Eq. (2) the velocity dependence in the two-body function is averaged over the velocity space and then compensated by the insertion of the one-body function. The approximation decouples the two-particle correlations in the velocity space, while it still preserves the correlation in the coordinate space.

The velocity-averaged two-particle distribution function is expressible in terms of the two-point density-density correlation function,

$$\int d^3v'd^3vG_{CA}(\mathbf{x}',\mathbf{v}';\mathbf{x},\mathbf{v};t)=\langle n_C(\mathbf{x}')n_A(\mathbf{x})\rangle(t) -\delta_{AC}\delta(\mathbf{x}-\mathbf{x}')\langle n_A(\mathbf{x}t)\rangle\ . \quad (4)$$

Substituting Eq. (4) into Eq. (1), one obtains

$$\left[\frac{\partial}{\partial t}+\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{x}}-\frac{1}{m_A}\frac{\partial\hat{\Phi}_A}{\partial \mathbf{x}}\cdot\frac{\partial}{\partial \mathbf{v}}\right]F_A(\mathbf{x},\mathbf{v};\mathbf{t}) =\frac{1}{m_A}\frac{\partial}{\partial \mathbf{v}}\cdot\int d\mathbf{x}'\frac{\partial\psi_{AC}(|\mathbf{x}-\mathbf{x}'|)}{\partial \mathbf{x}}f_A(\mathbf{x},\mathbf{v};\mathbf{t})[\langle n_C(\mathbf{x}')n_A(\mathbf{x})\rangle(t)-\delta_{AC}\delta(\mathbf{x}-\mathbf{x}')\langle n_A(\mathbf{x}t)\rangle]\ . \quad (5)$$

The last term in the equation represents the self-interaction of particles, and does not contribute to the integral.

We are interested in calculating the linear response of the system. Thus, linearizing Eq. (5) and taking Fourier transforms, we obtain

$$(\omega-\mathbf{k}\cdot\mathbf{v})F_A^{(1)}(\mathbf{k}\omega;\mathbf{v})+\frac{1}{m_A}\hat{\Phi}_A(\mathbf{k}\omega)\mathbf{k}\cdot\frac{\partial}{\partial \mathbf{v}}F_A^{(0)}(\mathbf{v}) =-\frac{1}{m_An_A}\frac{1}{V}\sum_{\mathbf{q}}\mathbf{q}\cdot\frac{\partial F_A^{(0)}(\mathbf{v})}{\partial \mathbf{v}}\psi_{AC}(q) \times\langle n_A(\mathbf{k}-\mathbf{q})n_C(\mathbf{q})\rangle^{(1)}(\omega)\ . \quad (6)$$

Here, the superscripts stand for the order in the external perturbation. The two-point density-density function can be separated into its irreducible (or proper) and singular parts:

$$\langle n_A(\mathbf{k}-\mathbf{q})n_C(\mathbf{q})\rangle^{(1)}(\omega)=\langle n_A(\mathbf{k}-\mathbf{q})n_C(\mathbf{q})\rangle^{(1)}_{\rm irr}(\omega) +\delta_{\mathbf{k}-\mathbf{q}}n_A\langle n_C(\mathbf{q})\rangle^{(1)}(\omega) +\delta_{\mathbf{q}}n_C\langle n_A(\mathbf{k})\rangle^{(1)}(\omega)\ , \quad (7)$$

and the singular-density term absorbed in a density response function. The irreducible part, on the other hand, can be formally expressed in terms of a "response function of the second kind" [16,18] (or "double-density function" [3,17]) $\hat{\Xi}_{ACD}(\mathbf{p},\mathbf{q};\omega)$:

$$\hat{\Xi}_{ACD}(\mathbf{p},\mathbf{q};\omega)\hat{\Phi}_D(\mathbf{k}\omega)=\langle n_A(\mathbf{p})n_C(\mathbf{q})\rangle^{(1)}_{\rm irr}(\omega)\ . \quad (8)$$

This latter, in turn, can be related [10] to the quadratic response function through the quadratic fluctuation-dissipation theorem [5,25]:

$$\hat{\Xi}_{ACD}(\mathbf{p},\mathbf{q};\omega) = -\frac{2}{\beta}\int d\mu\,\delta_-(\mu)[\hat{\chi}_{DAC}(\mathbf{p}\mu;\mathbf{q}\nu)+\hat{\chi}_{DAC}(\mathbf{p}\nu;\mathbf{q}\mu)]$$

$$\mathbf{k}=\mathbf{p}+\mathbf{q},\quad \omega=\mu+\nu\ . \tag{9}$$

The δ function is interpreted, as usual, through

$$\delta_-(\mu)=\lim_{o\to 0}\frac{-i}{2\pi}\frac{1}{\mu-io}=\tfrac{1}{2}\delta(\mu)-\frac{i}{2\pi}P\frac{1}{\mu}\ .$$

The OCP equivalent of the theorem was first derived by Golden and Kalman [2] in a different notation: the present formulation follows the works of Gu [16], Tao [17], and Tao and Kalman [3].

Substituting (7) and (8) into (6) and calculating the perturbed density, one finds

$$\langle n_A(\mathbf{k})\rangle^{(1)}(\omega)\equiv n_A(\mathbf{k}\omega)=\chi_A^{(0)}(\mathbf{k}\omega)\left[\delta_{AC}+\psi_{AB}(k)\hat{\chi}_{BC}(\mathbf{k}\omega)+\frac{1}{n_A V}\sum_{\mathbf{q}}\frac{\mathbf{q}\cdot\mathbf{k}}{k^2}\hat{\Xi}_{ABC}(\mathbf{p},\mathbf{q};\omega)\psi_{AB}(q)\right]\hat{\Phi}_C(\mathbf{k}\omega)\ ,$$

$$\mathbf{k}=\mathbf{p}+\mathbf{q},\quad \omega=\mu+\nu\ , \tag{10}$$

where $\chi_A^{(0)}$ is the linear density response function of the noninteracting gas; it is diagonal in species space:

$$\chi_A^{(0)}(\mathbf{k}\omega)=-\frac{1}{m_A}\int d^3v\frac{\mathbf{k}\cdot\dfrac{\partial F_A^{(0)}(v)}{\partial\mathbf{v}}}{\omega-\mathbf{k}\cdot\mathbf{v}}\ . \tag{11}$$

Comparing Eq. (10) with the relation for the density response function, Eq. (1), of paper I, one can derive, with some algebra, the relationship

$$\chi_{[AB]}(\mathbf{k}\omega)=\chi_A^{(0)}(\mathbf{k}\omega)[\delta_{AB}+v_{AB}(\mathbf{k}\omega)]\ . \tag{12}$$

The coupling function $v_{AB}(\mathbf{k}\omega)$ that embodies the correlational effects is now given by the expression

$$v_{AB}(\mathbf{k}\omega)=-\frac{2}{\beta n_A V}\sum_{\mathbf{q}}\psi_{AC}(q)\frac{\mathbf{q}\cdot\mathbf{k}}{k^2}\int d\mu\,\delta_-(\mu)[\chi_{BEF}(\mathbf{p}\mu;\mathbf{q}\nu)\eta_{EA}(\mathbf{p}\mu)\eta_{FC}(\mathbf{q}\nu)+\chi_{BEF}(\mathbf{p}\nu;\mathbf{q}\mu)\eta_{EA}(\mathbf{p}\nu)\eta_{FC}(\mathbf{q}\mu)]\ ,$$

$$\mathbf{p}=\mathbf{k}-\mathbf{q},\quad \nu=\omega-\mu\ . \tag{13}$$

The bracket notation $\chi_{[AB]}$ in the indices in (12) refers to the lack of manifest symmetry in the species indices A and B. Such a symmetry is required in view of the FDT than χ_{AB} must satisfy. Even though all the expressions obtained in concrete calculations performed for χ_{AB} on the basis of Eqs. (12) and (13) *do* obey the requisite symmetry, we have not been able to demonstrate that the structure of (13), in general, leads to a symmetric χ_{AB}. It is possible that the VAA may have a symmetry-breaking property. In order to maintain the symmetry of χ_{AB} even if this is the case, following GGN [9] we replace $\chi_{[AB]}$ by its symmetric projection:

$$\chi_{AB}=\tfrac{1}{2}(\chi_{[AB]}+\chi_{[BA]})\ . \tag{14}$$

Equation (13) is one of the central results of this paper. It generalizes the one-component result of Golden and Kalman [2] to multicomponent systems and recasts the multicomponent derivation of GGN [9] in the much more transparent and versatile language of the partial response functions. Our Eq. (13) can be shown to be equivalent to Eq. (41) of GGN, but GGN provide no calculational algorithm for the partial density response function χ_{AB}. Some further differences between Eq. (13) above and Eq. (41) of GGN are due to the slightly different definition of v_{AB} used by GGN: our definition is consistent with employing the matrix representation in species space.

Two particular limits of Eqs. (12)–(14) are of special interest. The first is the $\omega=0$ static limit. In this situation the result derived from (12) and (13) gives

$$\chi_{AB}(\mathbf{k}0)=\chi_A^{(0)}(\mathbf{k}0)\delta_{AB}+\delta\chi_{AB}(\mathbf{k}0)\ , \tag{15a}$$

$$\delta\chi_{AB}(\mathbf{k}0)=\frac{2}{k^2}\frac{1}{V}\sum_{\mathbf{q}}\mathbf{k}\cdot\mathbf{q}\varphi_{AC}(q)\chi_{BEF}(\mathbf{p}0;\mathbf{q}0)\times\eta_{EA}(\mathbf{p}0)\eta_{FC}(\mathbf{q}0)\ . \tag{15b}$$

In contrast to its $\omega\neq 0$ counterpart, (15) is *exact*: this follows from the general theorem that in the static limit the VAA is exact [2,19,24]. In Appendix B we explicitly show that (15) is indeed identical to a relationship derivable from the BGY hierarchy.

The other limit of interest is the one where $\omega\to\infty$. The coefficients of ω^{-2} and ω^{-4} in the high-frequency expansion of $\chi_{AB}(\mathbf{k}\omega)$, $\Lambda_{AB}^{(2)}(k)$ and $\Lambda_{AB}^{(4)}(k)$,

$$\Lambda_{AB}^{(2)}(k)=\frac{k^2 n_A}{m_A}\delta_{AB}\ , \tag{16a}$$

$$\Lambda^{(4)}_{AB}(k)=\frac{3k^4 n_A}{\beta m_A^2}\delta_{AB}+\frac{n_A}{m_A m_B}\sum_{\mathbf{q}}(\mathbf{q}\cdot\mathbf{k})^2[\,n_B\psi_{AB}(q)g_{AB}(p)-\delta_{AB}n_C\psi_{AC}(q)g_{CA}(q)] \tag{16b}$$

are again *exact*, since the VAA respects the ω^{-4} (third moment) sum rule [2,26].

The partial response functions χ_{AB} can be converted into the external response $\hat{\chi}_{AB}$ via Eq. (8) of paper I, which, in turn, though also artificial constructs, can be directly applied via the fluctuation-dissipation theorem to yield the partial dynamical structure functions $S_{AB}(\mathbf{k}\omega)$, which are of direct physical interest. The centrally important dielectric-response function can be obtained from the partial response function through the relationship displayed in Eq. (10), paper I.

The linear partial density response functions are now expressed in terms of the quadratic partial response functions. In order to achieve self-consistency, the reduction of $\chi_{ABC}(\mathbf{p}\mu;\mathbf{q}\nu)$ to combinations of $\chi(\mathbf{p}\mu)$ and $\chi(\mathbf{q}\nu)$ is to be established. Two approaches to achieve such a decomposition have been proposed and to some extent tested for the OCP: the dynamical superposition method of Golden and Kalman [2,6,9], and the UMFT representation of $\chi(\mathbf{p}\mu;\mathbf{q}\nu)$ of Tao and Kalman [3,4,17]. We have recently argued [4] that the latter is superior to the former in many respects, and rests on a more solid physical foundation. Thus here we follow the multispecies generalization of the method of Ref. [3]; this will be done in the next section.

One further observes that Eq. (23) possesses the order-raising property; i.e., the quadratic response function in a certain order of the coupling is linked to a linear response function that is one order higher in the coupling than the quadratic one. Consequently, if the quadratic response function is replaced by its RPA value (zeroth order in coupling), one obtains the linear partial response function to first order in coupling. This method works well in the weak-coupling limit and will be pursued in Sec. IV.

III. SELF-CONSISTENCY CONDITION FOR STRONG COUPLING

In order to derive the self-consistency condition for $v(\mathbf{k}\omega)$, we first generalize the customary mean-field expression

$$\chi=\frac{\chi^{(0)}}{1+\psi G\chi^{(0)}}\ ,$$

formulated in terms of the dynamical mean field $G(\mathbf{k}\omega)$. The quantity $\mathbf{K}=\boldsymbol{\psi}\mathbf{G}$ is more appropriate for the purpose of generalization to the multispecies situation. We can define $K_{AB}(\mathbf{k}\omega)$ now through

$$\delta\Phi_A=-K_{CA}n_C\ , \tag{17}$$

where $\delta\Phi_A$ is the "local-field correction" to Φ_A induced by correlations. We can then write

$$\boldsymbol{\chi}=\boldsymbol{\chi}^{(0)}\boldsymbol{\Theta}^{-1}\ , \tag{18}$$

and obtain for $\boldsymbol{\Theta}$

$$\boldsymbol{\Theta}=1+\mathbf{K}\boldsymbol{\chi}^{(0)}\ , \tag{19}$$

or for $\mathbf{K}$

$$\mathbf{K}=\boldsymbol{\chi}^{-1}-\boldsymbol{\chi}^{(0)-1}\ ,$$

which demonstrates that $\mathbf{K}$, if properly constructed, also has to be symmetric.

There is an obvious relationship between the screening function $\boldsymbol{\Theta}$ and the coupling function $\mathbf{v}$ introduced earlier:

$$\mathbf{1}+\mathbf{v}=\boldsymbol{\Theta}^{-1} \tag{20a}$$

or

$$\mathbf{K}\boldsymbol{\chi}^{(0)}=-\mathbf{v}\boldsymbol{\Theta}\ . \tag{20b}$$

In view of (18), ϵ can be expressed as

$$\epsilon=\boldsymbol{\Delta}\boldsymbol{\Theta}^{-1}\ , \tag{21}$$

with

$$\boldsymbol{\Delta}=1-\boldsymbol{\psi}\boldsymbol{\chi}^{(0)}+\mathbf{K}\boldsymbol{\chi}^{(0)}=1-\boldsymbol{\psi}(1-\mathbf{G})\boldsymbol{\chi}^{(0)}\ . \tag{22}$$

The principal approximation now consists of assuming the existence of a universal mean field (UMF) [27], acting on the quadratic response function as well and leading to the introduction of the ansatz for the quadratic response function

$$\chi_{ABC}(\mathbf{p}\mu;\mathbf{q}\nu)=\Theta^{-1}_{PA}(\mathbf{k}\omega)\chi^{(0)}_P(\mathbf{p}\mu;\mathbf{q}\nu)\Theta^{-1}_{PB}(\mathbf{p}\mu)\Theta^{-1}_{PC}(\mathbf{q}\nu)\ ,\quad \mathbf{k}=\mathbf{p}+\mathbf{q},\ \ \omega=\mu+\nu\ . \tag{23}$$

The analogous OCP relationship was used by Tao and Kalman [3]. Nevertheless, it should be realized that, in contrast to Eq. (18), where a properly chosen $\mathbf{K}(\mathbf{k}\omega)$ can reproduce any $\chi(\mathbf{k}\omega)$, Eq. (23) represents an approximation for $\chi_{ABC}(\mathbf{p}\mu;\mathbf{q}\nu)$, irrespective of the structure of $\mathbf{K}$.

We can now inject the ansatz (23) into (13) and (20b), which then immediately results in the desired self-consistency condition:

$$K_{AC}(\mathbf{k}\omega)\chi^{(0)}_C(\mathbf{k}\omega)=\frac{2}{\beta n_A V}\sum_{\mathbf{q}}\frac{\mathbf{k}\cdot\mathbf{q}}{k^2}\int d\mu\,\delta_-(\mu)[\,\chi^{(0)}_C(\mathbf{p}\nu;\mathbf{q}\mu)\Delta^{-1}_{CA}(\mathbf{p}\nu)\Delta^{-1}_{CB}(\mathbf{q}\mu)+\chi^{(0)}_C(\mathbf{p}\mu;\mathbf{q}\nu)\Delta^{-1}_{CA}(\mathbf{p}\mu)\Delta^{-1}_{CB}(\mathbf{q}\nu)]\psi_{AB}(q)\ ,\quad \mathbf{k}=\mathbf{p}+\mathbf{q},\ \ \omega=\mu+\nu\ . \tag{24}$$

Equation (24) in conjunction with (22) determines **K**. However, the results made earlier concerning the symmetry problem with respect to the species indices of χ_{AB} still hold; thus we determine χ_{AB} by (14) with

$$\chi_{[AB]}(\mathbf{k}\omega)=\chi_A^{(0)}\Theta_{AB}^{-1}(\mathbf{k}\omega) . \tag{25}$$

Equation (24) represents a rather formidable set of integral equations. In order to appreciate, however, the relative simplicity one has acquired by the use of the partial response formalism and the application of the novel decomposition technique for $\chi_{ABC}(\mathbf{p}\mu;\mathbf{q}\nu)$, one should compare it with the combined relationships (43), (49a)–(49c), and (50a)–(50c) in GGN [9], which represent the corresponding formulas arrived at in the dynamical superposition approximation. Moreover, it should be noted that $\chi_C^{(0)}(\mathbf{q}\mu;\mathbf{p}\nu)$ in (24), the noninteracting gas value of the quadratic response function, is a well-known and simple function [5]:

$$\chi_C^{(0)}(\mathbf{q}\nu;\mathbf{p}\mu)=\frac{\beta}{2m_C}\int d^3v\frac{F_A^{(0)}(\mathbf{v})}{(\omega-\mathbf{k}\cdot\mathbf{v})^2}\times\left[\frac{\mathbf{k}\cdot\mathbf{p}\mathbf{q}\cdot\mathbf{v}}{\nu-\mathbf{q}\cdot\mathbf{v}}+\frac{\mathbf{k}\cdot\mathbf{q}\mathbf{p}\cdot\mathbf{v}}{\mu-\mathbf{p}\cdot\mathbf{v}}\right] . \tag{26}$$

With some additional assumptions, consisting of ignoring plasmon pole contributions and exploiting the analytic properties of (26), the frequency integral in (24) becomes doable, thereby reducing the dimensionality and considerably simplifying the structure of the integral equation [3,4]. We do not pursue this line of thought here, since it belongs more properly to the general problem of solving the integral equation (24), which is not the concern of the present paper. As to the good features of the VAA, as exhibited in the intermediate state Eq. (13), the satisfaction of the ω^{-4} high-frequency sum rule is preserved by Eq. (24). The exactness of the formalism in the static limit is, however, violated, although (24) still represents a reasonable approximation [3] in the $\omega=0$ limit.

IV. WEAK-COUPLING LIMIT

In this section we employ the general formula to derive the first-order perturbational correction to the partial response function for weak coupling. The resulting expression is valid for arbitrary $\mathbf{k}$ and ω values, but it is still approximate, insofar as it is based on the VAA. The important $k=0$ limit is, however, as discussed below, in complete agreement with the corresponding rigorous perturbation-theoretical calculation. So are, as pointed out in Sec. II, the $\omega=0$ and $\omega\to\infty$ limit results. These facts and our experience with the VAA as applied to the OCP in the weak-coupling case reinforce our belief that the results Eqs. (28) and (32) below represent a good approximation and can be usefully applied to replace the cumbersome rigorous perturbation-theoretical derivation.

Now, starting with Eq. (12), the first-order correction to the partial density response function is given as

$$\chi^{(1)}(\mathbf{k}\omega)=\chi^{(0)}(\mathbf{k}\omega)\mathbf{v}^{(1)}(\mathbf{k}\omega) , \tag{27}$$

where the superscript designates the order in the coupling. The coupling function, to the first order in the coupling, as inferred from Eq. (13), is given as

$$v_{AB}^{(1)}(\mathbf{k}\omega)=-\frac{2}{n_A\beta V}\sum_{\mathbf{q}}\int d\mu\frac{\mathbf{k}\cdot\mathbf{q}}{k^2}\delta_-(\mu)\times[\chi_B^{(0)}(\mathbf{p}\nu;\mathbf{q}\mu)\eta_{BA}(\mathbf{p}\nu)\eta_{BC}(\mathbf{q}\mu)+\chi_B^{(0)}(\mathbf{p}\mu;\mathbf{q}\nu)\eta_{BA}(\mathbf{p}\mu)\times\eta_{BC}(\mathbf{q}\nu)]\psi_{CA}(q) , \tag{28}$$

where η and ϵ are understood to be the respective RPA values of the dielectric matrix and its inverse,

$$\epsilon_{AB}(\mathbf{k}\omega)=\delta_{AB}-\psi_{AB}(k)\chi_B^{(0)}(\mathbf{k}\omega) . \tag{29}$$

$\chi_{ABC}^{(0)}$, the quadratic density response function of the noninteracting system similarly to its linear counterpart, is diagonal in species space and is given above in Eq. (26). Equation (26) substituted into Eq. (28) now provides an explicit expression for the partial density response functions with an arbitrary pseudopotential to the first order in the coupling. It should be noted that no approximation in addition to the VAA is needed to do this calculation: the considerations of Sec. III do not apply here.

In the case of a pure Coulomb potential as the interaction potential $\psi_{AB}(q)$ becomes factorizable,

$$\psi_{AB}(q)=\varphi_{AB}(q)=Z_AZ_B\varphi(q) , \tag{30}$$

and, in addition to (30), we have

$$\eta_{AB}(\mathbf{k}\omega)=\delta_{AB}+\varphi_{AB}\frac{\chi_B^{(0)}(\mathbf{k}\omega)}{\epsilon(\mathbf{k}\omega)} \tag{31}$$

and

$$\eta_{BC}\psi_{CA}=\frac{\psi_{BA}}{\epsilon} . \tag{32}$$

Then, using (29) with some straightforward algebra, one obtains

$$v_{AB}^{(1)}(\mathbf{k}\omega)=-\frac{2}{n_A\beta V}\sum_{\mathbf{q}}\int d\mu\frac{\mathbf{q}\cdot\mathbf{k}}{k^2}\delta_-(\mu)\left[\delta_{BA}\varphi_{BA}(q)\left[\frac{\chi_B^{(0)}(\mathbf{p}\nu;\mathbf{q}\mu)}{\epsilon(\mathbf{q}\mu)}+\frac{\chi_B^{(0)}(\mathbf{p}\mu;\mathbf{q}\nu)}{\epsilon(\mathbf{q}\nu)}\right]+\varphi_{BA}(q)\varphi_{BA}(p)\left[\frac{\chi_B^{(0)}(\mathbf{p}\nu;\mathbf{q}\mu)\chi_A^{(0)}(\mathbf{p}\nu)}{\epsilon(\mathbf{p}\nu)\epsilon(\mathbf{q}\mu)}+\frac{\chi_B^{(0)}(\mathbf{p}\mu;\mathbf{q}\nu)\chi_A^{(0)}(\mathbf{p}\mu)}{\epsilon(\mathbf{p}\mu)\epsilon(\mathbf{q}\nu)}\right]\right] ,$$

$$\nu=\omega-\mu, \quad \mathbf{p}=\mathbf{k}-\mathbf{q} . \tag{33}$$

This formula combined with Eq. (28) reduces the computation of the partial response function and thus of the dielectric function for arbitrary wave-vector and frequency values to relatively simple quadratures.

Equation (33) can be compared with the corresponding exact first-order perturbation result calculated in paper I. This comparison is done in Appendix A. Also relegated to Appendix A is the comparison of the evaluation of (33) and of the exact expression in the so-called "static screening approximation" [by letting $\epsilon(\mathbf{p}\mu)\to\epsilon(\mathbf{p}0)$, $\epsilon(\mathbf{p}\omega-\mu)\to\epsilon(\mathbf{p}0)$ in the denominators of integrand]. It is especially in this approximation that the relative simplicity of the VAA expression emerges.

We now concentrate on the especially important long-wavelength ($k=0$) limit of the dielectric-response function, which provides information on the dc conductivity and on the plasmon frequency shift. To obtain this, $\chi_{AB}(\mathbf{k}\omega)$ has to be calculated to order $O(k^2)$. To this order, $\chi_A^{(0)}(\mathbf{k}\omega)$ and $\chi_A^{(0)}(\mathbf{p}\mu;\mathbf{q}\nu)$ have the simple limits

$$\lim_{\mathbf{k}\to 0}\chi_A^{(0)}(\mathbf{k}\omega)=\frac{k^2 n_A}{\omega^2 m_A} \tag{34}$$

and

$$\lim_{\mathbf{k}\to 0}\chi_B^{(0)}(\mathbf{p}\mu;\mathbf{q}\nu)=\frac{\mathbf{k}\cdot\mathbf{q}}{2m_B\omega^2}[\chi_B^{(0)}(\mathbf{q}\nu)-\chi_B^{(0)}(\mathbf{p}\mu)]\ . \tag{35}$$

Hence, using (34) and (35) in (28) and (29), the first-order correction to the partial density response function in this limit is given by

$$\chi_{AB}^{(1)}(\mathbf{k}\to 0\omega)=\frac{1}{\omega^4 m_A m_B\beta V}\sum_{\mathbf{q}}(\mathbf{q}\cdot\mathbf{k})^2\int d\mu\,\delta_-(\mu)\times(\eta_{BA}\tilde{\eta}_{BC}-\tilde{\eta}_{BA}\eta_{BC})\times(\chi_B^{(0)}-\tilde{\chi}_B^{(0)})\psi_{CA}(q)\ , \tag{36}$$

where $\chi^{(0)}=\chi^{(0)}(\mathbf{q}\mu)$, $\eta=\eta(\mathbf{q}\mu)$, $\tilde{\chi}^{(0)}=\chi^{(0)}(\mathbf{q}\omega-\mu)$, and $\tilde{\eta}=\eta(\mathbf{q}\omega-\mu)$.

The above expression is given with a general pseudopotential. The symmetry of χ_{AB} now can be demonstrated, and thus no symmetrization is required. One can also see by inspection that this expression exactly coincides with the rigorous perturbation calculational result, which has been derived in paper I. Indeed, it is quite remarkable that after making the VAA approximation, the result at $k=0$ in the first order of coupling is still exact. It can also be shown that in the case of a pure Coulomb potential the dielectric function derived from Eq. (46) is equivalent to the result given in GGN [9], Eqs. (53a)–(53c).

Since, as we have pointed out, the results of this section in the $k=0$ limit coincide with the exact perturbation formula derived in paper I (see also Ref. [10]), the reader is referred to that paper and to the references therein for the discussion of the physical implications of the results obtained, and for results of the concrete computations concerning electron-ion plasmas and the binary ionic mixture. Finally, we note that in the OCP limit the expression (46) becomes identically zero, as it should, for there is no deviation from the RPA behavior at $k=0$ for a one-component system.

V. CONCLUSIONS

In this paper we have calculated the dielectric-response function and the partial density response functions (which are related to the dynamical structure functions through fluctuation dissipation relations) for a multicomponent plasma in the velocity average approximation. The electron-ion plasma and the binary ionic mixture are the physical systems that are prime candidates for the application of these results. Our model incorporates a generalized pseudopotential as the interaction between the particles: the role of a non-Coulombic pseudopotential is crucial for the electron-ion plasma and is of importance for various ionic plasmas. Our derivation is based on the velocity average approximation. As a result of the consistent application of the partial response function formalism in its matrix form, a compact expression is obtained that determines the linear response functions in terms of the quadratic response [Eqs. (12), (13), and (14)]. This result is, then, used in two different ways: for arbitrary or strong coupling ($\Gamma\gtrsim 1$) we establish a dynamical mean-field theory formula that provides a self-consistency criterion for the calculation of the partial response functions and the dielectric-response function [Eqs. (19), (24), and (25)]. For weak coupling ($\gamma\ll 1$), we calculate the partial response functions and the dielectric-response function to $O(\gamma)$ and compare them with the rigorous perturbation calculational results. For finite k, we show how a convenient static screening approximation can be set up (cf. Appendix A).

The DMFT based on the velocity average approximation combined with the application of the quadratic fluctuation-dissipation theorem has proven to be a powerful approach to the calculation of the dynamical properties of Coulomb systems [6,7]. The versatility of the method as applied to binary systems is well demonstrated by the present paper. The mean-field expression Eq. (24), valid for arbitrary coupling, has a number of remarkable properties. First, it has the correct weak-coupling limit, as demonstrated by the structural equivalence of (24) and (28). (Note that for $\gamma\ll 1$, $\Delta^{-1}\cong\eta$.) This is not a trivial matter, since in the derivation of Eq. (24) an additional approximation, the UMF assumption, has been used. The low-Γ expression, Eq. (28), in turn, is very satisfactory, in view of its exactness both in the $\omega=0$ and $k=0$ limits. Second, the high-Γ expression itself, although not exact any more in the static $\omega=0$ limit (because the UMF approximation breaks the original exactness property of the VAA) still yields a very good static expression, as indicated in Refs. [3] and [4]. Third, the high-frequency ω^{-4} sum rule is always satisfied.

Further commenting on the strong-coupling static behavior, we note that it is well known that the hypernetted-chain (HNC) approximation provides extremely good results, as verified by comparison with Monte Carlo simulation data [11]. The present approximation, even though it yields a satisfactory static limit (in

the one-component case one recovers the results of Totsuji and Ichimaru [28]), is still inferior to the HNC method. However, the principal merit of the DMFT approach is its ability to correctly handle dynamical processes.

No concrete computations are performed in this paper, but our experience with the one-component system [7] shows that such calculation, even though not simple, is feasible. Our goal has been to establish a tractable formalism for future work and to show that, the substantial intrinsic complexity of the multispecies formalism notwithstanding, the calculations can be kept within manageable bounds. We expect that the formalism we have derived will be usefully applied to the calculation of the dynamical response and collective-mode behavior of correlated electron-ion and ion-ion systems.

ACKNOWLEDGMENTS

We wish to thank Kenneth I. Golden for many useful conversations and for sharing his insights, frustrations, and unpublished works with us and for his cooperation in comparing our results with those of GGN. This work has been supported in part by the National Science Foundation under Grant No. ECS-8713337.

APPENDIX A

In this appendix we display both the VAA result in the weak-coupling limit [Eq. (33)] and the result obtained from the exact perturbation calculation, borrowed from paper I (to facilitate comparison, we consider bare Coulomb interaction only, but generalization to the case of a general pseudopotential is feasible):

$$\chi^{(1)}_{[AB]}(\mathbf{k}\omega)=-\frac{2\chi^{(0)}_A(\mathbf{k}\omega)}{n_A\beta V}\sum_{\mathbf{q}}\frac{\mathbf{q}\cdot\mathbf{k}}{k^2}\int d\mu\,\delta_-(\mu)\left[Z_A^2Z_B^2\varphi(q)\varphi(p)\left[\frac{\chi^{(0)}_B(\mathbf{p}\nu;\mathbf{q}\mu)\chi^{(0)}_A(\mathbf{p}\nu)}{\epsilon(\mathbf{p}\nu)\epsilon(\mathbf{q}\mu)}+\frac{\chi^{(0)}_B(\mathbf{p}\mu;\mathbf{q}\nu)\chi^{(0)}_A(\mathbf{q}\mu)}{\epsilon(\mathbf{p}\mu)\epsilon(\mathbf{q}\nu)}\right]\right.$$
$$\left.+\delta_{AB}Z_A^2\varphi(q)\left[\frac{\chi^{(0)}_B(\mathbf{p}\nu;\mathbf{q}\mu)}{\epsilon(\mathbf{q}\mu)}+\frac{\chi^{(0)}_B(\mathbf{p}\mu;\mathbf{q}\nu)}{\epsilon(\mathbf{q}\nu)}\right]\right]\quad(\mathrm{VAA}),\tag{A1}$$

$$\chi^{(1)}_{AB}(\mathbf{k}\omega)=\tfrac{1}{2}(\chi^{(1)}_{[AB]}(\mathbf{k}\omega)+\chi^{(1)}_{[BA]}(\mathbf{k}\omega)),\tag{A2}$$

and

$$\chi^{(1)}_{AB}(\mathbf{k}\omega)=-\frac{4}{\beta V}\sum_{\mathbf{q}}\int d\nu\,\delta_-(\mu)\left[Z_A^2Z_D^2\frac{\varphi(q)\varphi(p)}{\epsilon(\mathbf{q}\nu)\epsilon(\mathbf{p}\mu)}\chi^{(0)}_A(\mathbf{p}\mu;\mathbf{q}\nu)\chi^{(0)}_B(\mathbf{p}\mu;\mathbf{q}\nu)\right.$$
$$\left.-\frac{\delta_{AB}}{24}\frac{\beta^2n_AZ_A^2}{m_A}\mathbf{k}\cdot\mathbf{q}\varphi(q)\frac{\partial^2}{\partial\omega^2}\left[\frac{T_A(\mathbf{k}\omega;\mathbf{p}\nu)}{\epsilon(\mathbf{q}\mu)}+\frac{T_A(\mathbf{k}\omega;\mathbf{p}\mu)}{\epsilon(\mathbf{q}\nu)}-2\frac{T_A(\mathbf{k}\omega;\mathbf{p}0)}{\epsilon(\mathbf{q}0)}\right]\right]$$
$$(\mathrm{exact}),\tag{A3}$$

with

$$T_B(\mathbf{k}\omega;\mathbf{q}\nu)\equiv-\frac{1}{n_B(\beta m_B)^2}\int d^3v\frac{\mathbf{k}\cdot\mathbf{p}\,\mathbf{q}\cdot\frac{\partial}{\partial\mathbf{v}}F^{(00)}_B(\mathbf{v})}{(\omega-\mathbf{k}\cdot\mathbf{v})^2(\nu-\mathbf{q}\cdot\mathbf{v})}\,.\tag{A4}$$

We note that there is some structural similarity between the two expressions. Both consist of a "collective" and a "scattering" contribution (cf. the discussion in paper I): the former is characterized by a proportionality with e^4 and by a double ϵ denominator; the latter is proportional to $\delta_{AB}e^2$ and has a single ϵ denominator. The differences manifest themselves as a decomposition of $\chi^{(0)}_A(\mathbf{p}\mu;\mathbf{q}\nu)$ into linear $\chi^{(0)}_A$ in the first term of the VAA expression, and as the approximation of $\partial T/\partial\omega^2$ by an algebraic expression in the second term. We also observe the evident symmetry in (A3), lacking in the VAA expression. Thus, it is quite remarkable to witness that they become identical in the $\mathbf{k}\to0$, $\omega=0$, and $\omega\to\infty$ limits.

A popular approximation scheme [29,30] for the evaluation of integrals of the type (A1) and (A3) is the "static-screening approximation" (SSA), which consists of ignoring contributions from the poles of denominator and replacing $\epsilon(\mathbf{p}\mu)$ and $\epsilon(\mathbf{p}\nu)$ by the static $\epsilon(\mathbf{p}0)\equiv\epsilon(\mathbf{p})$. The approximation, however, is not unambiguous: there is no unique prescription as to at what particular stage the approximation is to be implemented. Considerable care has to be exercised to ensure that obvious physical requirements are not violated by the approximation [10]. In particular, $\epsilon^{(1)}(\mathbf{k}=\mathbf{0},\omega)$ has to vanish in the OCP or symmetric ($Z_1/m_1=Z_2/m_2$) limit. One can convince oneself that this is accomplished if the SSA is formulated as follows:

$$\chi^{(1)}_{[AB]}(\mathbf{k}\omega)=-\frac{2\chi^{(0)}_A(\mathbf{k}\omega)}{k^2n_A\beta V}\sum_{\mathbf{q}}\int d\mu\frac{\mathbf{q}\cdot\mathbf{k}}{\epsilon(\mathbf{q})\epsilon(\mathbf{p})}\delta_-(\mu)$$
$$\times\{\delta_{BA}Z_A^2\varphi(q)[\chi^{(0)}_B(\mathbf{p}\nu;\mathbf{q}\mu)\epsilon(\mathbf{p}\nu)+\chi^{(0)}_B(\mathbf{p}\mu;\mathbf{q}\nu)\epsilon(\mathbf{p}\mu)]$$
$$+Z_A^2Z_B^2\varphi(q)\varphi(p)[\chi^{(0)}_B(\mathbf{p}\nu;\mathbf{q}\mu)\chi^{(0)}_A(\mathbf{p}\nu)+\chi^{(0)}_B(\mathbf{p}\mu;\mathbf{q}\nu)\chi^{(0)}_A(\mathbf{p}\mu)]\}\quad(\mathrm{VAA}).\tag{A5}$$

For the VAA expression, the SSA is performed after combining terms in (A1) over two common denominators $\epsilon(\mathbf{q}\mu)\epsilon(\mathbf{p}\nu)$ and $\epsilon(\mathbf{q}\nu)\epsilon(\mathbf{p}\mu)$. For the exact perturbation expression it is difficult to find a SSA exhibiting the right limiting behavior. However, by subtracting the $k=0$ term that leads to a nonvanishing contribution to $\epsilon^{(1)}(\mathbf{k}=0\omega)$ in the OCP or symmetric limits, the consistency can be restored [31]:

$$\chi^{(1)}_{AB}(\mathbf{k}\omega)=-\frac{4}{\beta V}Z_A^2Z_B^2\sum_{\mathbf{q}}\frac{\varphi(q)\varphi(p)}{\epsilon(\mathbf{q})\epsilon(\mathbf{p})}\int d\mu\,\delta_-(\mu)\chi^{(0)}_A(\mathbf{q}\nu;\mathbf{p}\mu)\chi^{(0)}_B(\mathbf{q}\nu;\mathbf{p}\mu)$$
$$+\delta_{AB}\frac{Z_A^2}{\omega^4m_A^2\beta V}\sum_{\mathbf{q}}\varphi(q)\frac{(\mathbf{q}\cdot\mathbf{k})^2}{\epsilon^2(\mathbf{q})}\int d\mu\,\delta_-(\mu)[\chi^{(0)}_B(\mathbf{q}\mu)\epsilon(\mathbf{q}\nu)+\chi^{(0)}_B(\mathbf{q}\nu)\epsilon(\mathbf{q}\mu)-\chi^{(0)}_B(\mathbf{q}\mu)\epsilon(\mathbf{q}\mu)]\quad\text{(exact)}\,. \tag{A6}$$

The analytic evaluation of (A5) [but not (A6)] seems to be possible, but is not within the scope of the present paper. We note, however, one interesting aspect concerning the structure of the VAA $\chi_{AB}(\mathbf{k}\omega)$. It is known [18] that the VAA, when applied to the OCP, exhibits one important defect: $\mathrm{Im}\epsilon(\mathbf{k}\omega)$ to $O(k^2)$ fails to reproduce the well-known "dominant" $\gamma\ln\gamma$ coefficient. On the other hand, we can observe that the VAA does generate for $\mathrm{Im}\epsilon(\mathbf{k}\omega)$ of the two-component system a $\gamma\ln\gamma$ dominant term, at least for $k=0$. It is interesting now to speculate about the behavior of $\mathrm{Im}\epsilon(\mathbf{k}\omega)$ for finite $\mathbf{k}$: does the dominant term survive to $O(k^2)$ (as one would expect from the analyticity of the k behavior of $\epsilon(\mathbf{k}\omega)$, or do, for finite k, the OCP and the two-component systems share the problematic missing of the dominant term?

APPENDIX B

In this appendix we show that the static Bogoliubov-Green-Yvon (BGY) hierarchy leads to the same relationship for $\chi_{AB}(\mathbf{k}0)$ as the VAA. Since, as we have emphasized, in the static limit the VAA is exact, this is expected. However, the explicit demonstration is probably still useful.

We focus on the second BGY equation, which links the static two-particle distribution $G_{AB}(\mathbf{x}_1,\mathbf{v}_1;\mathbf{x}_2,\mathbf{v}_2)$ to the static three-particle distribution $H_{ABC}(\mathbf{x}_1,\mathbf{v}_1;\mathbf{x}_2,\mathbf{v}_2;\mathbf{x}_3,\mathbf{v}_3)$:

$$\left[\mathbf{v}_1\cdot\frac{\partial}{\partial\mathbf{x}_1}+\mathbf{v}_2\cdot\frac{\partial}{\partial\mathbf{x}_2}-\frac{1}{m_A}\frac{\partial}{\partial\mathbf{x}_1}\psi_{AB}(\mathbf{x}_1-\mathbf{x}_2)\cdot\frac{\partial}{\partial\mathbf{v}_1}-\frac{1}{m_B}\frac{\partial}{\partial\mathbf{x}_2}\psi_{AB}(\mathbf{x}_1-\mathbf{x}_2)\cdot\frac{\partial}{\partial\mathbf{v}_2}\right]G_{AB}(\mathbf{x}_1,\mathbf{v}_1;\mathbf{x}_2,\mathbf{v}_2)$$
$$=-\int d^3x_3\int d^3v_3\left[\frac{1}{m_A}\frac{\partial}{\partial\mathbf{x}_1}\psi_{AC}(\mathbf{x}_1-\mathbf{x}_3)\cdot\frac{\partial}{\partial\mathbf{v}_1}+\frac{1}{m_B}\frac{\partial}{\partial\mathbf{x}_2}\psi_{BC}(\mathbf{x}_2-\mathbf{x}_3)\cdot\frac{\partial}{\partial\mathbf{v}_2}\right]H_{ABC}(\mathbf{x}_1,\mathbf{v}_1;\mathbf{x}_2,\mathbf{v}_2;\mathbf{x}_3,\mathbf{v}_3)\,. \tag{B1}$$

Exploiting now that in equilibrium the distribution functions factorize into space-dependent and Maxwellian velocity-dependent parts

$$G_{AB}(\mathbf{x}_1,\mathbf{v}_1;\mathbf{x}_2\mathbf{v}_2)=\bar{G}(\mathbf{x}_1,\mathbf{x}_2)F(v_1)F(v_2)\,,$$
$$H_{ABC}(\mathbf{x}_1,\mathbf{v}_1;\mathbf{x}_2\mathbf{v}_2;\mathbf{x}_3,\mathbf{v}_3)=\bar{H}_{ABC}(\mathbf{x}_1-\mathbf{x}_3,\mathbf{x}_2-\mathbf{x}_3)\times F(v_1)F(v_2)F(v_3)\,, \tag{B2}$$

etc., and introducing the Fourier transforms

$$\bar{G}_{AB}(\mathbf{x}_1,\mathbf{x}_2)=\frac{1}{V}\sum_{\mathbf{k}}ei\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)\bar{G}_{AB}(\mathbf{k})\,,$$
$$\bar{H}_{ABC}(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)=\frac{1}{V}\sum_{\mathbf{pq}}e^{i\mathbf{p}\cdot(\mathbf{x}_1-\mathbf{x}_3)}e^{i\mathbf{q}\cdot(\mathbf{x}_2-\mathbf{x}_3)}\bar{H}_{ABC}(\mathbf{p},\mathbf{q})\,, \tag{B3}$$

one obtains the equation

$$\mathbf{k}\cdot(\mathbf{v}_1-\mathbf{v}_2)\left[\bar{G}_{AB}(\mathbf{k})+\frac{\beta}{V}\sum_{p}\frac{\mathbf{k}\cdot\mathbf{p}}{k^2}\psi_{AB}(p)\bar{G}_{AB}(\mathbf{k}-\mathbf{p})\right]$$
$$=-\mathbf{k}\cdot\mathbf{v}_1\frac{\beta}{V}\sum_{p}\frac{\mathbf{k}\cdot\mathbf{p}}{k^2}\psi_{AC}(p)\bar{H}_{ABC}(\mathbf{k}-\mathbf{p},-\mathbf{k})$$
$$+\mathbf{k}\cdot\mathbf{v}_2\frac{\beta}{V}\sum_{\mathbf{p}}\frac{\mathbf{k}\cdot\mathbf{p}}{k^2}\psi_{BC}(p)\bar{H}_{BAC}(\mathbf{k}-\mathbf{p},-\mathbf{k})\,. \tag{B4}$$

Since G_{AB} is necessarily symmetric in the species indices, (B4) can be combined with its $A\leftrightarrow B$ counterpart. Furthermore, it is useful to introduce the cumulant expansion

$$\bar{G}_{AB}(\mathbf{k})=\frac{N_AN_B}{V}\left[\delta_{\mathbf{k}}+\frac{1}{V}g_{AB}(k)\right]\,,$$
$$\bar{H}_{AB}(\mathbf{p},\mathbf{q})=\frac{N_AN_BN_C}{V}\left[\delta_{\mathbf{p}}\delta_{\mathbf{q}}+\frac{1}{V}[g_{AC}(p)\delta_{\mathbf{q}}+g_{BC}(q)\delta_{\mathbf{p}}+g_{AB}(p)\delta_{\mathbf{k}}]+\frac{1}{V^2}h_{ABC}(\mathbf{p},\mathbf{q})\right]\,. \tag{B5}$$

The resulting expression is

$$g_{AB}(k)+\beta\psi_{AB}(k)+\frac{\beta}{V}\sum_{\mathbf{p}}\frac{\mathbf{k}\cdot\mathbf{p}}{k^2}\psi_{AB}(p)g_{AB}(\mathbf{k}-\mathbf{p})+\frac{\beta n_C}{2}[\psi_{AC}(k)g_{AC}(k)+\psi_{BC}(k)g_{BC}(k)]$$
$$=-\frac{\beta n_C}{2}\frac{1}{V}\sum_{\mathbf{p}}\frac{\mathbf{k}\cdot\mathbf{p}}{k^2}[\psi_{AC}(p)h_{ABC}(\mathbf{k}-\mathbf{p},-\mathbf{k})+\psi_{BC}(p)h_{BAC}(\mathbf{k}-\mathbf{p},-\mathbf{k})]\ . \quad \text{(B6)}$$

Equation (B6) is the final product of the BGY derivation, expressing two-particle correlations in terms of three-particle correlations. To cast the result in the language of response functions, we introduce the (conventional) two- and three-point structure functions

$$S_{AB}(\mathbf{k})=\frac{1}{V}\langle\bar{n}_A(\mathbf{k})\bar{n}_B(-\mathbf{k})\rangle\ ,$$
$$S_{CAB}(\mathbf{p},\mathbf{q})=\frac{1}{V}\langle\bar{n}_A(\mathbf{p})\bar{n}_B(\mathbf{q})\bar{n}_C(-\mathbf{p}-\mathbf{q})\rangle\ . \quad \text{(B7)}$$

Here $\bar{n}_A(\mathbf{k})$, etc. are the Fourier components of the static density fluctuations (i.e., their deviations from their average n_A, etc. values).

S_{AB} and S_{ABC} can be decomposed (note that the normalizations used here are different from those used in Ref. [25]) as

$$S_{AB}(\mathbf{k})=\delta_{AB}n_A+n_An_Bg_{AB}(k)\ ,$$
$$S_{CAB}(\mathbf{p},\mathbf{q})=\delta_{ABC}n_A+\delta_{AB}n_Bn_Cg_{BC}(k)+\delta_{BC}n_Cn_Ag_{CA}(p)+\delta_{CA}n_An_Bg_{AB}(q)+n_An_Bn_Ch_{ABC}(\mathbf{p},\mathbf{q})\ . \quad \text{(B8)}$$

In addition, S_{AB} and S_{ABC} satisfy the linear and the quadratic static fluctuation dissipation theorems

$$\beta S_{AB}(\mathbf{k})=-\hat{\chi}_{AB}(\mathbf{k}0)\ ,$$
$$\frac{\beta^2}{2}S_{CAB}(\mathbf{p},\mathbf{q})=\hat{\chi}_{CAB}(\mathbf{p}0;\mathbf{q}0)\ . \quad \text{(B9)}$$

The combination of (B7), (B8), and (B9) now leads to

$$-\chi^{(0)}_{AB}(\mathbf{k}0)+\tfrac{1}{2}[\epsilon^{(0)}_{CA}(\mathbf{k}0)\hat{\chi}_{CB}(\mathbf{k}0)+\hat{\chi}_{AC}(\mathbf{k}0)\epsilon^{(0)}_{CB}(\mathbf{k}0)]$$
$$=\frac{1}{V}\sum_{\mathbf{p}}\frac{\mathbf{k}\cdot\mathbf{p}}{k^2}[\psi_{AC}(p)\hat{\chi}_{BCA}(\mathbf{p}0;\mathbf{q}0)+\psi_{BC}(p)\hat{\chi}_{ACB}(\mathbf{p}0;\mathbf{q}0)]\ , \quad \text{(B10)}$$

which is equivalent to the combined Eqs. (14) and (15) in the main text.

[1] H. Zhang and G. Kalman, preceding paper, Phys. Rev. A **45**, 5935 (1992).
[2] K. I. Golden, G. Kalman, and M. B. Silevitch, Phys. Rev. Lett. **33**, 1544 (1974); K. I. Golden and G. Kalman, Phys. Rev. A **19**, 2112 (1979).
[3] Z. C. Tao and G. Kalman, Phys. Rev. A **43**, 973 (1991).
[4] G. Kalman and Z. C. Tao, Phys. Rev. A **43**, 7073 (1991).
[5] G. Kalman and X. Y. Gu, Phys. Rev. A **36**, 3399 (1987); K. I. Golden, G. Kalman, and M. B. Silevitch, J. Stat. Phys. **6**, 87 (1972).
[6] P. Carini, G. Kalman, and K. I. Golden, Phys. Lett. **78A**, 450 (1980); P. Carini and G. Kalman, *ibid.* **105A**, 229 (1984).
[7] M. Minella, G. Kalman, K. I. Golden, and P. Carini (unpublished).
[8] J. P. Hansen, E. L. Pollock, and I. R. McDonald, Phys. Rev. Lett. **32**, 277 (1974); J. P. Hansen, I. R. McDonald, and E. L. Pollock, Phys. Rev. A **11**, 1025 (1975).
[9] K. I. Golden, F. Green, and D. Neilson, Phys. Rev. A **31**, 3529 (1985); **32**, 1669 (1985); see also K. I. Golden and G. Kalman, *ibid.* **14**, 1802 (1976).
[10] H. Zhang, Ph.D. thesis, Boston College, 1991.
[11] W. D. Kraeft, D. Kremp. W. Ebling, and G. Röpke, *Quantum Statistics of Charged Particle Systems* (Akademie-Verlag, Berlin, 1986), Chap. 5.2.
[12] J. P. Hansen and I. R. McDonald, Phys. Rev. Lett. **41**, 1379 (1978); Phys. Rev. A **23**, 2041 (1981).
[13] H. Hellmann, J. Chem. Phys. **3**, 61 (1935); T. Dunn and A. A. Broyles, Phys. Rev. **157**, 156 (1967); C. Deutsch and M. M. Gombert, J. Math. Phys. **17**, 1077 (1976); A. A. Barker, J. Chem. Phys. **55**, 1751 (1971); R. G. Storer, J. Math. Phys. **9**, 964 (1968); F. J. Rogers, Phys. Rev. A **29**, 868 (1983).
[14] G. Kalman and K. I. Golden, Phys. Rev. A **29**, 844 (1984).
[15] P. Vashishta, P. Bhattacharrya, and K. S. Sigwi, Phys. Rev. B **10**, 5108 (1974).
[16] X. Y. Gu, Ph.D. thesis, Boston College, 1988.
[17] Z. C. Tao, Ph.D. thesis, Boston College, 1990.
[18] K. I. Golden and G. Kalman, Ann. Phys. (N.Y.) **143**, 160 (1982).
[19] J. Coste, Nucl. Fusion **5**, 284 (1965); **5**, 293 (1965).
[20] H. Zhang, G. Kalman, M. Minella, J. Jasperse, and K. I. Golden (unpublished).
[21] K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjölander, Phys. Rev. **176**, 589 (1968); K. S. Singwi, A. Sjölander, M. P. Tosi, and R. H. Land, Phys. Rev. B **1**, 1044 (1970).
[22] S. Ichimaru, Phys. Rev. A **2**, 494 (1970); H. Totsuji and S. Ichimaru, Prog. Theor. Phys. **50**, 753 (1973).
[23] G. Kalman, in *Strongly Coupled Plasmas,* edited by G. Kalman (Plenum, New York, 1978).
[24] G. Kalman, T. Datta, and K. I. Golden, Phys. Rev. A **12**, 1125 (1975).
[25] K. I. Golden and De-xin Lu, Stat. Phys. **29**, 281 (1982).
[26] J. P. Hansen, I. R. McDonald, and P. Vieillefosse, Phys. Rev. A **20**, 2590 (1979).
[27] G. Paasch and A. Heinrich, Phys. Status Solidi B **102**, 323

(1980).
[28] H. Totsuji and S. Ichimaru, Prog. Theor. Phys. **50**, 753 (1973); **52**, 42 (1974).
[29] M. Baus, Phys. Rev. A **15**, 290 (1977).
[30] P. Carini, G. Kalman, and K. I. Golden, Phys. Rev. A **26**, 1686 (1982).
[31] G. Kalman and K. I. Golden, Phys. Rev. A **41**, 5516 (1990).