Theory of partial response functions in multicomponent plasmas

G. Kalman
Department of Physics, Boston College, Chestnut Hill, Massachusetts 02167

K. I. Golden
Department of Electrical and Computer Engineering, Northeastern University, Boston, Massachusetts 02115
(Received 21 June 1983)

A new approach to the partial response functions in multicomponent plasmas is introduced. Central to the approach is that the density response function responding to the total (plasma plus external) field and a newly introduced dielectric matrix in species space are regarded as the primary quantities. A considerable simplification is achieved this way. Correlational terms to $O(\gamma)$ and pair-correlation functions both for ion-electron and binary-ion-mixture plasmas are calculated. Finally, the partial response functions in the mean-field-theory approximation are analyzed and it is shown that the consistency requirement based on the required symmetry of the response function is not always satisfied.

I. INTRODUCTION

The crucial role played by the dielectric and other closely related response functions such as polarizabilities, density response functions, etc. in the theory of plasmas and other many-body systems has long been recognized. One of the important ways through which information from the response functions is generated is the set of relationships known as linear and nonlinear fluctuation-dissipation theorems (FDTs). They allow one to calculate correlation functions and static and dynamic structure functions from the usually more easily accessible response functions. Nevertheless, for multicomponent systems these relationships lead to a peculiar problem which is due to the fact that for systems consisting of, for instance, K species, the number of physical polarizabilities is K, but the number of correlation functions and structure functions is $\frac{1}{2}K(K+1)$. Some time ago Vashishta, Bhattacaryya, and Singwi[1] suggested a way of handling the multicomponent situation. They introduced the concept of "partial" response functions (partial density responses and partial polarizabilities) describing the response of the system to fictitious external fields which act on each of the species independently. In their paper Vashishta *et al.*[1] derived simple relationships for the partial response functions in the framework of the Singwi-Tosi-Land-Sjolander (STLS) mean-field-theory[2] approximation. In a subsequent work the present authors[3] exploited the concept of partial response functions to set up a general framework for various static approximation schemes for strongly coupled plasmas. In particular, the two mean-field theories, STLS and TI (Totsuji-Ichimaru[4]), and the more general velocity-average approximation due to Golden, Kalman, and Silevitch[5] (GKS) were discussed. The concept of partial nonlinear response functions was also introduced in that paper.[3] In a later work, the results were reviewed by Kalman.[6] Even though we were able to achieve considerable progress in the development of a two-component formalism and in establishing general relationships, the formalism very soon became rather unwieldy and lost all transparency. In a recent work Golden and Lu[7] discussed nonlinear external (quadratic) partial response functions in the random-phase approximation, but the formalism suffered again from lack of transparency.

While the concept of partial response functions is a powerful formal tool, it should be clearly understood that it is not more than that. Partial response functions are not directly observable quantities. This is so because the fields that we contemplated in the definition of partial response functions, namely, fields that act on one type of plasma species only, never occur in actual physical systems. Nevertheless, the concept is perfectly reasonable. All that it requires is that each plasma species, in addition to its actual electric charge, be endowed with a (weak) fictitious "species charge"[6,7] which can interact only (i) with its corresponding perturbing field, or (ii) with another particle carrying a similar species charge. Even though such "species charges", in general, do not exist, there is nothing physically inconsistent in adding them to the system and, once they have completed their task, in letting them vanish.

In the present paper we take a fresh look at the general formalism of partial response functions and at their application in strongly coupled plasma approximations. Our present approach is based on a few simple observations, which, however, not only render the existing formalism incomparably more transparent, but also allow one to do the calculations with ease much beyond the point they have been carried to previously. First, we adopt a matrix formulation in species space and we introduce the new concept of partial dielectric matrix. Second, while previous discussions were directed exclusively at the external partial response functions, we define and analyze the structurally simpler total (as contrasted to external) partial response functions, i.e., response functions responding to the combined total (external plus plasma) field. Third, for the correlational calculations we base our work on the representation of correlational effects through the quadratic response function; the equivalence of this approach to the more conventional BGY hierarchy for the one-component system has already been demonstrated.[8]

Prominent among the multispecies systems to which the partial-response-function formalism applies is the electron-ion plasma (tcp). The classical treatment of such systems is, however, fraught with difficulties, which stem from the inadequate description of bound states. A simple way to avoid the difficulties was suggested by a number of workers.[9] It consists of the introduction of a modified (softened) Coulomb potential between electrons and ions [i.e., of replacing the bare Coulomb potential $\phi(r)$ by $(1-e^{-\mu r})\phi(r)$]. At the same time quantum diffraction effects in the electron-electron interaction and the effect of the van der Waals repulsion between ions can also be phenomenologically described through similarly modified electron-electron and ion-ion interactions, but with a different value of μ. Similarly, exchange effects can be included through a more general expression given by Deutsch *et al.*[9(a)] In each case the effective interaction can be considered as an analytic approximation to the exact quantities derived from the corresponding Slater sum. Thus the effective-interaction potential itself can be represented by a matrix in species space as well. In the present work we use this effective-interaction matrix without any restriction; in particular, we do not assume that the various interspecies potentials have the same spatial structures or, in other words, we allow for the determinant of the effective-interaction potential $||\psi(r)||$ to be different from zero. As a result, the emergence of $||\psi||$ leads to important structural effects in the formalism.

This work goes substantially beyond the results of earlier approaches. In addition to setting up the formalism along the line outlined above in Sec. II, in Secs. III and IV we give a succinct derivation and generalization of the linear and quadratic partial response functions in the random-phase approximation (RPA). In Sec. V we go beyond the RPA (although limited to static response functions) and calculate first-order correlational corrections. Combining the results into the full (as contrasted to partial) dielectric response function, we recover the earlier result of Coste.[10] In Sec. VI we apply the results of Sec. V to derive second-order corrections to various pair-correlation functions. Since we do not exploit charge neutrality for the noninert species, our results pertain to binary-ionic-mixture plasmas as well, for which the derivation of these higher-order pair-correlation functions is new. For the charge neutralized tcp, the earlier results of Yatom and Shima[11] are recovered.

In Sec. VII we focus on strongly coupled plasmas in the mean-field approximation. We discuss the derivation of the partial response functions in this approximation, which in the present formalism can be done without further specifying the approximation scheme. In further discussing the individual mean-field theories, we pay attention to a question that has already emerged in our earlier work[3] (but was not correctly answered): whether the required symmetry in species space is observed in the particular scheme. Our results in this section can be regarded as a generalization of the results of Vashihta *et al.*[1] and as a further development of our earlier work.[3]

II. FORMALISM

We consider a system consisting of two species. The two species might be thought of as electrons and ions, with the charge neutrality linking their respective densities, or as two species of ions, with independent concentrations in a neutralizing background, etc. Actually, restricting the number of species to two, rather than allowing for a multispecies system with an arbitrary number of components, is not important and most of the results of this paper can be trivially generalized to apply to such systems.

The interaction Hamiltonian is taken as

$$V=\frac{1}{2}\frac{1}{\mathscr{V}}\sum_{\vec{k}\,(\neq\vec{0})} n^{\bar{A}}_{\vec{k}}\psi^{\bar{A}\bar{B}}_{\vec{k}}n^{\bar{B}}_{-\vec{k}}+V^0 . \tag{1}$$

V^0 is a compensating constant whose precise value is not relevant for our purpose, the volume factor $\mathscr{V}$ will be omitted in most of the sequel ("unit volume"). Summation over repeated and barred species indices is understood and will be followed (but no summation over unbarred repeated indices will be implied).

The matrix of the interaction potential $\psi^{AB}_{\vec{k}}$, apart from being symmetric, is not restricted in any way. That is, no relationship is assumed between the various elements ψ^{AA}, ψ^{BB}, and ψ^{AB} $(A\neq B)$. The introduction of such a general potential is motivated by a number of different considerations: (i) Quantum diffraction effects and screening by the core electrons for high-Z ions render the ion-ion, ion-electron, and electron-electron effective interactions not only different from the bare Coulomb potential, but also substantially different from each other; (ii) the various mean-field theories invoked for the calculation of response functions in strong coupling situations are based on the idea of "effective potentials" which are necessarily species dependent, even when the physical potentials are not; (iii) in order to contemplate a partial response by the individual species to an external perturbation, one constructs a model in which, in addition to the physical interaction, an additional fictitious interaction, diagonal in species space, operates between the particles (which are endowed with a fictitious species charge X_Ae allowing them to interact with members of their own species only).

For the case of the bare Coulomb interaction

$$\psi^{AB}_{\vec{k}}=\phi^{AB}_{\vec{k}}\equiv Z_AZ_B\phi_{\vec{k}} , \qquad \phi_{\vec{k}}=\frac{4\pi e^2}{k^2} \tag{2}$$

is distinguished by the property

$$||\psi||=0 . \tag{3}$$

With diffraction and other corrections

$$\psi^{AB}_{\vec{k}}=\bar{\phi}^{AB}_{\vec{k}}\equiv\phi^{AB}_{\vec{k}}B^{AB}_{\vec{k}} , \tag{4}$$

where the factor $B^{AB}_{\vec{k}}$ is usually taken as

$$B^{AB}_{\vec{k}}=\frac{\mu^2_{AB}}{\mu^2_{AB}+k^2} . \tag{5}$$

Finally, with the fictitious species interaction added, we have

$$\psi^{AB}_{\vec{k}}=\bar{\phi}^{AB}_{\vec{k}}+X_A X_B \delta^{AB}\phi_{\vec{k}} \ .$$

The details of the interaction potential will be, however, of little consequence, except that for the bare Coulomb case, the vanishing of $||\psi||$ will lead to important simplifications.

Consider now the perturbation of the system by a (fictitious) external species field acting, by definition, on one species only. The corresponding potential of the external force, $\hat{\Phi}^B$ for species B, and the resulting first-order density perturbation in species A are linked by the (external) density response function matrix $\hat{\chi}^{AB}$:

$$n^{(1)A}=\hat{\chi}^{A\bar{B}}\hat{\Phi}^{\bar{B}} \ . \quad (6)$$

Similarly, when the total field Φ^B, including the plasma field $\check{\Phi}^B$,

$$\Phi^B=\hat{\Phi}^B+\check{\Phi}^B \quad (7)$$

is considered as the perturbation,

$$n^{(1)A}=\chi^{A\bar{B}}\Phi^{(1)\bar{B}} \ . \quad (8)$$

It is understood that $\chi^{AB}=\chi^{AB}(\vec{k}\omega)$, etc., that is, all the response functions are wave-vector and frequency dependent.

Obviously,

$$\check{\Phi}^A=\psi^{A\bar{B}}n^{\bar{B}}=\psi^{A\bar{B}}\hat{\chi}^{\bar{B}\bar{C}}\hat{\Phi}^{\bar{C}}=\psi^{A\bar{B}}\chi^{\bar{B}\bar{C}}\Phi^{\bar{C}} \ , \quad (9)$$

from which it follows that if we define the dielectric response function matrix ϵ^{AB} by

$$\hat{\Phi}^A=\epsilon^{A\bar{B}}\Phi^{(1)\bar{B}} \ , \quad (10)$$

then (in simplified matrix notation)

$$\underline{\epsilon}=\mathbb{1}-\underline{\psi}\,\underline{\chi} \quad (11)$$

and, defining $\underline{\eta}=\underline{\epsilon}^{-1}$,

$$\underline{\eta}=\mathbb{1}+\underline{\psi}\,\underline{\hat{\chi}} \ . \quad (12)$$

The relationship between $\underline{\chi}$ and $\underline{\hat{\chi}}$ is then

$$\underline{\hat{\chi}}=\underline{\chi}\,\underline{\eta} \ . \quad (13)$$

Equations (6)–(13) are rather obvious, though not quite trivial generalizations of the corresponding single species relations. Note, however, the order of the various quantities, in particular in (13). Note also that $\epsilon^{AB}\neq\epsilon^{BA}$. We will also need

$$\underline{\tilde{\epsilon}}=\mathbb{1}-\underline{\chi}\,\underline{\psi} \ . \quad (14)$$

In view of the fact that both $\underline{\chi}$ and $\underline{\hat{\chi}}$ are symmetric (this latter property is discussed below), $\tilde{\epsilon}^{AB}=\epsilon^{BA}$.

The dispersion relation for the longitudinal collective modes of the system now derive from the consistency condition of the system of equations (10) with the external excitation $\hat{\Phi}^A=0$:

$$||\underline{\epsilon}||=\mathbb{1}-\mathrm{tr}(\underline{\psi}\,\underline{\chi})+||\underline{\psi}||\,||\underline{\chi}||=0 \ . \quad (15)$$

The physical (scalar) dielectric function can conveniently be defined through the charge-density response. The charge density of species A is

$$\rho_A=eZ_A n^A \quad (16)$$

and the total charge density is evidently

$$\rho=eZ_{\bar{A}}n^{\bar{A}}=eZ_{\bar{A}}\hat{\chi}^{\bar{A}\bar{B}}\hat{\Phi}^{\bar{B}} \ . \quad (17)$$

The perturbation, in general, cannot of course be expressed merely in terms of the charge density. However, in practice, the perturbing wavelength is long enough to justify $k \ll \mu^{AB}$. In this situation $\psi^{AB}_{\vec{k}}\simeq Z_A\phi_{\vec{k}}Z_B$ and

$$\hat{\Phi}^B=Z_B Z_{\bar{C}}\hat{n}^{\bar{C}}\phi_{\vec{k}}$$
$$=\frac{1}{e}\phi_{\vec{k}}Z_B\hat{\rho} \ . \quad (18)$$

Combining (17) with (18) results in

$$\rho=\phi_{\vec{k}}Z_{\bar{A}}\hat{\chi}^{\bar{A}\bar{B}}Z_{\bar{B}}\hat{\rho} \ , \quad (19)$$

providing the external polarizability of species A, $\hat{\alpha}^A$, and the full external polarizability $\hat{\alpha}$ as

$$\hat{\alpha}^A=-\phi_{\vec{k}}Z_A\hat{\chi}^{A\bar{B}}Z_{\bar{B}} \ ,$$
$$\hat{\alpha}=\sum_A\hat{\alpha}^A=-\mathrm{tr}(\underline{\psi}\,\underline{\hat{\chi}}) \ . \quad (20)$$

Similar relations exist for the total polarizabilities

$$\alpha^A=-\phi_{\vec{k}}Z_A\chi^{A\bar{B}}Z_{\bar{B}} \ ,$$
$$\alpha=\sum_A\alpha^A=-\mathrm{tr}(\underline{\psi}\,\underline{\chi}) \ , \quad (21)$$

leading to the usual relationship between the polarizabilities and the dielectric response function ϵ,

$$\epsilon=1+\alpha=(1-\hat{\alpha})^{-1} \ . \quad (22)$$

There is no immediate relationship between the scalar ϵ and the matrix ϵ^{AB}. Also, there is a lack of consistency between the expressions obtained for $\hat{\alpha}$ as

$$\hat{\alpha}=\frac{\alpha}{\epsilon}=-\frac{1}{\epsilon}\mathrm{tr}(\underline{\psi}\,\underline{\chi}) \quad (23)$$

and as

$$\hat{\alpha}=\mathrm{tr}(\underline{\psi}\,\underline{\hat{\chi}})=-\mathrm{tr}(\underline{\psi}\,\underline{\chi}\,\underline{\epsilon}^{-1}) \ . \quad (24)$$

All this is not surprising in view of the approximate character of the derivation for α. Nevertheless, as long as the long wavelength limit is consistently imposed, or ψ is otherwise factorizable with $||\underline{\psi}||=0$, the consistency is restored and, as comparison of (15), (21), and (22) shows,

$$\epsilon=||\underline{\epsilon}|| \ . \quad (25)$$

Moreover, (23) and (24) are identical since

$$\mathrm{tr}[\underline{\gamma}(\mathbb{1}+\underline{\bar{\gamma}})]=\mathrm{tr}\underline{\gamma}+||\underline{\gamma}|| \ ,$$
$$\underline{\gamma}=\underline{\psi}\,\underline{\chi} \ , \quad (26)$$
$$\underline{\bar{\gamma}}=\text{cofactor of } \underline{\gamma} \ .$$

Two additional remarks are in order at this point. First, there is a certain arbitrariness obtained in defining ϵ^{AB} through the potential-potential response. Should one, for example, adopt the field-field response as the quantity around which ϵ^{AB} evolves, $\psi^{A\bar{C}}\chi^{\bar{C}B}$ would be replaced by $(Z_B/Z_A)\psi^{A\bar{C}}\chi^{\bar{C}B}$. Nevertheless, as it is easily seen, the only quantity of direct physical relevance $||\epsilon||$ would remain unchanged. As a second observation, one should note that we have avoided the definition of a partial polarizability α^{AB}. The introduction of such a quantity is neither natural, nor especially useful.

We now turn to the review of partial quadratic response functions. Again, the central role is played by the density-potential response functions $\hat{\chi}^{ABC}$ and χ^{ABC}. The second-order-density response is expressed as

$$n^{(2)A}(\vec{k},\omega)=\frac{1}{2\pi}\frac{1}{\mathscr{I}}\sum_{\vec{p},\vec{q}}\int d\nu\int d\mu\hat{\chi}^{A\bar{B}\bar{C}}(\vec{k},\omega;\vec{p},u,\vec{q},\nu)\times\hat{\Phi}^{\bar{B}}(\vec{p},\mu)\hat{\Phi}^{\bar{C}}(\vec{q},\nu)\delta_{\vec{k}-\vec{p}-\vec{q}}\delta(\omega-\mu-\nu)\ . \tag{27}$$

In the following we will omit the explicit indication of the $\vec{p}$, $\vec{q}$, μ, and ν summations and integrations, and the notation

$$n^{(2)A}=\hat{\chi}^{A\bar{B}\bar{C}}\hat{\Phi}^{\bar{B}}\hat{\Phi}^{\bar{C}} \tag{28}$$

will be understood to be equivalent to (27). A similar definition yields χ^{ABC}.

$$n^{(2)A}=\chi^{A\bar{B}\bar{C}}\Phi^{(1)\bar{B}}\Phi^{(1)\bar{C}}+\chi^{A\bar{B}}\Phi^{(2)\bar{B}}\ . \tag{29}$$

Comparison of (28) and (29) provides, in view of (10), the relationship

$$\hat{\chi}^{ABC}=\eta^{\bar{P}A}\chi^{\bar{P}\bar{Q}\bar{R}}\eta^{\bar{Q}B}\eta^{\bar{R}C}\ . \tag{30}$$

Quadratic polarizabilities can be derived within the long wavelength approximation as before

$$\begin{aligned}\rho^{(2)}&=eZ_{\bar{A}}n^{(2)\bar{A}}\\&=eZ_{\bar{A}}\hat{\chi}^{\bar{A}\bar{B}\bar{C}}\psi^{\bar{B}\bar{D}}_{\vec{p}}\psi^{\bar{C}\bar{E}}_{\vec{q}}\hat{n}^{\bar{D}}\hat{n}^{\bar{E}}\\&=eZ_{\bar{A}}\hat{\chi}^{\bar{A}\bar{B}\bar{C}}Z_{\bar{B}}Z_{\bar{D}}Z_{\bar{C}}Z_{\bar{E}}\phi_{\vec{p}}\phi_{\vec{q}}\hat{n}^{\bar{D}}\hat{n}^{\bar{E}}\\&=\frac{1}{e}Z_{\bar{A}}\hat{\chi}^{\bar{A}\bar{B}\bar{C}}Z_{\bar{B}}Z_{\bar{C}}\phi_{\vec{p}}\phi_{\vec{q}}\hat{\rho}\hat{\rho}\ .\end{aligned} \tag{31}$$

In contrast, however, to the linear theory where the two popular definitions of $\hat{\alpha}$, namely, $\hat{\alpha}=-\delta\rho/\delta\hat{\rho}$ and $\hat{\alpha}=-\delta E/\delta\hat{E}$ are equivalent, in the quadratic theory the corresponding quantities $-\delta^2\rho/\delta\hat{\rho}\,\delta\hat{\rho}$ and $-\delta^2 E/\delta\hat{E}\,\delta\hat{E}$ are not. While (31) leads to a "polarizability" based on the first relationship, we would rather adopt the electric field related polarizability which then acquires an additional factor, with the result

$$\begin{aligned}&\hat{\alpha}^{A}(\vec{p},\mu;\vec{q},\nu)=i\phi^{A\bar{B}\bar{C}}_{\vec{p}\,\vec{q}}\hat{\chi}^{A\bar{B}\bar{C}}(\vec{p},\mu;\vec{q},\nu)\ ,\\&\hat{\alpha}=\sum_A\hat{\alpha}^{A}=i(\underline{\phi}_{\vec{p}\,\vec{q}}\cdot\underline{\hat{\chi}})\end{aligned} \tag{32}$$

and

$$\begin{aligned}&\alpha^{A}(\vec{p},\mu;\vec{q},\nu)=i\phi^{ABC}_{\vec{p}\,\vec{q}}\chi^{A\bar{B}\bar{C}}(\vec{p},\mu;\vec{q},\nu)\ ,\\&\alpha=\sum_A\alpha^{A}=i(\underline{\phi}_{\vec{p}\,\vec{q}}\cdot\underline{\chi})\ m\end{aligned} \tag{33}$$

with

$$\phi^{ABC}_{\vec{p}\,\vec{q}}=\frac{4\pi e^3}{pq\,|\,\vec{p}+\vec{q}\,|}Z_AZ_BZ_C\ . \tag{34}$$

$(a\cdot b)$ is the contraction of a and b.

Finally, we discuss the symmetries of the linear and quadratic partial response functions. $\hat{\chi}^{AB}(\vec{k},\omega)$ satisfies the fluctuation-dissipation theorem which links it to $\langle n^{A}_{\vec{k}}(\omega)n^{*B}_{\vec{k}}(\omega)\rangle$ from which its symmetry under $A\leftrightarrow B$ interchange follows. $\chi^{AB}(\vec{k},\omega)$ obeys a similar symmetry as can be seen by recalling that $\chi=\hat{\chi}(1+\psi\hat{\chi})^{-1}$ and by representing $(1+\psi\hat{\chi})$ through its infinite series. These symmetries, however, as has already been pointed out, do not induce a similar symmetry in $\epsilon^{AB}(\vec{k},\omega)$, which, in general, is an asymmetric matrix.

The quadratic $\hat{\chi}^{ABC}(\vec{p},\mu;\vec{q},\nu)$ satisfies the nonlinear fluctuation-dissipation theorem which links it to $\langle n^{*A}_{\vec{p}+\vec{q}}(\mu+\nu)n^{B}_{\vec{p}}(\mu)n^{C}_{\vec{q}}(\nu)\rangle$. This establishes the symmetry of $\hat{\chi}$ under the interchange of the last two indices accompanied by the simultaneous interchange of the corresponding wave-vector and frequency arguments. There is, however, no symmetry with respect to interchange with the first index, since the analytic behavior of $\hat{\chi}$ with respect to the frequency $\omega=\mu+\nu$ on the one hand, and with respect to μ and ν on the other hand, are different. Nevertheless, in the static limit ($\mu=0$, $\nu=0$) the "triangle symmetry" with respect to the three vectors $-\vec{k}=(\vec{p}+\vec{q})$, $\vec{p},\vec{q}$ is not broken and therefore, $\hat{\chi}^{ABC}(\vec{p},0;\vec{q},0)\equiv\hat{\chi}^{ABC}_{\vec{p}\,\vec{q}}$ has a complete interchange symmetry with respect to any two of the three indices, accompanied by the simultaneous interchange of the wave-vector variables. Similar symmetry relations prevail for $\chi^{ABC}(\vec{p},\mu;\vec{q},\nu)$ as is easily demonstrated by examining the relationships $\chi^{ABC}=\epsilon^{A\bar{P}}\hat{\chi}^{\bar{P}\bar{Q}\bar{R}}\epsilon^{\bar{Q}B}\epsilon^{\bar{R}C}$.

III. RPA CALCULATION: LINEAR RESPONSE

The approach employed by earlier workers and also by our earlier work[3] for the calculation of the partial response functions generates the *external* (screened) response function $\hat{\chi}$. Indeed, the total response function χ is not even defined in these formalisms. The usual method, however, in the theory of the ordinary response functions emphasizes the total response function as the primary quantity. Such a method is feasible and not only more natural but also more expedient in the present case as well, and is discussed below.

The essential difference between $\hat{\chi}^{AB}(\vec{k},\omega)$ and $\chi^{AB}(\vec{k},\omega)$ within the RPA is that while the former, in general, possesses both diagonal and off-diagonal elements, the latter is always *diagonal.* This follows immediately from the fact that once the total species field is regarded as a perturbation, since it acts on its own species only, there is no mechanism by which it could couple to the density of any other species. In contrast, the external field as a perturbation is accompanied by the perturbations originating from all the other species indirectly excited by it through the interspecies coupling. This statement can be corroborated by the inspection of the Vlasov equation, as written down for the case when the external perturbation is explicitly displayed,

$$-i(\omega-\vec{k}\cdot\vec{v})F^{(1)A}(\vec{k},\omega;\vec{v})-i\left[\psi_{\vec{k}}^{A\bar{B}}n^{(1)\bar{B}}(\vec{k},\omega)\vec{k}\cdot\frac{\partial}{\partial\vec{v}}+\hat{\Phi}^{A}(\vec{k},\omega)\vec{k}\cdot\frac{\partial}{\partial\vec{v}}\right]F^{(0)A}(v)=0 \tag{35}$$

and when it is subsummed in the total field

$$-i(\omega-\vec{k}\cdot\vec{v})F^{(1)A}(\vec{k},\omega;\vec{v})-i\Phi^{(1)A}(\vec{k},\omega)\vec{k}\cdot\frac{\partial}{\partial\vec{v}}F^{(0)A}(v)=0\ . \tag{36}$$

Since in (35) both $F^{(1)A}$ (i.e., $n^{(1)A}$) and $n^{(1)B}$ are linked to $\hat{\Phi}^{A}$, while in (36) only $F^{(1)A}$ is linked to Φ^{A}, the difference is evident. Thus,

$$\chi^{AB}=\delta^{AB}\chi_{B}\ , \tag{37}$$

where χ_A (or χ_0 in index-free notation) is the surviving diagonal part of χ^{AB}, also,

$$\hat{\chi}^{AB}=\chi_{A}\eta^{AB}\ . \tag{38}$$

Explicitly we have

$$\hat{\chi}^{11}=\chi_1(1-\psi_{\vec{k}}^{22}\chi_2)\frac{1}{||\epsilon||}\ ,\qquad \hat{\chi}^{12}=\chi_1\psi_{\vec{k}}^{12}\chi_2\frac{1}{||\epsilon||}=\hat{\chi}^{21}\ , \tag{39}$$

with

$$||\epsilon||=1-\psi_{\vec{k}}^{11}\chi_1-\psi_{\vec{k}}^{22}\chi_2-\chi_1\chi_2||\psi_{\vec{k}}||\ . \tag{40}$$

Equations (39) and (40), in a somewhat lesser generality, have already been given by Refs. 1 and 3. The explicit RPA expression for $\chi_{\vec{A}}(\vec{k},\omega)$ is identical to the familiar one-component plasma (ocp) expression.[11] Here we note the simple static result

$$\chi_{A}(\vec{k},0)=-\beta n_{A}\equiv\chi_{A}\ . \tag{40a}$$

IV. RPA CALCULATION: QUADRATIC RESPONSE

Considerations similar to those given above apply to the difference between the quadratic external and total partial response functions. The latter is diagonal in the RPA, while the former is not. Again, a comparison of the quadratic Vlasov equation written down with the external perturbation

$$-i(\omega-\vec{k}\cdot\vec{v})F^{(2)A}(\vec{k},\omega;\vec{v})-i\psi_{\vec{k}}^{A\bar{B}}n^{(2)\bar{B}}(\vec{k},\omega)\vec{k}\cdot\frac{\partial}{\partial\vec{v}}F^{(0)A}(v)$$
$$-i\frac{1}{2\pi}\frac{1}{\mathscr{I}}\sum_{\vec{q}}\int d\mu\left[\psi_{\vec{q}}^{A\bar{B}}n^{(1)\bar{B}}(\vec{q},\mu)\vec{q}\cdot\frac{\partial}{\partial\vec{v}}+\hat{\Phi}^{A}(\vec{q},\mu)\vec{q}\cdot\frac{\partial}{\partial\vec{v}}\right]F^{(1)A}(\vec{k}-\vec{q},\omega-\mu;\vec{v})=0 \tag{41}$$

and in terms of the total field, only

$$-i(\omega-\vec{k}\cdot\vec{v})F^{(2)A}(\vec{k},\omega;\vec{v})-i\psi_{\vec{k}}^{A\bar{B}}n^{(2)B}(\vec{k},\omega)\vec{k}\cdot\frac{\partial}{\partial\vec{v}}F^{(0)A}(v)$$
$$-i\frac{1}{2\pi}\frac{1}{\mathscr{I}}\sum_{\vec{q}}\int d\mu\,\Phi^{(1)A}(\vec{q},\mu)\vec{q}\cdot\frac{\partial}{\partial\vec{v}}F^{(1)A}(\vec{k}-\vec{q},\omega-\mu;\vec{v})=0\ , \tag{42}$$

with the defining equations (28) and (29), proves the assertion.

The simple result is [see Eq. (30)], with χ_A as the surviving diagonal part of χ^{ABC},

$$\chi^{ABC}(\vec{q},\mu;\vec{p},\nu)=\delta^{AB}\delta^{CB}\chi_{A}(\vec{q},\mu;\vec{p},\nu) \tag{43}$$

$$\hat{\chi}^{ABC}(\vec{q},\mu;\vec{p},\nu)=\eta^{\bar{M}A}(\vec{k},\omega)\chi_{\bar{M}}(\vec{q},\mu;\vec{p},\nu)\eta^{\bar{M}B}(\vec{q},\mu)\times\eta^{\bar{M}C}(\vec{p},\nu)\ , \tag{44}$$
$$\vec{k}=\vec{p}+\vec{q},\quad \omega=\mu+\nu\ .$$

The two elements from which the others can be trivially generalized are explicitly given as follows:

$$\chi^{111}=[(1-\psi^{22}_{\vec{k}}\chi_2)X_1(1-\psi^{22}_{\vec{q}}\chi_2)(1-\psi^{22}_{\vec{p}}\chi_2)+(\psi^{21}_{\vec{k}}\chi_1)X_2(\psi^{21}_{\vec{q}}\chi_2)(\psi^{21}_{\vec{p}}\chi_2)]\frac{1}{||\epsilon||\,||\epsilon||\,||\epsilon||}\,, \quad (45)$$

$$\chi^{112}=[(1-\psi^{22}_{\vec{k}}\chi_2)X_1(1-\psi^{22}_{\vec{q}}\chi_2)(\psi^{12}_{\vec{p}}\chi_2)+(\psi^{21}_{\vec{k}}\chi_1)X_2(\psi^{21}_{\vec{q}}\chi_1)(1-\psi^{11}_{\vec{p}}\chi_1)]\frac{1}{||\epsilon||\,||\epsilon||\,||\epsilon||}\,,$$

$$\vec{k}=\vec{p}+\vec{q},\quad \omega=\mu+\nu\,, \quad (46)$$

with an obvious assignment of the wave-vector and frequency arguments. A less general equivalent of (45) and (46) where, however, the identification of the simple origin of the rather complicated final expressions is missing, has been reported before.[7] The explicit expression for $X_A(\vec{q},\mu;\vec{p},\nu)$, similarly to its linear counterpart, is identical to the ocp expression.[12] Again, we note the simple static result

$$X_A(\vec{q},0;\vec{p},0)=\tfrac{1}{2}\beta^2 n_A \equiv X_A\,. \quad (46a)$$

V. CORRELATIONAL CONTRIBUTIONS FOR WEAK COUPLING

The weak coupling correlation correction [to first order in the plasma parameter $(\gamma=\kappa^3/4\pi n)$] is of interest both structurally and as to the physical information it provides. From the structural point of view $\underline{\chi}$, to this order, ceases to be diagonal but shows an interesting factorization property. The most important physical information that can be inferred from the results of the calculation concerns the pair-correlation function and the static structure factor.

The calculation presented here is done in the static limit $(\omega=0)$ only. The full ω-dependent calculation of $\chi(\vec{k},\omega)$ to order γ would be an affair of much greater complexity and difficulty, as can be judged from the corresponding one-component calculation.[10] The method we follow for the static calculation is based on the variant of the quadratic fluctuation-dissipation theorem[13] which relates the perturbed two-point function $\langle n(\vec{x}_1)n(\vec{x}_2)\rangle^{(1)}$ and the equilibrium three-point function $\langle n(\vec{x}_1)n(\vec{x}_2)n(\vec{x}_3)\rangle^{(0)}$. In terms of their Fourier transforms one has

$$\langle n^A_{\vec{p}} n^B_{\vec{q}}\rangle^{(1)}=-\beta(S^{AB\bar{C}}_{\vec{p}\,\vec{q}}+N^A\delta_{\vec{p}}S^{B\bar{C}}_{\vec{q}}+N^B\delta_{\vec{q}}S^{A\bar{C}}_{\vec{p}})\hat{\Phi}^{\bar{C}}_{\vec{k}}\,, \quad (47)$$

where $S^{AB}_{\vec{q}}$ is the usual (linear) structure factor

$$S^{AB}_{\vec{q}}=\frac{1}{\mathscr{I}}(\langle n^A_{\vec{k}} n^B_{-\vec{k}}\rangle^{(0)}-N^AN^B\delta_{\vec{k}})\,, \quad (48)$$

$$S^{ABC}_{\vec{p}\,\vec{q}}=\frac{1}{\mathscr{I}}(\langle n^A_{\vec{p}} n^B_{\vec{q}} n^C_{-(\vec{p}+\vec{q})}\rangle^{(0)}-N^A\delta_{\vec{p}}S^{BC}_{\vec{q}}-N^B\delta_{\vec{q}}S^{CA}_{\vec{p}+\vec{q}}-N^C\delta_{\vec{p}+\vec{q}}S^{AB}_{\vec{p}}-N^AN^BN^C\delta_{\vec{p}}\delta_{\vec{q}})\,. \quad (49)$$

Another formulation of the quadratic FDT which will be used relates $S^{ABC}_{\vec{p}\,\vec{q}}$ to the quadratic response function $\hat{\chi}^{ABC}_{\vec{p}\,\vec{q}}$ by

$$\hat{\chi}^{ABC}_{\vec{p}\,\vec{q}}=\frac{\beta^2}{2}S^{ABC}_{\vec{p}\,\vec{q}}\,. \quad (50)$$

This should be compared with the corresponding linear relationship

$$\hat{\chi}^{AB}_{\vec{k}}=-\beta S^{AB}_{\vec{k}}\,. \quad (50a)$$

The calculation of the correlational contribution to $\underline{\chi}$ now proceeds by considering the first equation of the BGY hierarchy which states that

$$n^{(1)A}_{\vec{k}}=-\beta\left[\frac{1}{\mathscr{I}}\sum_{\vec{q}}\frac{\vec{k}\cdot\vec{q}}{k^2}\psi^{A\bar{B}}_{\vec{q}}\langle n^{\bar{B}}_{\vec{q}} n^A_{\vec{k}-\vec{q}}\rangle^{(1)}+n_A\hat{\Phi}^A_{\vec{k}}\right]. \quad (51)$$

Using now successively (47) and (50), one finds

$$n^{(1)A}_{\vec{k}}=\beta\left[\frac{\beta}{k^2}\sum_{\vec{q}}\vec{k}\cdot\vec{q}\psi^{A\bar{B}}_{\vec{q}}S^{A\bar{B}\bar{C}}_{\vec{k}-\vec{q},\vec{q}}+\beta n_A\psi^{A\bar{B}}_{\vec{k}}S^{\bar{B}\bar{C}}_{\vec{k}}-n_A\delta^{A\bar{C}}\right]\hat{\Phi}^{\bar{C}}_{\vec{k}} \quad (52)$$

$$=\left[\frac{2}{k^2}\sum_{\vec{q}}\vec{k}\cdot\vec{q}\psi^{A\bar{B}}_{\vec{q}}\hat{\chi}^{A\bar{B}\bar{C}}_{\vec{k}-\vec{q},\vec{q}}-\beta n_A(\delta^{A\bar{C}}+\psi^{A\bar{B}}_{\vec{k}}\hat{\chi}^{\bar{B}\bar{C}}_{\vec{k}})\right]\hat{\Phi}^{\bar{C}}_{\vec{k}} \quad (53)$$

or

$$\underline{\underline{\epsilon}}\,\underline{\hat{\chi}}=\underline{\chi}_0+\underline{\hat{v}}\,, \quad (54)$$

with[3]

$$\hat{v}^{AC}_{\vec{k}}=\frac{2}{k^2}\sum_{\vec{q}}\vec{k}\cdot\vec{q}\psi^{A\bar{B}}_{\vec{q}}\hat{\chi}^{A\bar{B}C}_{\vec{k}-\vec{q},\vec{q}}\,,$$
$$\epsilon^{AB}_{\vec{k}}=\delta^{AB}-\psi^{AB}_{\vec{k}}\chi_B\,. \quad (55)$$

Equations (54) and (55) provide the correlational contribution through $\hat{v}$ to arbitrary order in the coupling. To obtain the lowest, i.e., first-order contribution, we set

$$\underline{\hat{\chi}}=\underline{\hat{\chi}}_0+\delta\underline{\hat{\chi}} \quad (56)$$

and replaces $\hat{\chi}^{ABC}_{\vec{p}\,\vec{q}}$ by its RPA value [cf. (44)]

$$\delta\hat{\chi}^{AB}_{\vec{k}}=\eta^{\bar{C}A}_{\vec{k}}\hat{v}^{\bar{C}B}_{\vec{k}}=-\frac{\beta}{k^2}\eta^{\bar{M}A}_{\vec{k}}\eta^{\bar{S}B}_{\vec{k}}\chi_{\bar{S}}\sum_{\vec{q}}\vec{k}\cdot\vec{q}\psi^{\bar{M}\bar{N}}_{\vec{q}}\eta^{\bar{S}\bar{M}}_{\vec{p}}\eta^{\bar{S}\bar{N}}_{\vec{q}}\,, \quad (57)$$
$$\vec{p}=\vec{k}-\vec{q}\,.$$

From the relationship $\underline{\chi}=\underline{\hat{\chi}}\,\underline{\epsilon}$, it follows that

$$\delta\underline{\chi}=\underline{\underline{\epsilon}}\,\delta\underline{\hat{\chi}}\,\underline{\epsilon} \quad (58)$$

and thus

$$\delta\chi^{AB}_{\vec{k}}=-\frac{\beta}{k^2}\sum_{\vec{q}}\vec{k}\cdot\vec{q}\psi^{A\bar{N}}_{\vec{q}}\eta^{B\bar{N}}_{\vec{q}}\eta^{BA}_{\vec{p}}\chi_B,\quad \vec{p}=\vec{k}-\vec{q}\,. \quad (59)$$

The required symmetry of χ (or of $\hat{\chi}$) ($\chi^{AB}=\chi^{BA}$) is not manifest. It can, however, be observed by the explicit calculation of its elements which we now display:

$$\delta\chi^{11}_{\vec{k}}=-\frac{\beta}{k^2}\sum_{\vec{q}}\frac{\vec{k}\cdot\vec{q}}{||\epsilon_{\vec{q}}||\,||\epsilon_{\vec{p}}||}\times(\psi^{11}_{\vec{q}}-\chi_2||\underline{\psi}_{\vec{q}}||)(1-\psi^{22}_{\vec{p}}\chi_2)\chi_1\,,$$

$$\delta\chi^{12}_{\vec{k}}=-\frac{\beta}{k^2}\sum_{\vec{q}}\frac{\vec{k}\cdot\vec{q}}{||\epsilon_{\vec{q}}||\,||\epsilon_{\vec{p}}||}\psi^{12}_{\vec{q}}\psi^{12}_{\vec{p}}\chi_1\chi_2,\quad \vec{p}=\vec{k}-\vec{q}\,. \tag{60}$$

In our earlier work[3] the lack of manifest symmetry led us to the erroneous statement that the symmetry was broken by the approximation procedure. This is apparently not the case.

We now specialize to the case of pure Coulomb interaction

$$\psi^{AB}_{\vec{k}}=Z_AZ_B\phi_{\vec{k}}\,. \tag{61}$$

One easily finds

$$\delta\chi^{11}_{\vec{k}}=\beta\frac{\kappa_1^2}{k^2}\sum_{\vec{q}}\vec{k}\cdot\vec{q}^{\,q^2}\frac{1}{\epsilon_{\vec{q}}\epsilon_{\vec{p}}}\left[1+\frac{\kappa_2^2}{p^2}\right]$$
$$=-\beta\frac{\kappa_1^4}{k^4}\sum_{\vec{q}}\frac{\vec{k}\cdot\vec{q}}{k^2}\frac{\alpha_{\vec{q}}}{\epsilon_{\vec{q}}}\frac{\alpha_{\vec{p}}}{\epsilon_{\vec{p}}}\,, \tag{62a}$$

$$\delta\chi^{12}_{\vec{k}}=-\beta\frac{\kappa_1^2\kappa_2^2}{\kappa^4}\sum_{\vec{q}}\frac{\vec{k}\cdot\vec{q}}{k^2}\frac{\alpha_{\vec{q}}\alpha_{\vec{p}}}{\epsilon_{\vec{q}}\epsilon_{\vec{p}}},\quad p=\vec{k}-\vec{q} \tag{62b}$$

with

$$\alpha_{\vec{q}}=\kappa^2/q^2\,,$$
$$\kappa^2=\kappa_1^2+\kappa_2^2\,, \tag{63}$$
$$\kappa_A^2=4\pi e^2 n_A\beta Z_A^2\,,$$
$$\epsilon_{\vec{q}}=1+\alpha_{\vec{q}}\,.$$

The $\vec{q}$ summation can easily be done:

$$\frac{1}{\mathscr{I}}\sum_{\vec{q}}\frac{\vec{k}\cdot\vec{q}}{k^2}\frac{\alpha_{\vec{q}}\alpha_{\vec{p}}}{\epsilon_{\vec{q}}\epsilon_{\vec{p}}}$$
$$=\frac{1}{(2\pi)^2}\frac{1}{x}\kappa^3\times\int dy\,y^3\int d\mu\,\mu\frac{1}{(1+y^2)(1+x^2+y^2-2\mu xy)}$$
$$=\gamma nP_{\vec{k}},\quad \vec{p}=\vec{k}-\vec{q},\quad x=\frac{k}{\kappa} \tag{64}$$

where γ is the nominal coupling parameter

$$\gamma=\frac{\kappa^3}{4\pi n}$$

and

$$n=n_1+n_2\,,$$
$$P_{\vec{k}}=P(x)=\frac{1}{2x}\tan^{-1}\frac{x}{2}\,. \tag{65}$$

Thus (62a) and (62b) can be combined into

$$\delta\chi^{AB}_{\vec{k}}=-\gamma\beta n\frac{\kappa_A^2\kappa_B^2}{\kappa^4}P_{\vec{k}}\,. \tag{66}$$

The correlational correction to the polarizability can be evaluated according to (20);

$$\delta\alpha_{\vec{k}}=\gamma\zeta^2\frac{1}{x^2}P_{\vec{k}}\,. \tag{67}$$

The effective charge ζ is given by

$$\zeta=\frac{Z_{\bar{A}}\kappa_{\bar{A}}^2}{\kappa^2}=\frac{Z_{\bar{A}}^3n_{\bar{A}}}{Z_{\bar{A}}^2n_{\bar{A}}}\,. \tag{68}$$

We note that $\delta\alpha=0$ when $Z_1^3n_1+Z_2^3n_2=0$. In the charge-neutral case ($Z_1n_1+Z_2n_2=0$), this reduces to the well-known condition[10] $|Z_1|=|Z_2|$.

VI. PAIR-CORRELATION FUNCTIONS

The pair-correlation functions follow from the relationship

$$n_A(\delta^{AB}+n_Bg^{AB}_{\vec{k}})=S^{AB}_{\vec{k}} \tag{69}$$

and from the FDT (50a). To lowest order one finds

$$g^{11}_{\vec{k}}=-\beta\frac{\psi^{11}_{\vec{k}}+\beta n_2||\underline{\psi}_{\vec{k}}||}{||\epsilon_{\vec{k}}||}\,,$$

$$g^{12}_{\vec{k}}=-\beta\frac{\psi^{12}_{\vec{k}}}{||\epsilon_{\vec{k}}||}\,, \tag{70}$$

$$||\epsilon_{\vec{k}}||=1+\beta n_1\psi^{11}_{\vec{k}}+\beta n_2\psi^{22}_{\vec{k}}+\beta^2n_1n_2||\underline{\psi}_{\vec{k}}||\,.$$

We note that for nonfactorizable interaction ($||\underline{\psi}_{\vec{k}}||\neq 0$), $g^{11}_{\vec{k}}$ or $g^{22}_{\vec{k}}$ are not necessarily governed by the behavior of $\psi^{11}_{\vec{k}}$ or $\psi^{22}_{\vec{k}}$. In particular g can exhibit attractive features even for repulsive interaction. The details of this unusual behavior are discussed elsewhere.[16]

The next-order term in the pair-correlation functions can be calculated from $\delta\hat{\chi}$. The general expression, however, is too cumbersome to be displayed here. We will, nevertheless, consider, the Coulomb case in detail.

Using now, in addition to (69) and (50), (66) and (58), one finds

$$n_An_B\,\delta g^{AB}_{\vec{k}}=\gamma\frac{n}{\kappa^4}\kappa_{\bar{C}}^2\eta^{\bar{C}A}_{\vec{k}}\kappa_{\bar{D}}^2\eta^{\bar{D}B}_{\vec{k}}P_{\vec{k}}\,, \tag{71}$$

or, more explicitly, including the lowest-order term,

$$g^{11}_{\vec{k}} = -\beta Z_1^2 \frac{\phi_{\vec{k}}}{\epsilon_{\vec{k}}} + \gamma \frac{n}{n_1^2} \frac{\kappa_1^4}{\kappa^4} \left[1 + \left[1 - \frac{Z_2}{Z_1} \right] \frac{\kappa_2^2}{k^2} \right]^2 \frac{P_{\vec{k}}}{\epsilon^2_{\vec{k}}} , \tag{72}$$

$$g^{12}_{\vec{k}} = -\beta Z_1 Z_2 \frac{\phi_{\vec{k}}}{\epsilon_{\vec{k}}} + \gamma \frac{n}{n_1 n_2} \frac{\kappa_1^2 \kappa_2^2}{\kappa^4} \times \left[1 + \left[1 - \frac{Z_2}{Z_1} \right] \frac{\kappa_2^2}{k^2} \right] \cdot \left[1 + \left[1 - \frac{Z_1}{Z_2} \right] \frac{\kappa_1^2}{k^2} \right] \frac{P_{\vec{k}}}{\epsilon^2_{\vec{k}}} .$$

In a binary system where both $Z_1 > 0$ and $Z_2 > 0$, there is a qualitative difference between the behavior of the two correlation functions $\delta g^{11}_{\vec{k}}$ and $\delta g^{22}_{\vec{k}}$. If, for instance, $Z_2 > Z_1$ then $\delta g^{11}_{\vec{k}}$ and $\delta g^{12}_{\vec{k}}$ develop a nonmonotonic behavior, while $\delta g^{22}_{\vec{k}}$ stays monotonic.

For a charge-neutral system $(Z_1 n_1 + Z_2 n_2 = 0)$, a convenient form of (72) is

$$n_1 g^{11}_{\vec{k}} = \frac{|Z_1|}{|Z_1| + |Z_2|} \frac{-\alpha_{\vec{k}}}{\epsilon_{\vec{k}}} + \gamma \frac{|Z_1|}{|Z_2|} \left[1 + \frac{|Z_2|}{|Z_1|} \alpha_{\vec{k}} \right]^2 \frac{P_{\vec{k}}}{\epsilon^2_{\vec{k}}} , \tag{73}$$

$$\sqrt{n_1 n_2} g^{12}_{\vec{k}} = \frac{(|Z_1 Z_2|)^{1/2}}{|Z_1| + |Z_2|} + \frac{\alpha_{\vec{k}}}{\epsilon_{\vec{k}}} + \gamma \left[1 + \frac{|Z_2|}{|Z_1|} \alpha_{\vec{k}} \right] \left[1 + \frac{|Z_1|}{|Z_2|} \alpha_{\vec{k}} \right] \frac{P_{\vec{k}}}{\epsilon^2_{\vec{k}}} .$$

The charge-neutral expression (73) is equivalent to a form derived earlier from the second BGY equation by Yatom and Shima.[11] The general expression (72), valid also for binary systems, is, however, reported here for the first time.

VII. MEAN-FIELD THEORIES

For strong coupling various nonperturbative approximation methods have been developed for the ocp.[6,14] Prominent among these approaches are the mean-field theories whose principle thesis is that a static effective potential replacing the bare Coulomb potential in the reponse function can provide an adequate approximate description for the system. The question of generalization of the mean-field approximations for multispecies systems, of the correct incorporation of the effective potential in the partial response functions, and, finally, the question whether a particular approximation scheme preserves the required $\chi^{AB} = \chi^{BA}$ symmetry of the response functions, are not trivial and are the subjects of the present section.

For the purpose of the discussion of the response functions, we can now assume that a recipe for the determination of a static effective potential has been found such that

$$\psi^{AB}_{\vec{k}} \rightarrow \psi^{AB}_{\vec{k}} + \omega^{AB}_{\vec{k}} . \tag{74}$$

The replacement affects the interaction between particles, but has no bearing on the external potential, that is, on its relationship between the external density perturbation which remains

$$\hat{\phi}^A = \psi^{A\bar{C}}_{\vec{k}} \hat{n}_{\bar{C}} .$$

Similarly,

$$\phi^A = \psi^{A\bar{C}}_{\vec{k}} n_{\bar{C}} .$$

If this distinction is not made, one is led to the generalization of the early version of the mean-field theory, due to Hubbard,[15] the inadequacy of which is well known.[2,6] The calculation of the response function now can proceed along two possible avenues. One can consider either the external field $\hat{\phi}$ or the total field ϕ as the perturbation. While earlier works[1,3] followed exclusively the first approach, the second is considerably more transparent and natural, and will be adopted here. The simple observation which immediately provides the calculational prescription for the response function follows from the comparison of the mean-field equation with ϕ as a perturbation and the Vlasov equation with $\hat{\phi}$ as a perturbation. In the former situation the residual ω^{AB} interaction not included in ϕ^A plays the same role in coupling the different species to each other as the bare interaction ψ^{AB} in the latter situation. Thus, by defining a pseudodielectric matrix $\underline{e}$

$$\underline{e} = \underline{1} - \underline{\omega} \underline{\chi}_0 , \tag{75}$$

the expression for χ can be written down immediately as

$$\underline{\chi} = \underline{\chi}_0 \underline{e}^{-1} \tag{76}$$

or, more explicitly,

$$\chi^{11}(\vec{k},\omega) = \frac{1}{||\underline{e}(\vec{k},\omega)||} \chi_1(\vec{k},\omega)[1 - \omega^{22}_{\vec{k}} \chi_2(\vec{k},\omega)] ,$$
$$\chi^{12}(\vec{k},\omega) = \frac{1}{||\underline{e}(\vec{k},\omega)||} \chi_1(\vec{k},\omega) \chi_2(\vec{k},\omega) \omega^{12}_{\vec{k}} , \tag{77}$$

with

$$||\underline{e}|| = 1 - \omega^{11}\chi_1 - \omega^{22}\chi_2 + \chi_1 \chi_2 ||\underline{\omega}|| . \tag{78}$$

The external response function is then given by

$$\underline{\hat{\chi}} = \underline{\chi}_0 \underline{e}^{-1} \underline{\eta} , \tag{79}$$

where

$$\underline{\eta}^{-1} = \underline{\epsilon} = \underline{1} - \underline{\psi} \underline{\chi}_0 \underline{e}^{-1} . \tag{80}$$

On the other hand, adopting the picture where the external potential $\hat{\phi}$ is regarded as the primary perturbation, one can determine χ directly by observing that in this case the total effective potential $\psi^{AB}_{\vec{k}} + \omega^{AB}_{\vec{k}}$ couples the different species and thus introducing a second pseudodielectric matrix $\hat{\underline{e}}$:

$$\hat{\underline{e}} = \underline{1} - (\underline{\psi} + \underline{\omega}) \underline{\chi}_0 , \tag{81}$$

with the aid of which $\underline{\hat{\chi}}$ is expressed as

$$\underline{\hat{\chi}} = \underline{\chi}_0 \hat{\underline{e}}^{-1} . \tag{82}$$

Explicitly this becomes

$$\hat{\chi}^{11}(\vec{k},\omega)=\frac{1}{\|\hat{\underline{\epsilon}}(\vec{k},\omega)\|}\chi_1(\vec{k},\omega)[1-(\psi_{\vec{k}}^{22}+\omega_{\vec{k}}^{22})\chi_2(\vec{k},\omega)]\ ,$$
$$\hat{\chi}^{12}(\vec{k},\omega)=\frac{1}{\|\hat{\underline{\epsilon}}(\vec{k},\omega)\|}\chi_1(\vec{k},\omega)\chi_2(\vec{k},\omega)(\psi_{\vec{k}}^{12}+\omega_{\vec{k}}^{12})\ . \tag{83}$$

The equivalence of (82) and (79) follows immediately from the matrix relationship

$$(\underline{1}-\underline{A})^{-1}[\underline{1}-\underline{B}(\underline{1}-\underline{A})^{-1}]^{-1}=(\underline{1}-\underline{A}-\underline{B})^{-1}\ ,$$
$$\underline{A}=\underline{\omega}\underline{\chi}_0\ , \tag{84}$$
$$\underline{B}=\underline{\psi}\underline{\chi}_0\ .$$

Equation (83) is the relationship that has been given in earlier works.[1,3] It should be noted that in spite of the somewhat deceptive structure of (83), $\hat{\underline{\epsilon}}(\vec{k},\omega)$ is not the dielectric matrix of the system. It is $\underline{\epsilon}(\vec{k},\omega)$ as given by (80). Nevertheless, the dispersion relation is correctly provided by

$$\|\hat{\underline{\epsilon}}(\vec{k},\omega)\|=\|\underline{e}(\vec{k},\omega)\|\ \|\underline{\epsilon}(\vec{k},\omega)\|=0\ . \tag{85}$$

In order to establish a consistency condition for the mean-field theory, we expand (76) in γ and calculate the first-order term. Since ω is at least of order γ, one finds

$$\chi^{AB}=\chi_A(\delta^{AB}+\omega^{AB}\chi_B)\ . \tag{86}$$

Comparing this with (59) in the static limit one can conclude that to lowest order ω^{AB} has to satisfy

$$n_A\omega_{\vec{k}}^{AB}=\frac{1}{k^2}\sum_{\vec{q}}\vec{k}\cdot\vec{q}\psi_{\vec{q}}^{A\bar{N}}\eta_{\vec{q}}^{B\bar{N}}\eta_{\vec{p}}^{BA},\quad \vec{p}=\vec{k}-\vec{q}\ . \tag{87}$$

The simplest mean-field theory of Singwi, Tosi, Land, and Sjolander (STLS), when transcribed into multispecies language,[1,3] yields an effective potential determined by

$$\omega_{\vec{k}}^{AB}=\frac{1}{k^2}\sum_{\vec{q}}\vec{k}\cdot\vec{q}\psi_{\vec{q}}^{AB}g_{\vec{p}}^{AB},\quad \vec{p}=\vec{k}-\vec{q}\ . \tag{88}$$

Expanded to first order and combined with the FDT, (88) becomes

$$n_A\omega_{\vec{k}}^{AB}=\frac{1}{k^2}\sum_{\vec{q}}\vec{k}\cdot\vec{q}\psi_{\vec{q}}^{AB}\eta_{\vec{p}}^{BA},\quad \vec{p}=\vec{k}-\vec{q}\ . \tag{89}$$

There is an obvious discrepancy between (89) and (87), manifested by the absence of the $\eta_{\vec{q}}$ term in (89). This is not surprising. The defect of the STLS approximation in failing to reproduce the lowest-order perturbational correction in the ocp is well known.[6] On the other hand, the STLS approximation is entirely satisfactory as far as the required symmetry of ω^{AB} is concerned. Equation (88) provides a manifestly symmetric ω^{AB}.

The other known mean-field approximation scheme, which in the ocp case is known to be free of the abovementioned difficulty, is attributed to Ichimaru and Totsuji[4] (IT). It is based on a cluster decomposition of the three-body correlation function in a manner which is exact in the small-γ limit. In order to find the multicomponent generalization of the IT expression we start with the equivalent of Eq. (55) written in structure function language

$$\hat{v}_{\vec{k}}^{AC}=\frac{\beta^2}{k^2}\sum_{\vec{q}}\vec{k}\cdot\vec{q}\psi_{\vec{q}}^{A\bar{B}}S_{\vec{p},\vec{q}}^{A\bar{B}C},\quad \vec{k}=\vec{p}-\vec{q}\ . \tag{90}$$

To lowest order $S_{\vec{p}\,\vec{q}}^{ABC}$ is decomposable[3] as

$$S_{\vec{p}\,\vec{q}}^{ABC}=\delta^{AB}\delta^{AC}n_A+\delta^{AB}n_Bn_Cg_{\vec{k}}^{BC}+\delta^{BC}n_cn_Ag_{\vec{p}}^{CA}$$
$$+\delta^{CA}n_An_Cg_q^{AB}$$
$$+n_An_Bn_C(g_{\vec{p}}^{AB}g_{\vec{k}}^{BC}+g_{\vec{q}}^{BC}g_{\vec{p}}^{CA}+g_{\vec{k}}^{CA}g_{\vec{q}}^{AB})$$
$$+n_An_Bn_Cn_{\bar{D}}g_p^{A\bar{D}}g_{\vec{q}}^{B\bar{D}}g_{\vec{k}}^{C\bar{D}}\ . \tag{91}$$

The validity of (91) for arbitrary coupling is the basic assumption of the approximation. Substituting (91) into (90) one finds

$$\hat{v}_{\vec{k}}^{AC}=-\frac{\beta}{k^2}n_A\sum_{\vec{q}}\vec{k}\cdot\vec{q}\psi_{\vec{q}}^{A\bar{B}}(\delta_{\vec{q}}^{\bar{B}\bar{D}}+n_{\bar{B}}g_{\vec{q}}^{\bar{B}\bar{D}})g_{\vec{p}}^{A\bar{D}}\hat{\chi}_{\vec{k}}^{\bar{D}C}\ , \tag{92}$$
$$\vec{p}=\vec{k}-\vec{q}\ .$$

Combining (92) with (54) and then comparing the resulting relationship with (82) and (74), we can conclude that

$$\omega_{\vec{k}}^{AD}=\frac{1}{k^2}\sum_{\vec{q}}\vec{k}\cdot\vec{q}\psi_{\vec{q}}^{A\bar{B}}(\delta^{\bar{B}D}+n_{\bar{B}}g_{\vec{q}}^{\bar{B}D})g_{\vec{p}}^{AD},\quad \vec{p}=\vec{k}-\vec{q}\ . \tag{93}$$

The small-γ expansion of (93) can now again be compared with (87). The expansion yields

$$n_A\omega_{\vec{k}}^{AB}=\frac{1}{k^2}\sum_{\vec{q}}\vec{k}\cdot\vec{q}\psi_{\vec{q}}^{A\bar{N}}\eta_{\vec{q}}^{B\bar{N}}\eta_{\vec{p}}^{BA},\quad \vec{p}=\vec{k}-\vec{q}\ , \tag{94}$$

that is, it is in complete agreement with (87). This feature is again expected on the basis of the similar ocp behavior.

In contrast, however, to the STLS approximation, the structure of the $\omega_{\vec{k}}^{AB}$ in the IT approximation, Eq. (93), does not exhibit a manifest AB symmetry. To first order, of course, since $\omega_{\vec{k}}^{AB}$ agrees with the exact expression, the symmetry, nevertheless, emerges. As a quick calculation can show, however, this lucky state of affairs does not continue beyond the first order. Even in the second-order term the symmetry is explicitly broken. We must, therefore, conclude that in the multicomponent case the IT scheme is not acceptable.

VIII. CONCLUSIONS

We have demonstrated that a compact and transparent way of handling the rather unwieldy-looking partial response functions exists. The central idea in this formalism is the introduction of the partial density response functions responding to the *total* field, and of the dielectric matrix in species space. For a general interspecies interaction $\psi^{AB}(r)$ the determinant $\|\underline{\psi}\|$ plays an important role. Simple known results are recovered only when $\|\underline{\psi}\|=0$. We have displayed a relationship expressing the correlational part of the linear density response function in terms of the quadratic density response function. This is a generalization of the corresponding ocp relationship.[13]

Using this formalism we have been able to calculate with ease the first order $O(\gamma)$ correlational correction to the static partial density response function. From this the $O(\gamma^2)$ corrections to the pair-correlation functions g_{11}, g_{12}, and g_{22} followed both for charge-neutralized (electron-ion) and binary-ion-mixture plasmas. The latter displays a somewhat unexpected structure. Finally, we have analyzed the structure of the partial response functions in the mean-field-theory approximation in strongly coupled plasmas. We have found that the required symmetry of the response function is not automatically guaranteed, and could, indeed be violated.

ACKNOWLEDGMENTS

This work was partially supported by U. S. Air Force Office of Scientific Research AFOSR Grant No. 81-0089 and by National Science Foundation Grants ECS-81-18616 and ECS-81-07449.

---

[1]P. Vashishta, P. Bhattacaryya, and K. S. Singwi, Phys. Rev. B 10, 5108 (1974); Nuovo Cimento B 23, 172 (1974); see also P. C. Martin and J. Schwinger, Phys. Rev. 115, 1342 (1959) for an earlier introduction of similar ideas.

[2]K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjolander, Phys. Rev. 176, 589 (1968); K. S. Singwi, A. Sjolander, M. P. Tosi, and R. H. Land, Solid State Commun. 7, 1503 (1969); Phys. Rev. B 1, 1044 (1970).

[3]K. I. Golden and G. Kalman, Phys. Rev. A 14, 1802 (1976).

[4]S. Ichimaru, Phys. Rev. A 2, 494 (1970); H. Totsuji and S. Ichimaru, Progr. Theor. Phys. 50, 753 (1973); 52, 42 (1974); S. Ichimaru, in *Strongly Coupled Plasmas,* edited by G. Kalman (Plenum, New York, 1978).

[5]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).

[6]G. Kalman, in *Strongly Coupled Plasmas,* edited by G. Kalman (Plenum, New York, 1978).

[7]K. I. Golden and De-xin Lu, J. Stat. Phys. 29, 281 (1982).

[8]Y. Shima, H. Yatom, K. I. Golden, and G. Kalman, Phys. Rev. A 22, 2818 (1980).

[9]T. Dunn and A. A. Broyles, Phys. Rev. A 157, 156 (1967); M. M. Gombert and C. Deutsch, Phys. Lett. 47A, 473 (1974); C. Deutsch and M. M. Gombert, J. Math. Phys. 17, 1077 (1976); C. Deutsch, *ibid.* 17, 1404 (1976); W. Ebeling, W. D. Kraeft, and D. Kremp, *Theory of Bound States and Ionization Equilibrium in Plasmas and Solids* (Akademie, Berlin, 1976). (a) C. Deutsch, M. M. Gombert, and H. Minou, Phys. Lett. 66A, 381 (1979); (b) C. Deutsch, Y. Furutani, and M. M. Gombert, Phys. Reports 69, 86 (1981).

[10]J. Coste, Nucl. Fusion 5, 293 (1965).

[11]H. Yatom and T. Shima, Phys. Rev. A 18, 1291 (1978).

[12]See, e.g., S. Ichimaru, *Basic Principles of Plasma Physics* (Benjamin, New York, 1973).

[13]K. I. Golden and G. Kalman, Ann. Phys. (N.Y.) 143, 160 (1982).

[14]M. Baus and J. P. Hansen, Phys. Rep. 59, 1 (1980).

[15]J. Hubbard, Phys. Lett. 25A, 709 (1967).

[16]A. Kalman (unpublished).