Dynamical theory of strongly coupled two-dimensional Coulomb fluids in the weakly degenerate quantum domain

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We study the problem of dynamical response and plasma mode dispersion in strongly coupled twodimensional Coulomb fluids (2DCFs) in the weakly degenerate quantum domain. Adapting the nonlinear response function approach of Golden and Kalman [Phys. Rev. A **19**, 2112 (1979)] to the 2DCF, we construct a self-consistent approximation scheme for the calculation of the density response functions and plasma mode dispersion at long wavelengths. The basic ingredients in the construction are (i) the first kinetic equation in the Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy, (ii) the velocity-average-approximation (VAA) hypothesis, (iii) the quadratic fluctuation-dissipation theorem, and (iv) the dynamical superposition approximation (DSA) closure hypothesis. The reliability of the VAA-DSA theory can be assessed by observing that the principal coupling correction to the 2D temperature-dependent Lindhard function is identified as being precisely the part of the third-frequency-moment sum-rule coefficient proportional to the potential energy.

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I. INTRODUCTION

This paper addresses the problem of dynamical response and plasma mode dispersion in strongly coupled twodimensional Coulomb fluids in the weakly degenerate quantum domain. External magnetic fields are assumed to be entirely absent.

The two-dimensional Coulomb fluid (2DCF) is an idealized model one-component plasma (OCP) in which charged particle motions in a uniform rigid neutralizing background are restricted to a two-dimensional (2D) plane of zero thickness. The charges interact via the $\nu(r) = e^2/(\epsilon_s r)$ Coulomb potential, r being the separation distance in the plane and ϵ_s the dielectric constant of the substrate. In the classical (\hbar $\rightarrow 0$) domain, the coupling parameter $\Gamma_{cl} = \beta e^2 / (\epsilon_s a)$ is the customary measure of the strength of the particle correlations; $\beta^{-1} = k_B T$ is the 2D thermal energy and $a = 1/\sqrt{\pi n}$ is the interparticle distance. In the zero-temperature quantum domain the customary coupling parameter is $r_s = a/a_0$; a_0 $=\hbar^2 \epsilon_s / (m^* e^2)$ is the effective Bohr radius with m^* the effective mass. For arbitrary degeneracy, Γ $=e^{2}/(\epsilon_{s}a\langle E_{\rm kin}\rangle_{0})$ is the appropriate measure of the coupling strength, $\langle E_{\rm kin} \rangle_0$ being the average kinetic energy for a 2DCF of noninteracting particles; $\Gamma \rightarrow \Gamma_{cl}$ as $\hbar \rightarrow 0$ and $\Gamma \rightarrow 2r_s$ as $T \rightarrow 0$. The 2DCF is said to be strongly coupled when Γ > 1.

Over the past three decades a variety of theoretical approaches have been put forward for the calculation of the dynamical response and plasma mode behavior in the strongly coupled 2DCF. In the classical domain, formulas for the density response function and dispersion and damping of

the plasma mode excitations have been derived (i) by following a microscopic hydrodynamic approach [1], (ii) by adapting the conventional Singwi-Tosi-Land-Sjolander (STLS) [2] mean field theory approach to the 2D one-component plasma [3], (iii) by following an approach that combines the quadratic fluctuation-dissipation theorem (QFDT) with linearized moment equations for the plasma density, fluid velocity, pressure tensor, and heat-flow tensor [4], and (iv) by adapting the quasilocalized charge approximation (QLCA) [5] to the 2D OCP [6]. In the zero-temperature quantum domain, the density response function has been calculated and plasmon dispersion curves have been generated (v) by using the STLS approach-or a sum-rule version of it-with the 2D Vlasov density response function replaced by the Lindhard function [7-9]. (vi) via a 2D quantum kinetic equation treatment using a Mori memory function formalism that takes account of the dynamics of the exchange-correlation hole surrounding each electron [10], and (vii) more recently, by application of a quantum version [11] of the STLS approach to the 2D electron fluid [12].

The calculation of the dynamical response and plasma mode dispersion in the strongly coupled 2DCF at degeneracy levels somewhere between the classical and zero-temperature limits, is, to the best of our knowledge, a problem that has received very little attention. The present paper begins to explore this problem by considering the above calculation in the weakly degenerate quantum domain $\beta \epsilon_F = \beta \pi n \hbar^2 / m^* \leq (\beta \epsilon_F)_{\text{max}}$, where we take $(\beta \epsilon_F)_{\text{max}} \approx 0.1-0.2$. Examples of the strongly coupled 2DCF in the weakly degenerate quantum domain are (i) the 2D hole layer in a GaAs/Al_xGa_{1-x}As heterostructure $(n=2.5\times10^{10} \text{ cm}^{-2}, T$ = 5.78 K, $m^*=0.6m_e$, $\beta \epsilon_F=0.2$, $\Gamma=6.17$) [13] and (ii) the 2D electron layer trapped on the free surface of liquid helium $(n = 10^9 \text{ cm}^{-2}, T = 2.77 \text{ K}, \beta \epsilon_F = 0.01, \Gamma = 33.7)$ [14].

In calculating the dynamical response, we will suppose that a classical kinetic theory based response function approach, proposed some time ago by Golden and Kalman (GK) [15] for the 3D OCP, can be adapted to the weakly degenerate 2DCF of the present paper. This adaptation reasonably well approximates the dynamics provided that $\beta \epsilon_F$ is sufficiently small and exchange effects are properly taken into account. In Sec. III we propose a strategy suggested by the third-frequency-moment sum rule for incorporating exchange in the modified GK approach.

The principal building blocks for construction of the modified approach are (i) the first kinetic equation of the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy linking the one- and two-particle distribution functions (labeled f_1 and f_2) and (ii) the classical 2D QFDT linking quadratic response and three-point structure functions [16]. The central hypothesis of the theory, the velocity-average approximation (VAA) [see Eq. (20) below], supposes that the non-RPA (random-phase approximation) part of f_2 can be replaced by a suitably chosen momentum average.

In the GK theory, a chain of density-response-function equations can be generated solely from the first BBGKY kinetic equation by combining it with the hierarchy of fluctuation-dissipation theorems. This combination is made possible by the VAA, which converts the momentumdependent f_2 [in kinetic equation (19)] into a more tractable momentum-independent density-density nonequilibrium two-point function [see Eq. (21)]. The first equation in the VAA chain links linear and quadratic response functions, the second links quadratic and cubic response functions, and so on. Depending upon the degree of accuracy desired, one can truncate the chain at any level. If, for example, all equations after the first one are dropped, then closure is effected by approximating the quadratic density response function in terms of linear ones. This is the closure to be followed in the present paper. This procedure, first developed by GK for the 3D OCP [15] and referred to as the dynamical superposition approximation (DSA) is presented in Sec. V. The outcome is a self-consistent expression [Eqs. (29) and (67)] for the dynamical density response function featuring a dynamical local field correction that exactly reproduces the potential energy part [Eqs. (33) and (35)] of the third-frequency-moment sum-rule coefficient [17] in the high-frequency limit. This compliance with the sum rule makes it possible to incorporate exchange in the classical VAA-DSA formalism in a natural way, since the combined exchange-correlation effect resides in the potential energy through the static structure function [see Eq. (30)].

The plan of the paper is as follows. In Sec. II we introduce the dielectric and full and screened linear and quadratic density response functions via constitutive relations. Threepoint static and dynamical structure functions are next introduced and related to the quadratic response functions via the QFDT. The development of the approximation scheme is then carried out in three stages in Secs. III, IV, and V. In the stage-1 calculation, we establish the fundamental VAA-BBGKY kinetic equation for the weakly degenerate 2DCF. We next linearize and convert its right-hand-side nonequilibrium two-point density correlation function into equilibrium three-point structure functions via routine statistical mechanical linear response calculations. The resulting Eq. (29) for the screened linear response function features these latter as the Γ -dependent correction to the Lindhard function. In the stage-2 calculation (Sec. IV), we eliminate the threepoint structure functions in favor of the more accessible full and screened quadratic response functions by application of the QFDT. Self-consistency is then guaranteed at long wavelengths in the stage-3 calculation of Sec. V by approximating the quadratic density response functions in terms of linear ones. The first principal result of this paper, the non-RPA coupling correction (67), is expressed in terms of the exchange-correlation energy. The second principal result, a simple analytical formula for the long-wavelength dispersion of the plasma mode, is derived in Sec. VI from Eqs. (29) and (67). Conclusions and discussion follow in Sec. VII.

II. RESPONSE AND STRUCTURE FUNCTIONS

In this section we introduce quantities and relations central to the development of the VAA approach, namely, (i) linear and quadratic response functions; (ii) two- and threepoint structure functions; (iii) the QFDT linking the quadratic response and three-point structure functions.

Let $U_{tot}(\mathbf{r},t) = \hat{U}(\mathbf{r},t) + U_{pol}(\mathbf{r},t)$ be the total (screened) potential energy response to a weak external potential $\hat{\Phi}(\mathbf{r},t)$ acting at the in-plane (z=0) point \mathbf{r} within the 2D Coulomb fluid; U_{pol} is the induced (polarization) potential energy response to external potential energy $\hat{U}(\mathbf{r},t) = e\hat{\Phi}(\mathbf{r},t)$; e = -|e| for an electron fluid and e = +|e| for a hole fluid. The customary density response functions $\chi(\mathbf{q},\omega)$ (full) and $\chi_{sc}(\mathbf{q},\omega)$ (screened) are defined by the linear constitutive relations

$$\langle n_{\mathbf{q}} \rangle^{(1)}(\omega) = \chi(\mathbf{q}, \omega) \hat{U}(\mathbf{q}, \omega)$$
 (1)

$$= \chi_{\rm sc}(\mathbf{q}, \boldsymbol{\omega}) U_{\rm tot}^{(1)}(\mathbf{q}, \boldsymbol{\omega}); \qquad (2)$$

the superscript (1) denotes a first-order response to the external driving potential $\hat{\Phi}$; $n_{\mathbf{q}} = \Sigma_i \exp(-i\mathbf{q} \cdot \mathbf{x}_i)$ is the 2D Fourier transform of the microscopic density $n(\mathbf{r}) = \Sigma_j \delta(\mathbf{r} - \mathbf{x}_j)$ and the angular brackets denote the ensemble average; the in-plane wave vector $\mathbf{q} = (q_x, q_y)$. With the aid of $\chi_{sc}(\mathbf{q}, \omega)$ and $\nu(q) = 2\pi e^2/(\epsilon_s q)$ [the Fourier transform of the 2D potential $e^2/(\epsilon_s r)$] the dielectric response function is then

$$\boldsymbol{\epsilon}(\mathbf{q},\boldsymbol{\omega}) = 1 - \nu(q) \boldsymbol{\chi}_{\rm sc}(\mathbf{q},\boldsymbol{\omega}). \tag{3}$$

The χ - χ _{sc} relationship

$$\chi(\mathbf{q},\omega) = \frac{\chi_{\rm sc}(\mathbf{q},\omega)}{\epsilon(\mathbf{q},\omega)} \tag{4}$$

and the well-known expression

$$\frac{1}{\epsilon(\mathbf{q},\omega)} = 1 + \nu(q)\chi(\mathbf{q},\omega) \tag{5}$$

for the inverse dielectric response function readily follow from Eqs. (1)-(3).

We next define full and screened quadratic density response functions via the constitutive relations

$$\langle n_{\mathbf{q}} \rangle^{(2)}(\omega) = \frac{1}{\Omega} \sum_{\mathbf{q}'} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \chi(\mathbf{q}', \omega', \mathbf{q} - \mathbf{q}', \omega - \omega')$$
$$\times \hat{U}(\mathbf{q}', \omega') \hat{U}(\mathbf{q} - \mathbf{q}', \omega - \omega'),$$
(6)

$$n_{\mathbf{q}}^{(2)}(\omega) = \chi_{\rm sc}(\mathbf{q},\omega) U_{\rm pol}^{(2)}(\mathbf{q},\omega) + \frac{1}{\Omega} \sum_{\mathbf{q}'} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \chi_{\rm sc}(\mathbf{q}',\omega';\mathbf{q}-\mathbf{q}',\omega-\omega') \times U_{\rm tot}^{(1)}(\mathbf{q}',\omega') U_{\rm tot}^{(1)}(\mathbf{q}-\mathbf{q}',\omega-\omega');$$
(7)

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 Ω is the large but bounded area of the 2D system. The quadratic counterpart of Eq. (4),

$$\chi(\mathbf{q}', \omega'; \mathbf{q} - \mathbf{q}', \omega - \omega') = \frac{\chi_{\rm sc}(\mathbf{q}', \omega'; \mathbf{q} - \mathbf{q}', \omega - \omega')}{\epsilon(\mathbf{q}, \omega)\epsilon(\mathbf{q}', \omega')\epsilon(\mathbf{q} - \mathbf{q}', \omega - \omega')}, \qquad (8)$$

follows from Eqs. (6), (7), and (3), the constitutive relation $U_{\text{tot}}^{(1)}(\mathbf{q},\omega) = \hat{U}(\mathbf{q},\omega)/\epsilon(\mathbf{q},\omega)$, and the 2D second-order (in \hat{U}) Poisson equation $U_{\text{pol}}^{(2)}(\mathbf{q},\omega) = \nu(q) \langle n_{\mathbf{q}} \rangle^{(2)}(\omega)$.

The quadratic fluctuation-dissipation relations [16]

$$S(\mathbf{q}' - \mathbf{q}, t_1 = 0; \mathbf{q}, t_2 = 0)$$

$$= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega''}{2\pi} S(\mathbf{q}' - \mathbf{q}, \omega'; \mathbf{q}, \omega'')$$

$$= \frac{2}{n\beta^2} \operatorname{Re} \chi(\mathbf{q}' - \mathbf{q}, \omega' = 0; \mathbf{q}, \omega'' = 0), \qquad (9)$$

$$S(\mathbf{q}' - \mathbf{q}, \omega'; \mathbf{q}, \omega'')$$

$$= -\frac{4}{n\beta^2} \operatorname{Re} \left[\frac{1}{\omega' \omega''} \chi(\mathbf{q}' - \mathbf{q}, \omega'; \mathbf{q}; \omega'') - \frac{1}{\omega' (\omega' + \omega'')} \chi(-\mathbf{q}', -\omega' - \omega''; \mathbf{q}' - \mathbf{q}, \omega') - \frac{1}{\omega'' (\omega' + \omega'')} \chi(\mathbf{q}, \omega''; -\mathbf{q}', -\omega' - \omega'') \right]$$
(10)

connect the quadratic χ 's to the three-point structure function

$$S(\mathbf{q}' - \mathbf{q}, t_1; \mathbf{q}, t_2) = \frac{1}{N} \langle \delta n_{\mathbf{q}'}(0) \, \delta n_{\mathbf{q} - \mathbf{q}'}(-t_1) \, \delta n_{-\mathbf{q}}(-t_2) \rangle^{(0)}; \qquad (11)$$

the δn 's are microscopic fluctuating densities (e.g., $\delta n_q = n_q - N \delta_q$) and the $\langle \cdots \rangle^{(0)}$ brackets denote ensemble averaging over the equilibrium system. The useful triangle symmetry relations

$$\chi(\mathbf{q}-\mathbf{q}',0;-\mathbf{q},\omega) = \chi(\mathbf{q}',\omega;\mathbf{q}-\mathbf{q}',0), \qquad (12)$$

$$\chi(-\mathbf{q},\omega;\mathbf{q}',0) = \chi(\mathbf{q}',0;\mathbf{q}-\mathbf{q}',\omega)$$
(13)

are a consequence of the quadratic fluctuation-dissipation theorem (10) and the Kramers-Kronig relations that the four quadratic χ 's satisfy.

The classical quadratic fluctuation-dissipation relations (9) and (10) are central to the development of the theory and will be implemented in the stage-2 calculation of Sec. IV. The $O(\beta \hbar \omega/2)$ quantum correction [18] to the classical QFDT has been dropped in order to keep the mathematics tractable and to make possible the pivotal development of Sec. IV. This approximation would appear to be at the cost of some accuracy. However, at the weak degeneracies $(\beta \varepsilon_F|_{\text{max}} \approx 0.1 - 0.2)$ and low frequencies (the 2D plasma frequency) of interest in this paper, the cost can be kept to a minimum by confining our analysis to the long-wavelength domain (qa < 1). In any case, the approximation does not affect the essential qualitative feature of the 2D-plasma mode dispersion, namely, that exchange-correlation effects act to depress the mode frequency below its RPA value. This is to some extent borne out by the favorable quantitative comparison for qa values up to 0.5 between our Sec. VI plasmon frequency calculation at $\beta \epsilon_F = 0.2$ and $\Gamma = 10$ and the Ref. [10] quantum kinetic equation calculation at zero temperature and the equivalent coupling $r_s \approx \Gamma/2 = 5$.

III. STAGE-1 CALCULATION: VAA LINEAR RESPONSE

In this section we formulate the semiclassical VAA kinetic equation and from it we establish a relationship between $\chi(\mathbf{q}, \omega)$ and the three-point structure function. We then show that this relation very nearly satisfies the third-frequency-moment sum rule for arbitrary values of the coupling parameter.

Let $f_1(\mathbf{r}, \mathbf{k}, t)$ and $f_2(\mathbf{r}, \mathbf{k}; \mathbf{r}', \mathbf{k}'; t)$ be one- and twoparticle distribution functions; $\mathbf{r} = (x, y)$, $\mathbf{r}' = (x', y')$ and $\hbar \mathbf{k} = (\hbar k_x, \hbar k_y)$, $\hbar \mathbf{k}' = (\hbar k'_x, \hbar k'_y)$ are in-plane (z=0) position and momentum coordinates. The distribution functions are normalized to N and N(N-1) consistent with the moments

$$\frac{1}{2\pi^2} \int d\mathbf{k} f_1(\mathbf{r}, \mathbf{k}, t) = \langle n(\mathbf{r}) \rangle(t), \qquad (14)$$

$$\frac{1}{(2\pi^2)^2} \int d\mathbf{k} \int d\mathbf{k}' f_2(\mathbf{r}, \mathbf{k}; \mathbf{r}', \mathbf{k}'; t)$$

= $\langle n(\mathbf{r}) n(\mathbf{r}') \rangle(t) - \delta(\mathbf{r} - \mathbf{r}') \langle n(\mathbf{r}) \rangle(t);$ (15)

 $n(\mathbf{r})$ and $n(\mathbf{r}')$ in Eq. (15) are equal-time microscopic densities and the notation $\langle \cdots \rangle (t)$ refers to the time evolution carried by the Liouville distribution function.

The unperturbed state of the 2DCF is characterized by the equilibrium distributions

$$f_{1}^{(0)}(\mathbf{k}) = \frac{1}{1 + \exp\{\beta[\epsilon(\mathbf{k}) - \mu_{0}]\}},$$
 (16)

$$f_{2}^{(0)}(\mathbf{r},\mathbf{k};\mathbf{r}',\mathbf{k}') = f_{1}^{(0)}(\mathbf{k})f_{1}^{(0)}(\mathbf{k}')[1+h(|\mathbf{r}-\mathbf{r}'|)]; \quad (17)$$

 $\epsilon(\mathbf{k}) = \hbar^2 k^2 / (2m^*)$; the relation $\beta \mu_0 \equiv \mu_0 / (k_B T)$ = ln[exp($\beta \epsilon_F$)-1], derived from Eqs. (14) and (16), connects the chemical potential μ_0 for the noninteracting 2DCF to the 2D Fermi energy $\varepsilon_F = \pi n \hbar^2 / m^*$; $n = N/\Omega$ is the density of the unperturbed system; and

$$h(|\mathbf{r}-\mathbf{r}'|) = \frac{1}{N} \sum_{\mathbf{q}} [S(q)-1] \exp[i\mathbf{q} \cdot (\mathbf{r}-\mathbf{r}')] \quad (18)$$

is the equilibrium pair correlation function defined in terms of the static two-point structure function $S(q) \equiv S(q,t=0)$.

The introduction of the weak potential energy perturbation $\hat{U}(\mathbf{r},t)$ into the equilibrium system brings about the incremental responses $\delta f_1(\mathbf{r},\mathbf{k},t) = f_1(\mathbf{r},\mathbf{k},t) - f_1^{(0)}(\mathbf{k})$ and $\delta f_2(\mathbf{r},\mathbf{k};\mathbf{r}',\mathbf{k}';t) = f_2(\mathbf{r},\mathbf{k};\mathbf{r}',\mathbf{k}';t) - f_2^{(0)}(\mathbf{r},\mathbf{k};\mathbf{r}',\mathbf{k}'); \quad \delta f_1$ $= f_1^{(1)} + f_1^{(2)} + \cdots$ and $\delta f_2 = f_2^{(1)} + f_2^{(2)} \cdots$. We wish to calculate the average first-order density response $\langle n_q \rangle^{(1)}(t)$ from the first BBGKY kinetic equation

$$Lf_{1}(\mathbf{r},\mathbf{k},t) \equiv \left[\frac{\partial}{\partial t} + \frac{\hbar \mathbf{k}}{m^{*}} \cdot \frac{\partial}{\partial \mathbf{r}} - \left(\frac{\partial \hat{U}(\mathbf{r},t)}{\partial \mathbf{r}}\right) \cdot \frac{1}{\hbar} \frac{\partial}{\partial \mathbf{k}}\right] f_{1}(\mathbf{r},\mathbf{k},t)$$
$$= \frac{1}{\hbar} \frac{\partial}{\partial \mathbf{k}} \cdot \frac{1}{2\pi^{2}} \int d\mathbf{r}' \int d\mathbf{k}' f_{2}(\mathbf{r},\mathbf{k};\mathbf{r}',\mathbf{k}';t)$$
$$\times \frac{\partial}{\partial \mathbf{r}} \frac{e^{2}}{|\mathbf{r}-\mathbf{r}'|}. \tag{19}$$

Paralleling the Ref. [15] procedure, we first convert the righthand side of Eq. (19) into a more tractable momentumindependent nonequilibrium two-point correlation function. This is accomplished by supposing that f_2 is well described by its momentum average in the restricted sense where only one of its momentum arguments is averaged out, viz.,

$$f_{2}(\mathbf{r},\mathbf{k};\mathbf{r}',\mathbf{k}';t) = \frac{1}{2} \frac{f_{1}(\mathbf{r},\mathbf{k},t)}{\langle n(\mathbf{r})\rangle(t)} \frac{1}{2\pi^{2}} \int d\mathbf{\bar{k}} f_{2}(\mathbf{r},\mathbf{\bar{k}};\mathbf{r}',\mathbf{k}';t) + \frac{1}{2} \frac{f_{1}(\mathbf{r}',\mathbf{k}',t)}{\langle n(\mathbf{r}')\rangle(t)} \frac{1}{2\pi^{2}} \times \int d\mathbf{\bar{k}}' f_{2}(\mathbf{r},\mathbf{k};\mathbf{r}',\mathbf{\bar{k}}';t).$$
(20)

The VAA ansatz (20) is exact when the system is in thermodynamic equilibrium [i.e., equilibrium distributions (16) and (17) rigorously satisfy Eq. (20)]. The resulting momentumspace double integral

$$\frac{f_1(\mathbf{r},\mathbf{k},t)}{\langle n(\mathbf{r})\rangle(t)}\frac{1}{(2\,\pi^2)^2}\int d\mathbf{\overline{k}}\int d\mathbf{k}' \ f_2(\mathbf{r},\mathbf{\overline{k}};\mathbf{r}',\mathbf{k}';t),$$

which replaces $(1/2\pi^2)\int d\mathbf{k}' f_2(\mathbf{r}, \mathbf{k}; \mathbf{r}', \mathbf{k}'; t)$ in Eq. (19), can now be expressed in terms of the nonequilibrium twopoint function $\langle n(\mathbf{r})n(\mathbf{r}')\rangle(t)$ via Eq. (15). The VAA kinetic equation accordingly takes the form

$$Lf_{1}(\mathbf{r},\mathbf{k},t) = \frac{1}{\hbar} \frac{\partial}{\partial \mathbf{k}} \frac{f_{1}(\mathbf{r},\mathbf{k},t)}{\langle n(\mathbf{r})\rangle(t)} \cdot \int d\mathbf{r}' \langle n(\mathbf{r})n(\mathbf{r}')\rangle(t)$$
$$\times \frac{\partial}{\partial \mathbf{r}} \frac{e^{2}}{|\mathbf{r}-\mathbf{r}'|}.$$
(21)

In the classical limit, Eq. (21) is known to be exact when the system is driven by a static perturbation. This follows from the fact that the perturbed distribution function in the presence of a static external perturbation is still a canonical distribution in terms of the perturbed Hamiltonian, and that it factorizes into momentum- and coordinate-dependent contributions [19].

The routine calculation of the first-order average density response consists in linearizing Eq. (21), taking its Fourier transform, solving for $f_1^{(1)}(\mathbf{q},\mathbf{k};\omega)$, and then taking the density moment per Eq. (14). One obtains

$$\langle n_{\mathbf{q}} \rangle^{(1)}(\omega) = \overline{\chi}_{0}(\mathbf{q},\omega) \left[\hat{U}(\mathbf{q},\omega) + \nu(q) \frac{1}{N} \sum_{\mathbf{q}'} \left(\frac{\mathbf{q} \cdot \mathbf{q}'}{qq'} \right) \times \langle n_{\mathbf{q}'} n_{\mathbf{q}-\mathbf{q}'} \rangle^{(1)}(\omega) \right].$$
(22)

The semiclassical Vlasov screened response function

$$\bar{\chi}_0(\mathbf{q},\omega) = -\frac{1}{2\pi^2\hbar} \int d\mathbf{k} \frac{(\mathbf{q}\cdot\partial/\partial\mathbf{k})f_1^{(0)}(\mathbf{k})}{\omega - (\hbar/m^*)\mathbf{q}\cdot\mathbf{k}}$$
(23)

calculated from Eq. (19) in the $f_2(\mathbf{r},\mathbf{k};\mathbf{r}',\mathbf{k}';t) = f_1(\mathbf{r},\mathbf{k},t)f_1(\mathbf{r}',\mathbf{k}',t)$ uncorrelated approximation, in fact, is the long-wavelength limit of the Lindhard function

$$\chi_0(\mathbf{q},\omega) = \frac{2}{\hbar\Omega} \sum_{\mathbf{k}} \frac{f_1^{(0)}(\mathbf{k} - (\mathbf{q}/2)) - f_1^{(0)}(\mathbf{k} + (\mathbf{q}/2))}{\omega - (\hbar/m^*)\mathbf{q} \cdot \mathbf{k}}.$$
(24)

The nonequilibrium two-point function $\langle n_{\mathbf{q}'} n_{\mathbf{q}-\mathbf{q}'} \rangle^{(1)}(\omega)$, in turn, can be expressed in terms of equilibrium three-point functions through a straightforward statistical mechanical linear response calculation. One obtains

$$\langle n_{\mathbf{q}'} n_{\mathbf{q}-\mathbf{q}'} \rangle^{(1)}(\omega) = N(\delta_{\mathbf{q}-\mathbf{q}'} + \delta_{\mathbf{q}'}) \langle n_{\mathbf{q}} \rangle^{(1)}(\omega) -\beta n \Xi(\mathbf{q},\mathbf{q}',\omega) \hat{U}(\mathbf{q},\omega), \quad (25)$$

$$\Xi(\mathbf{q},\mathbf{q}',\boldsymbol{\omega}) = S(\mathbf{q}'-\mathbf{q},t=0;\mathbf{q},t=0) + \frac{i\omega}{2\pi} \int_{-\infty}^{\infty} d\omega' \int_{-\infty}^{\infty} d\omega'' \ \delta_{+}(\omega-\omega'') \times S(\mathbf{q}'-\mathbf{q},\omega';\mathbf{q},\omega''),$$
(26)

where $\delta_{\pm}(x) = (1/2) \,\delta(x) \pm (i/2\pi) P(1/x)$; the *P* symbol denotes the Cauchy principal value. The VAA *full* density response function expression

$$\chi(\mathbf{q},\omega) = \chi_0^{\text{RPA}}(\mathbf{q},\omega) [1 - \nu(q)K(\mathbf{q},\omega)]$$
(27)

then results from Eqs. (22), (25), and (1) with $\bar{\chi}_0(\mathbf{q},\omega)$ replaced by $\chi_0(\mathbf{q},\omega)$; $\chi_0^{\text{RPA}}(\mathbf{q},\omega) = \chi_0(\mathbf{q},\omega)/\epsilon_0(\mathbf{q},\omega)$ is the response in the RPA, $\epsilon_0(\mathbf{q},\omega) = 1 - \nu(q)\chi_0(\mathbf{q},\omega)$ being the Lindhard dielectric function. In the classical VAA, the key particle-particle correlation effects beyond the RPA reside in the coupling correction

$$K(\mathbf{q},\omega) \equiv \frac{\beta}{\Omega} \sum_{\mathbf{q}'} \left(\frac{\mathbf{q} \cdot \mathbf{q}'}{qq'} \right) \Xi(\mathbf{q},\mathbf{q}',\omega)$$
(28)

with $\Xi(\mathbf{q},\mathbf{q}',\omega)$ given by Eq. (26). The equally compact VAA expression for the *screened* density response,

$$\chi_{\rm sc}(\mathbf{q},\omega) = \chi_0(\mathbf{q},\omega) [1 - \nu(q) K_{\rm sc}(\mathbf{q},\omega)], \qquad (29)$$

readily follows from Eqs. (27) and (4) and introduction of the screened coupling correction $K_{\rm sc}(\mathbf{q},\omega)$ via the definition $K(\mathbf{q},\omega) = K_{\rm sc}(\mathbf{q},\omega)/\epsilon(\mathbf{q},\omega)$ paralleling Eq. (4). In adapting the classical VAA formalism to the weakly degenerate quantum domain, we are, in effect, supposing that the temperature-dependent exchange also resides in the threepoint structure functions that comprise the $K_{\rm sc}$ and K coupling corrections. This completes the stage-1 derivation.

The VAA screened coupling correction, in its final longwavelength form (67) below, is expressed in terms of the static two-point structure function $S(q) \equiv S(q,t=0)$ via the potential energy per particle

$$V = \frac{1}{2\Omega} \sum_{\mathbf{q}'} \nu(q') [S(q') - 1].$$
(30)

Unfortunately, static structure function and equilibrium pair correlation function data for the 2DCF in the weakly degenerate quantum domain are unavailable so that the potential energy input to Eq. (67) has to be determined by some other means. One strategy is proposed below in connection with the third-frequency-moment sum-rule [17] analysis.

At high frequencies, the VAA expression for $\chi(\mathbf{q}, \omega)$ very nearly reproduces the third-frequency-moment sum-rule coefficient. To demonstrate this, we need to evaluate $\chi(\mathbf{q}, \omega)$ in the $\omega \rightarrow \infty$ limit. Following the procedure of Ref. [15], one obtains

$$\operatorname{Re} \Xi(\mathbf{q}, \mathbf{q}', \omega \to \infty)$$

$$= \lim_{\omega \to \infty} \frac{1}{\omega^{2}} \left[\left(\frac{\partial}{\partial t'} + \frac{\partial}{\partial t''} \right)^{2} S(\mathbf{q}', t'; \mathbf{q} - \mathbf{q}', t'') \right]_{t' = t'' = 0}$$

$$= -\lim_{\omega \to \infty} \frac{1}{\beta m^{*} \omega^{2}} [(\mathbf{q} \cdot \mathbf{q}') S(|\mathbf{q} - \mathbf{q}'|)$$

$$+ \mathbf{q} \cdot (\mathbf{q} - \mathbf{q}') S(q')], \qquad (31)$$

whence the high-frequency expression

$$\operatorname{Re} \chi(\mathbf{q}, \omega \to \infty) = \lim_{\omega \to \infty} \left\{ \frac{nq^2}{m^* \omega^2} + \frac{nq^2}{m^* \omega^4} \left[\left(\frac{\hbar q^2}{2m^*} \right)^2 + \frac{3q^2 \langle E_{\mathrm{kin}} \rangle_0}{m^*} + \omega_{2D}^2(q) + D(\mathbf{q}) \right] \right\},$$
(32)

$$D(\mathbf{q}) = \frac{1}{m^* \Omega} \sum_{q'} \frac{(\mathbf{q} \cdot \mathbf{q}')^2}{q^2} \nu(q') [S(|\mathbf{q} - \mathbf{q}'|) - S(q')],$$
(33)

results from Eqs. (24), (27), (28), and (31); the kinetic energy term

$$\langle E_{\rm kin} \rangle_0 = \frac{1}{\epsilon_F} \int_0^\infty d\epsilon \frac{\epsilon}{1 + \exp[\beta(\epsilon - \mu_0)]}$$
 (34)

in Eq. (32) is the expectation value of the kinetic energy per electron for a noninteracting system. $D(\mathbf{q})$ is identified as precisely the term in the ω^3 sum-rule coefficient [17] that embodies the exchange-correlation effects through the static structure functions $S(|\mathbf{q}-\mathbf{q}'|)$ and S(q'). At long wavelengths,

$$D(q \to 0) = \frac{5}{8} \frac{q^2 V}{m^*}.$$
 (35)

As stated above, the complete lack of static structure function data for the 2DCF in the weakly degenerate quantum domain makes it necessary to determine V by some other means. One strategy is to replace Eq. (30) with the postulated decomposition

$$V(n,T) = \langle E_c \rangle(n,T) + \langle E_x \rangle(n,T)$$
(36)

in terms of the more accessible correlation and exchange energies per particle $\langle E_c \rangle(n,T)$ and $\langle E_x \rangle(n,T)$, respectively [see Eqs. (78)–(81) below]. Such a decomposition is consistent with the observations (i) that $V_{cl} = \langle E_c \rangle(n,T)$ in the classical limit and (ii) that the exchange contribution to V is the Hartree-Fock (HF) exchange energy per particle $\langle E_x \rangle(n,0)$ = $-0.6e^2/a$ in the T=0 limit [17(c)].

In the classical domain, the VAA expansion (32) is in every respect identical to the exact high-frequency expansion of Re $\chi(\mathbf{q}, \omega \rightarrow \infty)$ through $O(1/\omega^4)$. With the decomposition (36), this is very nearly the case in the weakly degenerate quantum domain—except for the discrepancy between the VAA($3q^2/m^*$) $\langle E_{kin} \rangle_0$ term (which is devoid of correlation effects) and its ω^3 sum-rule counterpart $(3q^2/m^*)\langle E_{kin} \rangle$ (which is not) [17(c)]. There is no way to remedy this defect of the VAA formalism.

IV. STAGE-2 REFORMULATION IN TERMS OF QUADRATIC DENSITY RESPONSE FUNCTIONS

The stage-2 development consists in using the QFDT to replace the three-point structure functions in the expression (28) for $K(\mathbf{q}, \omega)$ and in $K_{\rm sc}(\mathbf{q}, \omega) = \varepsilon(\mathbf{q}, \omega)K(\mathbf{q}, \omega)$ with the more accessible quadratic density response functions.

Since the three-point function $S(\mathbf{q}' - \mathbf{q}, \omega'; \mathbf{q}, \omega'')$ is ex-

pected to be nonsingular, the $\omega' = 0$, $\omega'' = 0$, and $\omega' = -\omega''$ singularities in Eq. (10) are spurious, and the QFDT remains unchanged if one stipulates that each denominator in Eq. (10) is a double principal-value denominator. With this understanding, injecting Eq. (10) into Eq. (28) leads to expressions that are amenable to Kramers-Kronig analysis. They are

$$\operatorname{Re} K(\mathbf{q}, \omega) = \frac{2}{\beta N} \sum_{\mathbf{q}'} \left(\frac{\mathbf{q} \cdot \mathbf{q}'}{q q'} \right) [\operatorname{Re} \chi(\mathbf{q}' - \mathbf{q}, 0; \mathbf{q}, 0) + I_1(\mathbf{q}, \mathbf{q}', \omega) - I_2(\mathbf{q}, \mathbf{q}', \omega) - I_3(\mathbf{q}, \mathbf{q}', \omega)],$$
(37a)

$$I_{1}(\mathbf{q},\mathbf{q}',\omega) = 2\omega \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega''}{2\pi} \times \operatorname{Re} \chi(\mathbf{q}'-\mathbf{q},\omega';\mathbf{q},\omega'') \times P \frac{1}{\omega'} P \frac{1}{\omega''} P \frac{1}{\omega-\omega''}, \quad (37b)$$

$$I_{2}(\mathbf{q},\mathbf{q}',\omega) = 2\omega \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega''}{2\pi} \times \operatorname{Re} \chi(-\mathbf{q}',-\omega'-\omega'';\mathbf{q}'-\mathbf{q},\omega') \times P \frac{1}{\omega'} P \frac{1}{\omega'+\omega''} P \frac{1}{\omega-\omega''}, \quad (37c)$$

$$I_{3}(\mathbf{q},\mathbf{q}',\omega) = 2\omega \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega''}{2\pi} \times \operatorname{Re} \chi(\mathbf{q},\omega'';-\mathbf{q}',-\omega'-\omega'') \times P \frac{1}{\omega''} P \frac{1}{\omega'+\omega''} P \frac{1}{\omega-\omega''}, \quad (37d)$$

$$\operatorname{Im} K(\mathbf{q}, \omega) = \frac{2}{\beta N} \sum_{\mathbf{q}'} \left(\frac{\mathbf{q} \cdot \mathbf{q}'}{q q'} \right) \operatorname{Re} \left[\omega \int_{-\infty}^{\infty} \frac{d \omega'}{2 \pi} \times \chi(-\mathbf{q}', -\omega - \omega'; \mathbf{q}' - \mathbf{q}, \omega') P \frac{1}{\omega'} P \frac{1}{\omega + \omega'} - \int_{-\infty}^{\infty} \frac{d \omega'}{2 \pi} \chi(\mathbf{q}' - \mathbf{q}, \omega'; \mathbf{q}, \omega) P \frac{1}{\omega'} + \int_{-\infty}^{\infty} \frac{d \omega'}{2 \pi} \chi(\mathbf{q}, \omega; -\mathbf{q}', -\omega - \omega') P \frac{1}{\omega + \omega'} \right].$$
(38)

Addressing first the reduction of $\operatorname{Re} K(\mathbf{q}, \omega)$, the evaluation of I_1 is facilitated by the partial-fraction expansion

$$I_{1}(\mathbf{q},\mathbf{q}',\omega) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \int_{-\infty}^{\infty} \frac{d\omega''}{\pi} \operatorname{Re} \chi(\mathbf{q}'-\mathbf{q},\omega';\mathbf{q},\omega'') \\ \times \left[P \frac{1}{\omega'} P \frac{1}{\omega''} + P \frac{1}{\omega'} P \frac{1}{\omega-\omega''} \right].$$
(39)

The subsequent reduction of Eq. (39) to

$$I_{1}(\mathbf{q},\mathbf{q}',\omega) = -\frac{1}{2}\operatorname{Re} \chi(\mathbf{q}-\mathbf{q}',0;-\mathbf{q},0) +\frac{1}{2}\operatorname{Re} \chi(\mathbf{q}-\mathbf{q}',0;-\mathbf{q},\omega)$$
(40)

via Hilbert transform operations follows from the observation that $\chi(\mathbf{q}' - \mathbf{q}, \omega'; \mathbf{q}, \omega'')$ is a plus function of its frequency arguments. The more involved evaluations of I_2 and I_3 similarly proceed from the partial-fraction expansions

$$I_{2}(\mathbf{q},\mathbf{q}',\omega) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \int_{-\infty}^{\infty} \frac{d\omega''}{\pi}$$

$$\times \operatorname{Re} \chi(-\mathbf{q}',-\omega'-\omega'';\mathbf{q}'-\mathbf{q},\omega')$$

$$\times \left[P \frac{1}{\omega'} P \frac{1}{\omega'+\omega''} - P \frac{1}{\omega+\omega'} P \frac{1}{\omega'+\omega''} + P \frac{1}{\omega'+\omega''} P \frac{1}{\omega-\omega''} + P \frac{1}{\omega-\omega''} P \frac{1}{\omega-\omega''} - P \frac{1}{\omega+\omega'} P \frac{1}{\omega-\omega''} \right],$$

$$(41)$$

$$I_{3}(\mathbf{q},\mathbf{q}',\omega) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \int_{-\infty}^{\infty} \frac{d\omega''}{\pi} \times \operatorname{Re} \chi(\mathbf{q},\omega'';-\mathbf{q}',-\omega'-\omega'') \times \left[P \frac{1}{\omega''} P \frac{1}{\omega'+\omega''} + P \frac{1}{\omega-\omega''} P \frac{1}{\omega'+\omega''} \right].$$

$$(42)$$

After some lengthy algebra entailing repeated Hilbert transform operations, Eq. (41) simplifies to

$$I_{2}(\mathbf{q},\mathbf{q}',\omega) = \frac{1}{2} \operatorname{Re} \chi(\mathbf{q}',0;\mathbf{q}-\mathbf{q}',0) - \frac{1}{2} \operatorname{Re} \chi(\mathbf{q}',0;\mathbf{q}-\mathbf{q}',\omega)$$
$$-\omega \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \operatorname{Im} \chi(\mathbf{q}',\omega';\mathbf{q}-\mathbf{q}',\omega-\omega')$$
$$\times P \frac{1}{\omega'} P \frac{1}{\omega-\omega'}. \tag{43}$$

Equation (42), as it stands, is not amenable to Kramers-Kronig analysis unless one first invokes the Poincaré-Bertrand theorem [15,20]. The steps in the reduction of the first integral are

$$\frac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \int_{-\infty}^{\infty} \frac{d\omega''}{\pi} \operatorname{Re} \chi(\mathbf{q}, \omega''; -\mathbf{q}', -\omega' - \omega'')$$

$$\times P \frac{1}{\omega''} P \frac{1}{\omega' + \omega''}$$

$$= \frac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega''}{\pi} P \frac{1}{\omega''} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} P \frac{1}{\omega' + \omega''}$$

$$\times \chi(\mathbf{q}, \omega''; -\mathbf{q}', -\omega' - \omega'') - \frac{1}{2} \operatorname{Re} \chi(\mathbf{q}, 0; -\mathbf{q}', 0)$$

$$= \frac{1}{2} \operatorname{Re} \chi(\mathbf{q}, 0; -\mathbf{q}', 0) - \frac{1}{2} \operatorname{Re} \chi(\mathbf{q}, 0; -\mathbf{q}', 0) = 0; \quad (44)$$

the last line results from the double Hilbert transform operation. The second integral in Eq. $(\underline{42})$ similarly vanishes. Thus,

$$I_3(\mathbf{q},\mathbf{q}',\omega) = 0. \tag{45}$$

The expression

$$\operatorname{Re} K(\mathbf{q}, \omega) = \frac{1}{\beta N} \sum_{\mathbf{q}'} \left(\frac{\mathbf{q} \cdot \mathbf{q}'}{q q'} \right) \\ \times \left[\omega \int_{-\infty}^{\infty} \frac{d \omega'}{\pi} \operatorname{Im} \chi(\mathbf{q}', \omega'; \mathbf{q} - \mathbf{q}', \omega - \omega') \right. \\ \left. \times P \frac{1}{\omega'} P \frac{1}{\omega - \omega'} + \operatorname{Re} \chi(\mathbf{q}', \omega; \mathbf{q} - \mathbf{q}', 0) \right. \\ \left. + \operatorname{Re} \chi(\mathbf{q}', 0; \mathbf{q} - \mathbf{q}', \omega) \right]$$
(46)

then results from Eqs. (<u>37</u>), (40), (43), and (45), and the triangle symmetry relation (<u>12</u>). The conversion of the expression (<u>38</u>) for Im $K(\mathbf{q}, \omega)$ into a form similar to Eq. (<u>46</u>) is a less daunting task. Replacing the last two integrals in Eq. (<u>38</u>) by their Hilbert transforms and using triangle symmetry relations (<u>12</u>) and (<u>13</u>), one readily obtains

$$\operatorname{Im} K(\mathbf{q}, \omega) = \frac{1}{\beta N} \sum_{\mathbf{q}'} \left(\frac{\mathbf{q} \cdot \mathbf{q}'}{q q'} \right) \\ \times \left[-\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \operatorname{Re} \chi(\mathbf{q}', \omega'; \mathbf{q} - \mathbf{q}', \omega - \omega') \right] \\ \times P \frac{1}{\omega'} P \frac{1}{\omega - \omega'} + \operatorname{Im} \chi(\mathbf{q}', \omega; \mathbf{q} - \mathbf{q}', 0) \\ + \operatorname{Im} \chi(\mathbf{q}', 0; \mathbf{q} - \mathbf{q}', \omega) \right].$$
(47)

The compact VAA coupling correction

$$K(\mathbf{q},\omega) = \frac{2}{\beta N} \sum_{\mathbf{q}'} \left(\frac{\mathbf{q} \cdot \mathbf{q}'}{qq'} \right) \int_{-\infty}^{\infty} d\omega' \,\delta_{-}(\omega') \\ \times [\chi(\mathbf{q}',\omega';\mathbf{q}-\mathbf{q}',\omega-\omega') \\ + \chi(\mathbf{q}',\omega-\omega';\mathbf{q}-\mathbf{q}',\omega')]$$
(48)

and its screened counterpart

$$K_{\rm sc}(\mathbf{q},\omega) = \frac{2}{\beta N} \sum_{\mathbf{q}'} \left(\frac{\mathbf{q} \cdot \mathbf{q}'}{qq'} \right) \int_{-\infty}^{\infty} d\omega' \,\delta_{-}(\omega') \\ \times \left[\frac{\chi_{\rm sc}(\mathbf{q}',\omega';\mathbf{q}-\mathbf{q}',\omega-\omega')}{\epsilon(\mathbf{q}',\omega')\epsilon(\mathbf{q}-\mathbf{q}',\omega-\omega')} + \frac{\chi_{\rm sc}(\mathbf{q}',\omega-\omega';\mathbf{q}-\mathbf{q}',\omega')}{\epsilon(\mathbf{q}',\omega-\omega')\epsilon(\mathbf{q}-\mathbf{q}',\omega')} \right]$$
(49)

follow from Eqs. (46), (47), (28), and (8). This completes the stage-2 derivation.

Earlier we mentioned that the classical $(\hbar \rightarrow 0)$ limit of VAA kinetic equation (21) is exact when the system is driven by a static perturbation. This implies that in the $\hbar \rightarrow 0$ limit the VAA expression (27) [with (28)] for $\chi(\mathbf{q}, \omega=0)$ is identical to the first equation in the static BBGKY hierarchy linking the equilibrium pair and ternary correlation functions. Then, by definition, VAA Eq. (29) [with (49)] must rigorously reproduce the classical $(\hbar \rightarrow 0)$ limit of the compressibility rule $\chi_{sc}^{exact}(\mathbf{q}\rightarrow 0, \omega=0) = -n(\partial P/\partial n)_T^{-1}$ for all fluid-phase values of the classical coupling parameter $\Gamma_{cl} = \beta e^2/a$. In the weakly degenerate quantum domain, however, the static VAA coupling correction

$$K_{\rm sc}(\mathbf{q}\to\mathbf{0},0) = \frac{2}{\beta n} \sum_{\mathbf{q}'} \left(\frac{\mathbf{q}\cdot\mathbf{q}'}{qq'}\right) \frac{\chi_{\rm sc}(\mathbf{q}',0;\mathbf{q}-\mathbf{q}',0)}{\epsilon(\mathbf{q}',0)\,\epsilon(\mathbf{q}-\mathbf{q}',0)},\tag{50}$$

when evaluated in the RPA limit, reproduces the dominant $O(\Gamma_{cl}^2 \ln \Gamma_{cl}^2)$ correlation energy part but not the $O(\Gamma_{cl} \sqrt{\beta \varepsilon_F})$ exchange energy part [see Eqs. (80) and (81) below] of the compressibility rule [21]. This discrepancy has no bearing whatsoever on the further evaluation of $K_{sc}(\mathbf{q} \rightarrow \mathbf{0}, \omega)$ in Sec. V, where a prescription for including exchange in the dynamics is guided by the more pivotal third-frequency-moment sum rule.

V. STAGE 3: DYNAMICAL SUPERPOSITION APPROXIMATION

Equations (29) and (49) constitute the central relations of the VAA. They determine the linear density response function in terms of quadratic ones. Closure can be achieved by postulating a decomposition of the latter in terms of the former applicable to the long-wavelength (small-q) domain of interest in the present paper. To accomplish this, we first analyze the semiclassical Vlasov function

$$\bar{\chi}_0(\mathbf{q}',\omega';\mathbf{q}-\mathbf{q}',\omega-\omega')$$

and show that it has a simple decomposition in terms of linear $\bar{\chi}_0$ pair clusters in the $q \rightarrow 0$ limit. This relationship will then be postulated to serve as the basis of the

self-consistency approximation for arbitrary coupling values.

The semiclassical Lindhard-like expression

$$\begin{split} \bar{\chi}_{0}(\mathbf{q}',\omega';\mathbf{q}'',\omega'') &= \frac{1}{(2\pi\hbar)^{2}} \int d\mathbf{k} \frac{1}{\omega - (\hbar/m^{*})(\mathbf{q}\cdot\mathbf{k})} \\ &\times \left[\left(\mathbf{q}' \cdot \frac{\partial}{\partial \mathbf{k}} \right) \frac{\mathbf{q}'' \cdot (\partial/\partial \mathbf{k}) f_{1}^{(0)}(\mathbf{k})}{\omega'' - (\hbar/m^{*})(\mathbf{q}''\cdot\mathbf{k})} \right. \\ &\left. + \left(\mathbf{q}'' \cdot \frac{\partial}{\partial \mathbf{k}} \right) \frac{\mathbf{q}' \cdot (\partial/\partial \mathbf{k}) f_{1}^{(0)}(\mathbf{k})}{\omega' - (\hbar/m^{*})(\mathbf{q}'\cdot\mathbf{k})} \right] \end{split}$$
(51)

for the screened quadratic response function is derived from Eqs. (7) and (14) with $f_1^{(2)}(\mathbf{q},\mathbf{k},\omega)$ calculated from the parent kinetic equation (19) in the uncorrelated approximation; $\mathbf{q}'' = \mathbf{q} - \mathbf{q}', \ \omega'' = \omega - \omega'$. The subsequent long-wavelength development of Eq. (51) in powers of $\alpha = |\hbar(\mathbf{q} \cdot \mathbf{k})/(m^*\omega)|$ through order α^3 then results in the following relationship between the quadratic and linear $\overline{\chi}_0$'s:

$$\bar{\chi}_{0}(\mathbf{q}',\omega';\mathbf{q}'',\omega'') = \frac{1}{2m^{*}} \sum_{j=1}^{3} \frac{j}{\omega^{j+1}} [A_{j}(\mathbf{q}',\omega') + A_{j}(\mathbf{q}'',\omega'')]$$
(52a)

$$+A_{j}(\mathbf{q}'',\boldsymbol{\omega}'')], \qquad (52a)$$

$$A_1(\mathbf{q}',\boldsymbol{\omega}') = (\mathbf{q} \cdot \mathbf{q}'') \bar{\chi}_0(\mathbf{q}',\boldsymbol{\omega}'), \qquad (52b)$$

$$A_2(\mathbf{q}',\omega') = \frac{1}{{q'}^2} (\mathbf{q} \cdot \mathbf{q}') (\mathbf{q} \cdot \mathbf{q}'') \omega' \bar{\chi}_0(\mathbf{q}',\omega'), \quad (52c)$$

$$A_{3}(\mathbf{q}',\boldsymbol{\omega}') = (\mathbf{q} \cdot \mathbf{q}'') \beta \left(\frac{\hbar}{m^{*}}\right)^{3} \frac{1}{2\pi^{2}} \int d\mathbf{k} (\mathbf{q} \cdot \mathbf{k})^{2} (\mathbf{q}' \cdot \mathbf{k})$$
$$\times \frac{f_{1}^{(0)}(\mathbf{k})[1 - f_{1}^{(0)}(\mathbf{k})]}{\boldsymbol{\omega}' - (\hbar/m^{*})(\mathbf{q}' \cdot \mathbf{k})}.$$
(52d)

Now rewrite the weak-coupling, long-wavelength value of $K_{\rm sc}$,

$$K_{0}(q \to 0, \omega) = \lim_{q \to 0} \frac{2}{\beta N} \sum_{\mathbf{q}'} \left(\frac{\mathbf{q} \cdot \mathbf{q}'}{q q'} \right) \int_{-\infty}^{\infty} d\omega' \, \delta_{-}(\omega') \\ \times \left[\frac{\overline{\chi}_{0}(\mathbf{q}', \omega'; \mathbf{q}'', \omega'')}{\overline{\epsilon}_{0}(\mathbf{q}', \omega') \overline{\epsilon}_{0}(\mathbf{q}'', \omega'')} + \frac{\overline{\chi}_{0}(\mathbf{q}', \omega''; \mathbf{q}'', \omega')}{\overline{\epsilon}_{0}(\mathbf{q}', \omega'') \overline{\epsilon}_{0}(\mathbf{q}'', \omega'')} \right],$$
(53)

in the more convenient form

$$K_{0}(q \to 0, \omega) = \frac{1}{\beta m^{*}} \sum_{j=1}^{3} \frac{j}{\omega^{j+1}} \lambda_{j}(q \to 0, \omega), \qquad (54)$$

$$\lambda_{j}(q,\omega) = \frac{1}{N} \sum_{\mathbf{q}'} \left(\frac{\mathbf{q} \cdot \mathbf{q}'}{qq'} \right) \int_{-\infty}^{\infty} d\omega' \,\delta_{-}(\omega') \\ \times \left[\frac{A_{j}(\mathbf{q}',\omega') + A_{j}(\mathbf{q}'',\omega'')}{\overline{\epsilon}_{0}(\mathbf{q}',\omega') \overline{\epsilon}_{0}(\mathbf{q}'',\omega'')} \right. \\ \left. + \frac{A_{j}(\mathbf{q}',\omega'') + A_{j}(\mathbf{q}'',\omega'')}{\overline{\epsilon}_{0}(\mathbf{q}'',\omega'') \overline{\epsilon}_{0}(\mathbf{q}'',\omega')} \right];$$
(55)
$$\mathbf{q}'' = \mathbf{q} - \mathbf{q}', \ \omega'' = \omega - \omega';$$

$$\overline{\boldsymbol{\epsilon}}_0(\mathbf{q}',\boldsymbol{\omega}') = 1 - \nu(\boldsymbol{q}')\overline{\boldsymbol{\chi}}_0(\mathbf{q}',\boldsymbol{\omega}'),$$

etc. Inserting Eqs. (52b)–(52d) into Eq. (55) and exploiting Kramers-Kronig relations, the subsequent evaluation of the λ_i 's through order q^3 yields

$$\lambda_{1}(q \to 0, \omega) = -\frac{q^{3} \gamma}{32 \pi e^{2}} (5 \ln \gamma + 9) + \frac{3}{8} q^{3} \frac{1}{N} \sum_{\mathbf{q}'} \frac{1}{q'} \nu(q') H_{0}(\mathbf{q}', \omega), \qquad (56)$$

$$\lambda_2(q \to 0, \omega) = \frac{3q^3 \gamma \omega}{16\pi e^2} - \frac{1}{8} \omega q^3 \frac{1}{N} \sum_{\mathbf{q}'} \frac{1}{q'} \nu(q') H_0(\mathbf{q}', \omega),$$
(57)

$$\lambda_3(q \rightarrow 0, \omega) = 0$$
 through $O(q^4)$, (58)

$$H_{0}(\mathbf{q}',\omega) = \int_{-\infty}^{\infty} d\omega' \,\delta_{-}(\omega') \frac{\overline{\chi}_{0}(\mathbf{q}',\omega')\overline{\chi}_{0}(\mathbf{q}',\omega-\omega')}{\overline{\epsilon}_{0}(\mathbf{q}',\omega')\overline{\epsilon}_{0}(\mathbf{q}',\omega-\omega')}.$$
(59)

In deriving the first right-hand-side terms of Eqs. (56) and (57), one encounters the long-wavelength $(q \rightarrow 0)$ RPA dielectric functions [17(c)] $\overline{\epsilon}_0(\mathbf{q}',0) = 1 + (\kappa/q')$ and $\overline{\epsilon}_0(\mathbf{q}',0) = 1 + (\kappa/q')$ $-\mathbf{q}',0) = 1 + (\kappa/|\mathbf{q}-\mathbf{q}'|); \ \kappa = (2m^*e^2/\hbar^2)[1 - \exp(-\beta\epsilon_F)]$ is the effective Fermi-Thomas wave number. In the weakly degenerate quantum domain, $\kappa \approx \kappa_D (1 - \beta \epsilon_F/2)$, where κ_D $=2\pi ne^2\beta$ is the classical Debye wave number. In Eqs. (56) and (57), we have introduced the modified plasma parameter $\gamma = \kappa^2 / (2\pi n) = 2r_s^2 [1 - \exp(-\beta \epsilon_F)]^2 \approx \gamma_{cl} (1 - \beta \epsilon_F) \ll 1; \text{ its}$ value in the classical limit, $\gamma_{cl} = \kappa_D^2/(2\pi n)$, is customarily used whenever a large number of particles populate the Deby circle, i.e., whenever $\gamma_{cl} \ll 1$. We have imposed the customary $q_{\text{max}} = \kappa / \gamma \approx 1 / \beta e^2$ inverse-impact-parameter cutoff to avoid the familiar 2D logarithmic divergence also encountered in the calculation of the 2D correlation energy from the Debye-Huckel structure function [22]. This divergence arises because in two dimensions the RPA treatment breaks down in the neighborhood of an electron where the induced charges exceed the background density. Equations (54), (56), (57), and (58) combine to give the small- γ VAA coupling correction

$$-\nu(q)K_0(q \to 0,\omega) = \frac{q^2}{\beta m^* \omega^2} [\mathfrak{R}_0^{\text{stat}} + \mathfrak{R}_0^{\text{dyn}}(\omega)], \quad (60)$$

$$\mathfrak{R}_0^{\text{stat}} = \frac{5}{16} \gamma \ln \gamma - \frac{3}{16} \gamma, \qquad (61)$$

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$$\mathfrak{R}_{0}^{\mathrm{dyn}}(\boldsymbol{\omega}) = -\frac{1}{8N} \sum_{q' \leqslant \kappa/\gamma} \nu^{2}(q') H_{0}(\mathbf{q}', \boldsymbol{\omega}).$$
(62)

To make contact with the ω^3 sum rule, we observe that at frequencies high compared with the plasmon frequency

$$H_0(\mathbf{q}',\omega\to\infty) \approx \frac{nq'^2}{m^*\omega^2} \frac{\bar{\chi}_0(\mathbf{q}',0)}{\bar{\epsilon}_0(\mathbf{q}',0)}.$$
 (63)

The high-frequency expansion

$$\chi_{\rm sc}(\mathbf{q},\omega\to\infty) = \frac{nq^2}{m^*\omega^2} + \frac{nq^2}{m^*\omega^4} \left[\left(\frac{\hbar q^2}{2m^*}\right)^2 + 3q^2 \frac{\langle E_{\rm kin}\rangle_0}{m^*} + \frac{q^2}{\beta m^*} \mathfrak{R}_0^{\rm stat} \right] + O\left(\frac{1}{\omega^6}\right)$$
(64)

then follows from Eqs. (29) and (60)-(63). In the classical limit, Eq. (64) reproduces the exact sum-rule expansion [17(b),(c)] for $\chi(\mathbf{q},\omega\rightarrow\infty)$ if and only if $[q^2/(\beta m^*)]\Re_0^{\text{stat}}$ is identified as the $q \rightarrow 0$, $\gamma_{cl} \ll 1$ value of $D^{cl}(\mathbf{q})$, the term in the classical ω^3 sum-rule coefficient that portrays non-RPA particle correlations. This identification is easily verified by using $D^{\rm cl}(q \rightarrow 0) = 5q^2 \langle E_c \rangle / (8m^*)$ with the correlation energy from Totsuji's cluster-expansion formula [23]

$$\beta \langle E_c \rangle (\gamma_{\rm cl}) = \frac{\gamma_{\rm cl}}{2} [\ln(2\gamma_{\rm cl}) + 0.1544]$$

$$(\gamma_{\rm cl} = \kappa_D^2 / (2\pi n) = 2\pi n e^4 \beta^2 \ll 1)$$
(65)

for the classical 2D electron gas. One readily obtains

$$D_0^{\rm cl}(q \to 0) = \frac{5q^2}{16m^*} \gamma_{\rm cl} [\ln \gamma_{\rm cl} + 0.8475], \qquad (66)$$

in agreement with $[q^2/(\beta m^*)]\Re_0^{\text{stat}}$ through order $\gamma_{\text{cl}} \ln \gamma_{\text{cl}}$ in the dominant term. But we have already noted that the VAA reproduces the potential energy part of the ω^3 sum rule in the weakly degenerate quantum domain for arbitrary values of the coupling parameter $\Gamma = e^2/(a\langle E_{kin} \rangle_0)$. It is therefore quite natural to identify $[q^2/(\beta m^*)]\Re^{\text{stat}}(\Gamma)$ as the Eq. (35) $D(q \rightarrow 0)$ for Γ arbitrary [see Eq. (67b) below]. The zero subscript is accordingly dropped here and in the following to reflect this hypothesis. This latter identification, in fact, is subsumed in the following closure hypothesis referred to as the dynamical superposition approximation: Eqs. (29) and (49) are made self-consistent by postulating that a decomposition of the quadratic χ 's in terms of linear ones, which prevails in the $(q/\omega) \rightarrow 0$ limit for weak coupling, can be relied upon as a paradigm for arbitrary coupling. Accordingly,

$$\nu(q)K_{\rm sc}(q \to 0,\omega) = -\frac{q^2}{\beta m^* \omega^2} [\Re^{\rm stat} + \Re^{\rm dyn}(\omega)],$$
(67a)

$$\Re^{\text{stat}} = \frac{5}{8} \beta V(n,T) = \frac{5}{8} \beta [\langle E_c \rangle(n,T) + \langle E_x \rangle(n,T)],$$
(67b)

$$\mathfrak{R}^{\rm dyn}(\boldsymbol{\omega}) = -\frac{1}{8N} \sum_{\mathbf{q}'} \nu^2(\boldsymbol{q}') H(\mathbf{q}', \boldsymbol{\omega}), \qquad (67c)$$

$$H(\mathbf{q}',\omega) = \int_{-\infty}^{\infty} d\omega' \,\delta_{-}(\omega') \,\frac{\chi_{\rm sc}(\mathbf{q}',\omega')\chi_{\rm sc}(\mathbf{q}',\omega-\omega')}{\epsilon(\mathbf{q}',\omega')\,\epsilon(\mathbf{q}',\omega-\omega')}.$$
(67d)

This completes the stage-3 development of the VAA-DSA theory.

Equations (29) and (67) combine into a self-consistent expression for $\chi_{sc}(q \rightarrow 0, \omega)$ with correlation energy data input from available Monte Carlo (MC) experiments and/or hypernetted chain (HNC) calculations. The actual task of solving Eq. (29) with Eq. (67) at arbitrary frequencies and Γ values is a formidable analytical/computational undertaking well beyond the scope of the present paper. At long wavelengths, however, it turns out that the expression (67c) is amenable to analysis in the neighborhood of the plasma frequency $\omega_{2D}(q) = [2 \pi n e^2 q / (\epsilon_s m^*)]^{1/2}$, making it possible to establish a tractable formula for the real part of the plasmon frequency $\omega(q \rightarrow 0)$ for Γ values such that $(\beta \epsilon_F) \Gamma_{cl} < 1$ [see Sec. II]. The analysis of Sec. VI elaborates on this.

VI. PLASMON DISPERSION

The dispersion relation for the longitudinal plasma mode is derived from the zeros of the dielectric response function

$$\boldsymbol{\epsilon}(\mathbf{q},\boldsymbol{\omega}(\mathbf{q})) = 1 - \nu(q) \chi_{\rm sc}(\mathbf{q},\boldsymbol{\omega}(\mathbf{q})), \tag{68}$$

with χ_{sc} given by Eqs. (29) and (67).

At long wavelengths, we observe that (q^2/ω^2) is at most of O(q) smallness in the vicinity of the plasmon frequency. With this in mind, the development of Eq. (29) with Eq. (67)in powers of (q^2/ω^2) gives

$$\boldsymbol{\epsilon}(q \to 0, \boldsymbol{\omega}) = 1 - \frac{\omega_{2\mathrm{D}}^2(q)}{\omega^2} \bigg(1 + \frac{3q^2}{m^* \omega^2} \langle E_{\mathrm{kin}} \rangle_0 + \frac{q^2}{\beta m^* \omega^2} [\Re^{\mathrm{stat}} + \Re^{\mathrm{dyn}}(\boldsymbol{\omega})] \bigg).$$
(69)

To further evaluate $\Re^{dyn}(\omega)$, we observe that for small q, $H(\mathbf{q}', \omega)$ can be Taylor expanded about $\omega = 0$ as follows:

.....

$$H(\mathbf{q}', \omega(\mathbf{q})) \approx H(\mathbf{q}', \omega_{2D}(q))$$

$$= \operatorname{Re} H(\mathbf{q}', 0) + i\omega_{2D}(q) \left[\frac{\partial}{\partial \omega} \operatorname{Im} H(\mathbf{q}', \omega) \right]_{\omega=0}$$

$$+ \cdots = \frac{1}{2} \left[\frac{\chi_{\mathrm{sc}}(\mathbf{q}', 0)}{\epsilon(\mathbf{q}', 0)} \right]^{2} + i\omega_{2D}(q) \frac{1}{2\pi}$$

$$\times P \int_{-\infty}^{\infty} \frac{d\omega'}{\omega'} \frac{\partial}{\partial \omega'} \left[\operatorname{Im} \frac{\chi_{\mathrm{sc}}(\mathbf{q}', \omega')}{\epsilon(\mathbf{q}', \omega')} \right]^{2}. \quad (70)$$

whence

 $\operatorname{Re} \mathfrak{R}^{\operatorname{dyn}}(\omega(\mathbf{q})) \equiv \operatorname{Re} \mathfrak{R}^{\operatorname{dyn}}$

$$\approx -\frac{1}{16N} \sum_{q' \leqslant q_{\max}} \nu^2(q') \left[\frac{\chi_{sc}(\mathbf{q}', 0)}{\boldsymbol{\epsilon}(\mathbf{q}', 0)} \right]^2,$$
(71)

$$\operatorname{Im} \mathfrak{R}^{\operatorname{dyn}}(\omega(\mathbf{q}))|_{\operatorname{corr}} \approx -\omega_{2D}(q) \frac{1}{16\pi N} \sum_{\mathbf{q}'} \nu^{2}(q') \\ \times P \int_{-\infty}^{\infty} \frac{d\,\omega'}{\omega'} \frac{\partial}{\partial\omega'} \left[\operatorname{Im} \frac{\chi_{\operatorname{sc}}(\mathbf{q}',\omega')}{\epsilon(\mathbf{q}',\omega')} \right]^{2}.$$

$$(72)$$

The steps in the derivation of Eq. (70) are detailed in the Appendix. Again, the q_{max} cutoff in Eq. (71) is imposed to avoid the ubiquitous 2D logarithmic divergence arising from the RPA-like structure of the quadratic response function inherent in the closure hypothesis. [To detect the divergence, go to the classical limit, replace $\chi_{\text{sc}}(\mathbf{q}', 0)/\varepsilon(\mathbf{q}', 0)$ with $-\beta n S(\mathbf{q}')$ via the fluctuation-dissipation theorem, and then observe that the latter tends to $-\beta n$ as $q' \rightarrow \infty$]. For $\Gamma < 1$ one customarily chooses $q_{\text{max}} = \kappa/\gamma$ as before, whereas for $\Gamma > 1$ one chooses $q_{\text{max}} = 1/a$. Concentrating on the latter domain, we observe that $\chi_{\text{sc}}(\mathbf{q}', 0)$ and $\epsilon(\mathbf{q}', 0)$ can be reasonably well approximated by the compressibility formulas

 $\chi_{\rm sc}^{\rm exact}(q' \rightarrow 0, \omega = 0) = -n(\partial P/\partial n)_T^{-1}$

and

$$\epsilon^{\text{exact}}(q' \rightarrow 0, \omega = 0) = 1 + \nu(q')n(\partial P/\partial n)_T^{-1}$$

over most of the summation interval $0 \le q' \le 1/a$. Substituting these expressions into Eq. (71) and performing the summation, one obtains

$$\operatorname{Re} \mathfrak{R}^{\operatorname{dyn}} \approx -\frac{\Gamma_{\operatorname{cl}}^{2}}{8[\beta(\partial P/\partial n)_{T}]^{2}} \ln \left[1 + \frac{\beta(\partial P/\partial n)_{T}}{2\Gamma_{\operatorname{cl}}}\right] + \frac{\Gamma_{\operatorname{cl}}^{2}}{8\beta(\partial P/\partial n)_{T}[\beta(\partial P/\partial n)_{T} + 2\Gamma_{\operatorname{cl}}]}.$$
 (73)

The expression (73) is bounded for all $\Gamma \ge 1$; this is true even at the Γ value where $\beta(\partial P/\partial n)_T = 0$: $\Re^{dyn} = -1/64$. The expression (72) for Im $\Re^{dyn}(\omega(\mathbf{q}))$ provides the VAA-DSA correlation-induced damping of the plasmon mode. Evaluating Eq. (72) at arbitrary coupling would entail solving Eq. (29) with Eq. (67), which, as we have already stated, is well beyond the scope of the present paper. However, Eq. (72) can be readily evaluated in the $\hbar \rightarrow 0$ limit for $\gamma_{cl} \ll 1$; using the Vlasov formula $\text{Im } \chi_0(\mathbf{q}', \omega') = -(\beta n \omega/q') \sqrt{\pi \beta m/2} \exp[-\beta m \omega'^2/(2q'^2)]$ and approximating $\varepsilon(q', \omega')$ by its static RPA value, one obtains

$$\operatorname{Im} \mathfrak{R}^{\operatorname{dyn}}(\boldsymbol{\omega}(\mathbf{q}))\big|_{\operatorname{corr}} \approx -\frac{\pi\sqrt{\pi}}{32} \gamma_{\operatorname{cl}} \sqrt{q/\kappa_D}.$$
(74)

We will return to Eq. (74) shortly when we discuss plasmon damping.

For calculation of the plasmon frequency, Eqs. (68), (69), and (67b) combine to give the biquadratic dispersion relation

$$\omega^4 - \omega_{2D}^2(q)\,\omega^2 - \omega_{2D}^2(q)s^2q^2 = 0,\tag{75}$$

$$s^{2} = 3 \, \frac{\langle E_{\rm kin} \rangle_{0}}{m^{*}} + \frac{5}{8} \, \frac{V}{m^{*}} + \frac{1}{\beta m^{*}} \, \Re^{\rm dyn}. \tag{76}$$

Addressing the dispersion part of the calculation, we solve Eq. (75) for the real part to obtain

Re
$$\omega(\mathbf{q}) = \frac{\omega_{2\mathrm{D}}(q)}{\sqrt{2}} [1 + \sqrt{1 + 4s_r^2 q^2 / \omega_{2\mathrm{D}}^2(q)}]^{1/2}$$
 (77a)

$$\approx \omega_{\rm 2D}(q) + \frac{s_r^2 q^2}{2\,\omega_{\rm 2D}(q)},\tag{77b}$$

where

$$s_r^2 = \operatorname{Re} s^2 = 3(\langle E_{kin} \rangle_0 / m^*) + 5V/(8m^*) + (1/\beta m^*) \operatorname{Re} \mathfrak{R}^{dyn}.$$

Equation (77b) follows from the small-q expansion of the radical in Eq. (77a). Equations (77), (76), and (73) describe the long-wavelength plasmon dispersion in weakly degenerate ($\beta \epsilon_F \leq 0.2$) 2D Coulomb fluids over a wide range of Γ values such that $(\beta \epsilon_F) \Gamma_{cl}$ is of order unity at most. A given pair of $(\Gamma, \beta \epsilon_F)$ values determines the $\langle E_{\rm kin} \rangle_0$, $\langle E_{\rm xc} \rangle$, and inverse compressibility $(\partial P/\partial n)_T$ inputs via Eqs. (78)–(81) and (83) below. While Monte Carlo [24,25] simulations and hypernetted chain [26] calculations have generated correlation-energy data for the 2D electron liquid in the classical [24,26] and zero-temperature quantum [25] domains, little, if any, such data are available at arbitrary degeneracy. For $(\beta \epsilon_F)_{\text{max}} = 0.1 - 0.2$, however, fairly reliable formulas for the interaction energy can be constructed either from the purely classical MC formula of Totsuji [23] or from Lado's HNC formula [26]. This is accomplished simply by adding a temperature-dependent exchange contribution. The modified formulas for the exchange-correlation energy are

$$\beta V(n,T) = \begin{cases} -1.12\Gamma_{\rm cl} + 0.71\Gamma_{\rm cl}^{1/4} - 0.38 + \beta \langle E_x \rangle (n,T) & (0.707 < \Gamma_{\rm cl} < 50), \\ 1.0052\Gamma_{\rm cl} + 0.0851 + 0/E_z \rangle (n,T) & (\Gamma_{\rm cl} > 20) \end{cases}$$
(78)

$$(-1.0952\Gamma_{\rm cl}+0.9851+\beta\langle E_x\rangle(n,T)) \qquad (\Gamma_{\rm cl}>30), \tag{79}$$

with the exchange energy given by the asymptotic formula [27]

$$\langle E_x \rangle(n,T) = 0.632 \sqrt{\beta \epsilon_F \langle E_x \rangle(n,T=0)}$$
 (80)

in terms of the Hartree-Fock exchange energy per particle [7]

$$\langle E_x \rangle (n, T=0) = -\frac{4\sqrt{2}}{3\pi} \frac{e^2}{a}.$$
 (81)

The inverse isothermal compressibility input to Eq. (73) is calculated from the *approximate* 2D equation of state formula

$$P = n \langle E_{\rm kin} \rangle_0 + \frac{2}{3} n \langle E_x \rangle(n,T) + \frac{1}{2} n \langle E_c \rangle(n,T)$$
(82)

that is exact in the classical limit [17(c)] and that best accommodates use of the fitted formulas (78) and (79). From Eq. (82), it can be shown that

$$\left(\frac{\partial P}{\partial n}\right)_{T} = \frac{\epsilon_{F}}{1 - \exp(-\beta\epsilon_{F})} + \frac{\partial}{\partial n}n(\frac{2}{3}\langle E_{x}\rangle(n,T) + \frac{1}{2}\langle E_{c}\rangle(n,T))$$
$$\approx \frac{1}{\beta}(1 + \frac{1}{2}\beta\epsilon_{F}) + \frac{\partial}{\partial n}n(\frac{2}{3}\langle E_{x}\rangle(n,T) + \frac{1}{2}\langle E_{c}\rangle(n,T))$$
(83)

valid for $(\beta \epsilon_F)_{max} = 0.1 - 0.2$ and arbitrary Γ . One cannot overstate the centrality of the ω^3 sum rule in the VAA-DSA description of plasma-mode dispersion: our calculations reveal that $|\text{Re } \mathcal{R}^{\text{dyn}}(\omega(\mathbf{q}))| \leq (5/8)\beta |V|$ for all Γ values, suggesting that the coupling correction to the long-wavelength RPA plasma-mode dispersion is entirely controlled by the potential energy part of the third-frequency-moment sumrule coefficient.

Dispersion curves based on Eq. (77a) are displayed in Figs. 1(a), 1(b), and 2 for the weakly degenerate and classical 2DCFs. The exceedingly thin RPA linewidths shown in Figs. 3 and 4 confirm that the 2D plasma waves are virtually unaffected by Landau damping at long wavelengths. As expected, the effect of the static exchange-correlation hole acts to depress the long-wavelength plasmon frequency below its RPA value, the deviation increasing with increasing Γ for fixed $\beta \epsilon_F$. Here the correlational contribution plays the dominant role. For example, at $\beta \epsilon_F = 0.2$ and $\Gamma = 5$ the exchange comprises 16–18% of the deviation for *qa* ranging from 0.1 to 0.5; at $\Gamma = 10$, its effect diminishes slightly to 14.9–17.4% over the same *qa* range.

VII. CONCLUSIONS AND DISCUSSION

In this paper, we have analyzed the dynamical response and long-wavelength plasmon dispersion in the strongly coupled 2DCF in the weakly degenerate quantum domain. Adopting the Ref. [15] methodology, we have developed a self-consistent approximation scheme [Eq. (29) with Eq. (67)] for calculation of the screened density response function $\chi_{sc}(\mathbf{q}, \omega)$ at long wavelengths. The basic ingredients in the construction of the approximation scheme are the first kinetic equation in the BBGKY hierarchy [Eq. (19)], the



FIG. 1. (a) Plasmon dispersion curves for $\beta \epsilon_F = 0.2$ and $\Gamma = 5$. The solid line, calculated from Eq. (77a), takes account of the static exchange-correlation effect. The dash-dotted line portrays the dispersion without the exchange and the dotted line is the RPA curve. (b) Plasmon dispersion curves for $\beta \epsilon_F = 0.2$ and $\Gamma = 10$ with the solid line calculated from Eq. (77a). The dash-dotted line leaves out the exchange and the dotted line is the RPA curve.

VAA hypothesis [Eq. (20)], the QFDT [Eqs. (9) and (10)], and the DSA closure hypothesis [Eq. (67)]. The VAA-DSA *dynamical* local field correction

$$G(\mathbf{q},\omega) = \frac{K_{\rm sc}(\mathbf{q},\omega)}{\chi_0(\mathbf{q},\omega)[1-\nu(q)K_{\rm sc}(\mathbf{q},\omega)]},\qquad(84)$$

with screened coupling correction $K_{sc}(\mathbf{q}, \omega)$ given by Eq. (67), provides the correspondence between Eq. (29) and the conventional mean field theory formula

$$\chi_{\rm sc}(\mathbf{q},\omega) = \frac{\chi_0(\mathbf{q},\omega)}{1 + \nu(q)G(\mathbf{q},\omega)\chi_0(\mathbf{q},\omega)}.$$
(85)

The $D(\mathbf{q})$ term in the high-frequency expansion (32) of $\chi^{VAA}(\mathbf{q},\omega)$ is identified as precisely the term in the third-



FIG. 2. Plasmon dispersion curves in the classical domain for Γ =5, 10, and 40. The solid lines, calculated from Eq. (77a), take account of the static correlation effect. Γ =5 labels the upper solid line, Γ =10 the middle line, and Γ =40 the bottom line. The dash-dotted lines are the corresponding RPA curves with the same Γ value ordering.

frequency-moment sum-rule coefficient [17(a),(d)] that accounts for exchange and correlation through the two-point static structure functions [see Eq. (33)]; at long wavelengths, $D(q \rightarrow 0)$ is proportional to the potential energy per particle. Given the complete lack of S(q) data for the 2DCF in the weakly degenerate quantum domain, we have postulated that the long-wavelength expression (35) for $D(q \rightarrow 0)$ can be replaced by the decomposition (36) as an alternative way of determining the potential energy in terms of the exchange and correlation energies calculated from formulas (78)–(81).

The VAA-DSA $G(\mathbf{q}, \omega)$, in contrast to the conventional [3,7,8,9] and quantum [12] STLS local field corrections, which do not satisfy the third-frequency-moment sum rule, (i) features the ω^3 sum-rule $D(q \rightarrow 0)$ coefficient as the cen-







FIG. 4. RPA linewidths at $\Gamma = 5$, 10, and 40 in the classical domain.

trally important element in the description of the coupling correction to the long-wavelength 2D-plasmon dispersion and (ii) gives a prescription for going beyond the RPA dynamics of single particle-hole pair excitations (Landau damping) by taking account of Coulomb correlation-induced damping [see Eq. (86) below].

A few remarks about plasma-mode damping in the classical limit and at weak coupling ($\gamma_{cl} \ll 1$), which could have relevance to the strongly coupled 2DCF in the weakly degenerate quantum domain. From Eq. (74), the correlational damping rate is calculated to be the $O(q^2)$ couplingdependent expression

Im
$$\omega(\mathbf{q}) = -\frac{\pi\sqrt{\pi}}{2^{3/4}32} \gamma_{cl}^{5/4} \omega_0 \left(\frac{q}{\kappa_D}\right)^2 \quad \omega_0 \equiv \sqrt{2\pi n e^2/(ma)}.$$
(86)

This result differs markedly from the damping rate predicted some time ago by Totsuji [23] and later confirmed by Lu and Golden in an independent calculation [28]. Using a semiphenomenological approach based on the Vlasov-Boltzmann equation, Totsuji's calculation reveals the existence of a lower-order overall O(q) coupling-independent collisional damping which survives even in the $\gamma_{cl}=0$ limit and which is accompanied by an upward shift in the Bohm-Gross plasmon dispersion, viz.,

$$\omega(\mathbf{q}) \approx \omega_{2\mathrm{D}}(q) \left[1 + \left(\frac{3}{2} + B\right) \frac{q}{\kappa_D} - iA\sqrt{\pi q/\kappa_D} \right], \quad (87)$$

where the collisional damping coefficient $A = \frac{3}{16}$, and where the concomitant collision-induced dispersion coefficient $B = 21 \pi/256$. Using a systematic formal expansion (in γ_{cl}) of the first two equations in the BBGKY hierarchy, Lu and Golden [28] arrive at the same structure (87) in the $\gamma_{cl}=0$ limit with $A = \frac{1}{8}$ and $B = 7 \pi/128$. [Satisfaction of the ω^3 sum rule is still assured since

$$\boldsymbol{\epsilon}_{\text{coll}}(q \rightarrow 0, \boldsymbol{\omega}; \boldsymbol{\gamma}_{\text{cl}} = 0) = \boldsymbol{\epsilon}(q \rightarrow 0, \boldsymbol{\omega}; \boldsymbol{\gamma}_{\text{cl}} = 0) - \boldsymbol{\epsilon}_{0}(q \rightarrow 0, \boldsymbol{\omega})$$

$$=i(\sqrt{\pi/4})[\omega_{2D}(q)/\omega]^5(q/\kappa_D)^{1/2}.]$$

By contrast A=0=B in the RPA ($\gamma=0$) limit of the present VAA-DSA mean field theory. Indeed, A=0=B for *all* 2D mean field theories in the classical and quantum domains. This irreconcilable disparity is a consequence of the fact that mean field theories do not take account of short-range dynamic collisions. The survival of the collisional effect in the $\gamma=0$ limit is related to the fact that, in two dimensions, the mean particle-particle collision frequency $[2\pi ne^2 \kappa_{\rm DH}/m]^{1/2}$ turns out to be entirely independent of the plasma parameter. This obtains even when calculated under the usual weakcoupling assumption that a test particle interacts weakly with a large population of field particles inside the Debye circle.

Given the possibility of the interesting small $7\pi/128$ upward shift, we expect that the VAA-DSA description of longwavelength plasmon dispersion is most accurate for $\Gamma_{\min} \approx 5$, beyond which short-range dynamic collisional effects are overwhelmed by exchange-correlation effects.

The question arises as to whether the VAA might be a promising approach to the calculation of dynamical response and plasmon dispersion in the 2DCF in the strongly degenerate quantum domain. Kalman and Rommel [29] have completed the first two stages of the quantum VAA calculation for the *zero-temperature* 2DCF. Some progress was made in the stage-3 development in that they calculated the Lindhard quadratic density response function equivalent of our Eq. (51). Their far more involved expression, however, suggests that the final step of establishing a quantum equivalent of the DSA closure scheme is a formidable task well beyond the scope of the present paper.

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APPENDIX

In this Appendix, we detail the steps in the evaluation of the first right-hand-side member of Eq. (70). We begin by writing Eq. (67d) in the more convenient form

$$H(\mathbf{q}',\omega) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{d\omega'}{\omega'} \frac{\chi_{\rm sc}(\mathbf{q}',\omega-\omega')}{\epsilon(\mathbf{q}',\omega-\omega')} \operatorname{Im} \frac{\chi_{\rm sc}(\mathbf{q}',\omega')}{\epsilon(\mathbf{q}',\omega')}.$$
 (A1)

Replacement of $\text{Im}[\chi_{sc}(\mathbf{q}', \omega')/\varepsilon(\mathbf{q}', \omega)]$ by its Hilbert transform (HT) accompanied by a partial fraction expansion (PFE) and application of the Poincaré-Bertrand (PE) theorem gives

$$H(\mathbf{q}',\omega) = \frac{1}{\pi^2} PP \int_{-\infty}^{\infty} \frac{d\omega'}{\omega'} \int_{-\infty}^{\infty} \frac{d\omega''}{\omega'-\omega''} \frac{\chi_{sc}(\mathbf{q}',\omega-\omega')}{\epsilon(\mathbf{q}',\omega-\omega')} \operatorname{Re} \frac{\chi_{sc}(\mathbf{q}',\omega'')}{\epsilon(\mathbf{q}',\omega'')} \quad (HT)$$

$$= \frac{1}{\pi^2} PP \int_{-\infty}^{\infty} d\omega' \int_{-\infty}^{\infty} \frac{d\omega''}{\omega'(\omega'-\omega'')} \frac{\chi_{sc}(\mathbf{q}',\omega-\omega')}{\epsilon(\mathbf{q}',\omega-\omega')} \operatorname{Re} \frac{\chi_{sc}(\mathbf{q}',\omega'')}{\epsilon(\mathbf{q}',\omega'')} \quad (PFE)$$

$$= -\frac{1}{\pi^2} PP \int_{-\infty}^{\infty} d\mu \int_{-\infty}^{\infty} \frac{d\nu}{\nu(\mu+\nu-\omega)} \frac{\chi_{sc}(\mathbf{q}',\mu)}{\epsilon(\mathbf{q}',\mu)} \operatorname{Re} \frac{\chi_{sc}(\mathbf{q}',\nu)}{\epsilon(\mathbf{q}',\nu)}$$

$$= \frac{\chi_{sc}(\mathbf{q}',\omega)\chi_{sc}(\mathbf{q}',0)}{\epsilon(\mathbf{q}',0)} - \frac{1}{\pi^2} PP \int_{-\infty}^{\infty} \frac{d\nu}{\nu} \int_{-\infty}^{\infty} \frac{d\mu}{\mu} + \nu-\omega} \frac{\chi_{sc}(\mathbf{q}',\mu)}{\epsilon(\mathbf{q}',\mu)} \operatorname{Re} \frac{\chi_{sc}(\mathbf{q}',\nu)}{\epsilon(\mathbf{q}',\mu)} (PB)$$

$$= \frac{\chi_{sc}(\mathbf{q}',\omega)\chi_{sc}(\mathbf{q}',0)}{\epsilon(\mathbf{q}',0)} + \frac{1}{\pi^2} PP \int_{-\infty}^{\infty} \frac{d\mu}{\mu} \int_{-\infty}^{\infty} \frac{d\nu}{(\omega-\mu)-\nu} \frac{\chi_{sc}(\mathbf{q}',\nu)}{\epsilon(\mathbf{q}',\nu)} \operatorname{Re} \frac{\chi_{sc}(\mathbf{q}',\mu)}{\epsilon(\mathbf{q}',\mu)}; \quad (\mu \leftrightarrow \nu) \text{ interchange.}$$
(A2)

Consequently,

$$H(\mathbf{q}',\omega) = \frac{\chi_{\rm sc}(\mathbf{q}',\omega)\chi_{\rm sc}(\mathbf{q}',0)}{\epsilon(\mathbf{q}',\omega)\epsilon(\mathbf{q}',0)} - \frac{i}{\pi}P\int_{-\infty}^{\infty}\frac{d\mu}{\mu}\frac{\chi_{\rm sc}(\mathbf{q}',\omega-\mu)}{\epsilon(\mathbf{q}',\omega-\mu)}\operatorname{Re}\frac{\chi_{\rm sc}(\mathbf{q}',\mu)}{\epsilon(\mathbf{q}',\mu)}$$
(A3)

by application of the Hilbert transformation to Eq. (A2). From Eqs. (A1) and (A3), it can then be shown that

$$-\frac{i}{\pi}P\int_{-\infty}^{\infty}\frac{d\mu}{\omega-\mu}\frac{\chi_{\rm sc}(\mathbf{q}',\omega-\mu)\chi_{\rm sc}^{*}(\mathbf{q}',\mu)}{\epsilon(\mathbf{q}',\omega-\mu)\epsilon^{*}(\mathbf{q}',\mu)} = \frac{\chi_{\rm sc}^{*}(\mathbf{q}',\omega)\chi_{\rm sc}(\mathbf{q}',0)}{\epsilon^{*}(\mathbf{q}',\omega)\epsilon(\mathbf{q}',0)}.$$
(A4)

Equation (A4) combined with

then gives

$$H(\mathbf{q}',0) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{d\mu}{\mu} \operatorname{Re} \frac{\chi_{\rm sc}(\mathbf{q}',\mu)}{\epsilon(\mathbf{q}',\mu)} \operatorname{Im} \frac{\chi_{\rm sc}(\mathbf{q}',\mu)}{\epsilon(\mathbf{q}',\mu)}$$
(A5)

$$H(\mathbf{q}',0) = \frac{1}{2} \left[\frac{\chi_{\rm sc}(\mathbf{q}',0)}{\boldsymbol{\epsilon}(\mathbf{q}',0)} \right]^2. \tag{A6}$$

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