Mean-Field Kinetic Theory of a Classical Electron Gas in a Periodic Potential. I. Formal Solution of the Vlasov Equation

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We study the static and dynamic behavior of a classical electron gas in the periodic potential created by an ionic lattice. Using the well-known Vlasov approximation, we derive a mean-field kinetic equation for the density-response function of the electrons. This equation is formally solved in terms of the trajectories of one electron in the mean-field equilibrium potential which determines the local electronic density. The mean-field expressions of the static and dynamic structure factors are then obtained through the fluctuation-dissipation theorem. These expressions are used to show that within the mean-field approximation the system is a conductor at all temperatures and for all dimensions.

1. INTRODUCTION

The classical Coulomb gas (CG) is made up of two species of particles with opposite charges e and $-e$. Two charges interact through the Coulomb potential defined as the solution of Poisson's equation in d dimensions. This potential is linear in one dimension, logarithmic in two dimensions, and inversely proportional to the distance in three dimensions. For $d \geqslant 2$, one has to introduce a short-range repulsive potential between oppositely charged particles in order to prevent their collapse. For $d = 2$, this additional potential is really essential to the stability only below the collapse temperature[1] $T_0 = e^2/2k_B$ (the system of point charges is stable above T_0 [1]).

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The CG is particularly interesting in two dimensions, where it undergoes a Kosterlitz–Thouless (KT) transition[2] from a low-temperature dielectric phase to a high-temperature plasma phase.[3] The KT transition is characterized by a discontinuity in the *response* of the system to an external static field, as materialized by the static dielectric constant, which is infinite in the plasma phase and finite in the dielectric phase. This transition is induced by the binding nature of the logarithmic potential: at low temperatures, each positive charge combines with a negative charge to form a dipolar molecule. Kosterlitz and Thouless[2] have proposed a semiheuristic argument which shows that the dielectric (dipole) phase is stable below $T_c = e^2/4k_B$, in the zero-density limit. Renormalization-group calculations[2,4] lead to a density-dependent transition temperature; when the density becomes small, this temperature goes to T_c. For higher densities, the KT transition should become a first-order transition between a dielectric gas and a conducting liquid.[5] In one dimension, the CG is always (at any temperature or density) a dielectric, as shown by an exact explicit calculation[6]; this is due to the strong binding nature of the $|x|$ potential. In three dimensions, the CG is expected to be always a plasma, at least in the fluid phase, since the Coulomb potential then vanishes at large distances.

The KT transition of the CG is characterized by a static criterion regarding the static-screening properties. This transition also should be characterized by a dynamic criterion with regard to the dc conductivity σ. The plasma phase should be conducting ($\sigma \neq 0$), since it contains free charges, whereas the dielectric phase should be insulating ($\sigma = 0$), since it contains only dipolar molecules. This dynamic aspect of the KT transition has been recently investigated through molecular dynamics (MD) experiments.[7,8] The authors[7,8] consider a spcial version of the CG, where the particles of one species (the "ions") are fixed at the sites of a periodic lattice while the particles of the other species (the "electrons") move in the periodic potential created by the fixed ions. The KT transition then becomes a *localization* transition for the mobile particles: at low temperatures, each electron is bound to a given ion, while above some threshold temperature the electrons diffuse throughout the lattice.[7,8] Since it is difficult to obtain accurate estimates of σ from MD simulations, Clerouin *et al.*[8] have only computed the self-diffusion constant D. As expected, D vanishes below some threshold temperature[2] depending on the density.

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[2] *A priori* this threshold temperature might be different from the one at which σ vanishes. Furthermore, both previous temperatures might be different from the KT temperature determined by the static criterion. In fact, intuitive physical arguments indicate that all these temperatures should be identical.

As illustrated by the MD simulations,[7,8] the fixed-ion model in two dimensions exhibits remarkable dynamic properties related to the KT transition. Furthermore, this model in three dimensions might reasonably describe superionic conductors.[9] The present series of papers is devoted to a mean-field analysis of the static and dynamic behavior of the fixed-ion model in d dimensions. In this analysis, the electron–electron interactions are treated in a mean-field approximation, while the electron–ion interactions are taken into account *exactly*. The latter prescription makes the mean-field calculations much more difficult than for the usual CG with two mobile species. Furthermore, and this is more essential, the exact treatment of the electron–ion interactions allows one to describe complicated coupling effects between the electron motion and the periodic structure of the lattice. The nontrivial character of the mean-field approach for the fixed-ion model led us to investigate the predictions of this theory at all temperatures, although the latter is expected to be only valid in the high-temperature regime. Our salient results have been summarized in a letter.[10] In the present paper (referred to as paper I), we formally solve the mean-field equations, and we study the nature of the phase predicted by the mean-field theory from both static and dynamic points of view. In papers II and III, we shall compute explicitly the mean-field quantities for $d = 1$ and $d = 2$, respectively. The corresponding results will be compared to exact (analytic) or MD data; in particular, emphasis will be put on the spectrum of the fluctuations and on the collective modes.

The present paper is organized as follows. In Section 2, we define the fixed-ion model. In Section 3, we derive a mean-field kinetic equation for the density-response function of the system, where the correlations between the electrons are neglected (Vlasov approximation). This equation is formally solved in Section 4. The man-field expressions of the static and dynamic structure factors are then obtained through the fluctuation-dissipation theorem in Sections 5 and 6. The static and dynamic criteria, which determine the phase of the system, are applied to these mean-field expressions. A short summary of the main results and some comments are given in Section 7.

2. THE FIXED-ION MODEL

In the fixed-ion model, the positive charges e (the ions) are fixed at the sites $\mathbf{R}_j$ of a periodic lattice. The negative charges $-e$ (the electrons) move in the periodic potential created by the ions. The mass of the electrons is m. The system is overall neutral, i.e., the number N_e of electrons is equal to the number N_i of ions, $N_e = N_i = N$. Thus, the mean-electron density ρ, $\rho = N/\Lambda$, where Λ is the measure of the system, reduces to $1/\Lambda_{\mathrm{WS}}$, where

A_{WS} is the measure of the Wigner–Seitz (WS) unit cell. The mean distance between the electrons is $a = [d\Gamma(d/2)/2\pi^{d/2}\rho]^{1/d}$, where $\Gamma(d/2)$ is the gamma function.

Two electrons separated by a distance r interact through the Coulomb potential $\phi_C(r)$ defined as the solution of Poisson's equation

$$\nabla^2 \phi_C(r) + \frac{2\pi^{d/2}}{\Gamma(d/2)} e^2 \delta(\mathbf{r}) = 0 \tag{2.1}$$

whose solutions are

$$\begin{array}{lll} \phi_C(x) = -e^2 |x| & \text{for} & d = 1 \\[4pt] \phi_C(r) = -e^2 \ln(r/L_s) & \text{for} & d = 2 \\[4pt] \phi_C(r) = e^2/r & \text{for} & d = 3 \end{array} \tag{2.2}$$

(L_s is an irrelevant scale length). The Fourier transform of $\phi_C(r)$,

$$\tilde{\phi}_C(k) = \int d\mathbf{k} \exp(i\mathbf{k} \cdot \mathbf{r}) \, \phi_C(r) \tag{2.3}$$

takes the simple form

$$\tilde{\phi}_C(k) = [2\pi^{d/2}/\Gamma(d/2)] e^2/k^2 \tag{2.4}$$

One electron and one ion separated by a distance r interact through the potential $\phi_{ie}(r)$,

$$\phi_{ie}(r) = \begin{cases} \phi_{SR}(r) & \text{for} \quad r < \delta \\ -\phi_C(r) & \text{for} \quad \delta < r \end{cases} \tag{2.5}$$

δ is a length characterizing the "size" of the ions. $\phi_{SR}(r)$ is a suitable short-range potential, which guarantees the stability of the system for $d \geqslant 2$. At this level, we do not need to specify the precise form of $\phi_{SR}(r)$. We shall only assume that $\phi_{ie}(r)$ is continuously differentiable everywhere. This assumption is motivated by purely technical reasons, the mean-field analysis becoming slightly more difficult to handle if $\phi_{SR}(r)$ includes hard cores. The long-wavelength properties of the system are not sensitive (from a qualitative point of view) to the detailed form of $\phi_{SR}(r)$. The total interaction potential of the finite system is

$$V_N(\mathbf{r}_1,...,\mathbf{r}_N) = \frac{1}{2} \sum_{i \neq j} \phi_C(|\mathbf{r}_i - \mathbf{r}_j|) + \sum_{i=1}^{N} V_L(\mathbf{r}_i) + V_{0,N} \tag{2.6}$$

where $\mathbf{r}_i$ is the position of the electron i, and $V_L(\mathbf{r})$ is the one-body potential created by the ions and seen by the electrons,

$$V_L(\mathbf{r}) = \sum_{\mathbf{R}_j} \phi_{ie}(|\mathbf{r} - \mathbf{R}_j|) \qquad (2.7)$$

and $V_{0,N}$ is a constant, which represents the ion–ion interactions.

We shall consider the infinite system defined by taking the thermodynamic limit $(\mathrm{TL})N \to \infty$, $\Lambda \to \infty$, $\rho = N/\Lambda$ being kept fixed. We assume the quantities of interest to be well-defined in the TL.[3] The equilibrium state of the infinite system is determined by the mean electron density ρ and by the inverse temperature $\beta = 1/k_B T$. The coupling constant $\Gamma = \beta e^2 a^{2-d}$ measures the strength of electrostatic interactions. The inverse of the Debye wavenumber $\kappa_D = [2\pi^{d/2}\beta e^2\rho/\Gamma(d/2)]^{1/2}$ is the characteristic screening length of the electrons. The inverse of the plasma frequency $\omega_p = [2\pi^{d/2}e^2\rho/m\Gamma(d/2)]^{1/2}$ is the natural time scale for the dynamics.

3. THE VLASOV APPROXIMATION

In this section we derive the basic mean-field equation for the density-response function. We follow the well-known procedure where one starts from the first equation of the BBGKY hierarchy in the presence of a time-dependent external potential. Neglecting the correlations between the electrons (Vlasov approximation), we then obtain the required mean-field equation.

Let $f^{(1)}(\mathbf{r}, \mathbf{v}; t)$ and $f^{(2)}(\mathbf{r}, \mathbf{v}; \mathbf{r}', \mathbf{v}'; t)$ be the phase-space one- and two-body distribution functions of the electrons subjected to the external potential $V_{\mathrm{ext}}(\mathbf{r}, t)$. The first equation of the BBGKY hierarchy reads

$$\left[\frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \frac{1}{m} \mathbf{F}_L(\mathbf{r}) \cdot \frac{\partial}{\partial \mathbf{v}} + F_{\mathrm{ext}}(\mathbf{r}, t) \cdot \frac{\partial}{\partial \mathbf{v}} \right] f^{(1)}(\mathbf{r}, \mathbf{v}, t)$$

$$+ \frac{1}{m} \frac{\partial}{\partial \mathbf{v}} \cdot \int d\mathbf{r}' \, d\mathbf{v}' \, f^{(2)}(\mathbf{r}, \mathbf{v}; \mathbf{r}', \mathbf{v}'; t) \, \mathbf{F}_C(\mathbf{r}' - \mathbf{r}) = 0 \qquad (3.1)$$

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[3] For $d = 2$, the existence of transport coefficients like D and σ is an open question. For systems with short-range forces, the self-diffusion constant computed from the Green–Kubo formula should diverge. Indeed, a simple physical argument[11] suggests that the self-velocity autocorrelation function decays like $1/t$ for long times t (this behavior can also be obtained by a hydrodynamic analysis.[12]) For Coulomb systems, the previous argument does not apply in its original form. However, a sophisticated mode-coupling analysis[13] shows that the long-time tails persist in a homogeneous electron gas, in agreement with MD simulations.[14] The extension of such an analysis to the present inhomogeneous system is not straightforward, and consequently D and σ might be finite. For $d = 1$, the status of D and σ is still more obscure.

$\mathbf{F}_L(\mathbf{r})$ is the periodic force deriving from $V_L(\mathbf{r})$,[4]

$$\mathbf{F}_L(r) = -\frac{\partial}{\partial \mathbf{r}} V_L(\mathbf{r}) \qquad (3.2)$$

$\mathbf{F}_{ext}(\mathbf{r}, t)$ is the external force,

$$\mathbf{F}_{ext}(\mathbf{r}, t) = -\frac{\partial}{\partial \mathbf{r}} V_{ext}(\mathbf{r}, t) \qquad (3.3)$$

and $\mathbf{F}_C(\mathbf{r}' - \mathbf{r})$ is the Coulomb force acting on an electron at $\mathbf{r}$ due to another electron located at $\mathbf{r}'$,

$$\mathbf{F}_C(\mathbf{r}' - \mathbf{r}) = -\frac{\partial}{\partial \mathbf{r}} \phi_C(|\mathbf{r}' - \mathbf{r}|) \qquad (3.4)$$

The last term of the left-hand side of (3.1) arises from the interactions between the electrons and depends on the two-body distribution function $f^{(2)}$. If we make the usual factorization ansatz,

$$f^{(2)}(\mathbf{r}, \mathbf{v}; \mathbf{r}', \mathbf{v}'; t) = f^{(1)}(\mathbf{r}, \mathbf{v}; t) f^{(1)}(\mathbf{r}', \mathbf{v}'; t) \qquad (3.5)$$

the exact equation (3.1) is replaced by an approximate closed equation for $f^{(1)}$, i.e.,

$$\left[\frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \frac{1}{m} \mathbf{F}_L(\mathbf{r}) \cdot \frac{\partial}{\partial \mathbf{v}} \right.$$

$$\left. + \frac{1}{m} \mathbf{F}_{ext}(\mathbf{r}, t) \cdot \frac{\partial}{\partial \mathbf{v}} + \frac{1}{m} \mathbf{F}_{MF}(\mathbf{r}, t) \cdot \frac{\partial}{\partial \mathbf{v}} \right] f^{(1)}(\mathbf{r}, \mathbf{v}; t) = 0 \qquad (3.6)$$

where $\mathbf{F}_{MF}(\mathbf{r}, t)$ is the mean-field force

$$\mathbf{F}_{MF}(\mathbf{r}, t) = \int d\mathbf{r}' \, d\mathbf{v}' \, f^{(1)}(\mathbf{r}', \mathbf{v}'; t) \, \mathbf{F}_C(\mathbf{r}' - \mathbf{r}) \qquad (3.7)$$

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[4] Strictly speaking, $V_L(\mathbf{r})$ diverges in the limit of an infinite system. This divergence causes no trouble, because it is canceled by the divergence appearing in the potential created by all the electrons. This cancellation could be made more explicit in (3.1) by introducing the truncated two-body distribution function,

$$f^{(2,T)} = f^{(2)}(\mathbf{r}, \mathbf{v}; \mathbf{r}', \mathbf{v}'; t) - f^{(1)}(\mathbf{r}, \mathbf{v}; t) f^{(1)}(\mathbf{r}', \mathbf{v}', t)$$

Then (3.1) takes a form where each term is well defined if one assumes that $f^{(2,T)}$ has a sufficiently strong clustering and $f^{(1)}$ satisfies the overall neutrality sum rule at any time. In the mean-field equations, $V_L(\mathbf{r})$ is always combined with the potential created by the electronic charge distribution $-e\rho(\mathbf{r})$ and the sum of these potentials is finite because of the neutrality of each Wigner–Seitz cell [see (3.11)].

The mean-field kinetic equation (3.6) is nothing but the particular form in the present case of the usual collisionless Vlasov equation.[15]

In the absence of external potential, the equilibrium phase-space density takes the form

$$f_{eq}^{(1)}(\mathbf{r}, \mathbf{v}) = \rho(\mathbf{r}) \, \varphi(v) \tag{3.8}$$

where $\rho(\mathbf{r})$ is the (periodic) equilibrium density of the electrons and $\varphi(v)$ is the normalized Maxwell–Boltzmann distribution,

$$\varphi(v) = (\beta m/2\pi)^{d/2} \exp(-\beta m v^2/2) \tag{3.9}$$

In the framework of the mean-field approach, $f_{eq}^{(1)}(\mathbf{r}, \mathbf{v})$ has to be computed as the stationary solution of (3.6) obtained by setting $\mathbf{F}_{ext}(\mathbf{r}, t) = 0$. This gives the following coupled mean-field equations for $\rho(\mathbf{r})$ and $V(\mathbf{r})$:

$$\rho(\mathbf{r}) = \rho(0) \exp\{-\beta[V(\mathbf{r}) - V(0)]\}$$
$$V(\mathbf{r}) = V_L(\mathbf{r}) + \int d\mathbf{r}' \, \phi_C(|\mathbf{r}' - \mathbf{r}|) \, \rho(\mathbf{r}') \tag{3.10}$$

These equations will be studied in detail in further publications. In this paper we do not need the explicit form of their solutions. Note only that both $\rho(\mathbf{r})$ and $V(\mathbf{r})$ have the periodicity of the lattice and depend on the temperature; furthermore, $\rho(\mathbf{r})$ does satisfy the neutrality sum rule

$$\int_{WS} d\mathbf{r} \, \rho(\mathbf{r}) = 1 \tag{3.11}$$

Now we assume the external potential to be weak and monochromatic,

$$V_{ext}(\mathbf{r}, t) = V_{ext} \exp(i\mathbf{k} \cdot \mathbf{r} - i\omega t) \tag{3.12}$$

and to have been switched on at $t = -\infty$ (ω has a small, positive, imaginary part) when the system was at equilibrium. This external potential induces in $f^{(1)}$ a change $\delta f^{(1)}$ with respect to the equilibrium distribution $f_{eq}^{(1)}$, i.e.,

$$f^{(1)}(\mathbf{r}, \mathbf{v}; t) = \rho(\mathbf{r}) \, \varphi(v) + \delta f^{(1)}(\mathbf{r}, \mathbf{v}; t) \tag{3.13}$$

Up to the lowest order in V_{ext}, $\delta f^{(1)}$ can be written as

$$\delta f^{(1)}(\mathbf{r}, \mathbf{v}; t) = \chi(\mathbf{r}, \mathbf{v}; \mathbf{k}, \omega) \, V_{ext} \exp(i\mathbf{k} \cdot \mathbf{r} - i\omega t) \tag{3.14}$$

where $\chi(\mathbf{r}, \mathbf{v}; \mathbf{k}, \omega)$ is a local, wavenumber- and frequency-dependent

response function. Replacing (3.13) and (3.14) in the Vlasov equation (3.6), and linearizing this equation with respect to V_{ext}, we find

$$\left[-i\omega + i\mathbf{k} \cdot \mathbf{v} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \frac{1}{m} \mathbf{F}(\mathbf{r}) \cdot \frac{\partial}{\partial \mathbf{v}} \right] \chi(\mathbf{r}, \mathbf{v}; \mathbf{k}, \omega)$$

$$= -\beta \rho(\mathbf{r}) \varphi(v) \mathbf{v} \cdot \left\{ i\mathbf{k} - \int d\mathbf{r}' \, d\mathbf{v}' \, \chi(\mathbf{r}', \mathbf{v}'; \mathbf{k}, \omega) \mathbf{F}_C(\mathbf{r}' - \mathbf{r}) \exp[i\mathbf{k} \cdot (\mathbf{r}' - \mathbf{r})] \right\}$$

$$(3.15)$$

which is the required mean-field equation for $\chi(\mathbf{r}, \mathbf{v}; \mathbf{k}, \omega)$. Here $\mathbf{F}(\mathbf{r})$ is the force deriving from the mean-field potential $V(\mathbf{r})$ determined from (3.10),

$$\mathbf{F}(\mathbf{r}) = -\frac{\partial}{\partial \mathbf{r}} V(\mathbf{r}) \tag{3.16}$$

In the homogeneous electron gas model, where the ions form a uniform background with charge density $e\rho$, the solutions of (3.10) are $\rho(\mathbf{r}) = \rho$ and $V(\mathbf{r}) = 0$. Then $\mathbf{F}(\mathbf{r})$ vanishes and the solution of (3.15) is straightforward[16]; in particular, χ is independent of $\mathbf{r}$ and its dependence on $\mathbf{v}$ is easily computed. In the present case, $\rho(\mathbf{r})$ and $V(\mathbf{r})$ are not constant, so $\mathbf{F}(\mathbf{r})$ does not vanish. Consequently, the dependence on $\mathbf{r}$ and $\mathbf{v}$ of χ is highly nontrivial and the resolution of (3.15) is much more difficult than in the homogeneous case. This difficulty arises from our "exact" treatment of the interactions between the electrons and the ions, or, in other words, from the nonlinearization of the Vlasov equation with respect to the periodic ionic potential $V_L(\mathbf{r})$.

4. THE RESPONSE FUNCTION

In this section, we derive the mean-field expression of the density response function $\chi(\mathbf{k}, \omega)$ averaged over one Wigner–Seitz cell,

$$\chi(\mathbf{k}, \omega) = \frac{1}{A_{WS}} \int_{WS} d\mathbf{r} \int_{\mathbb{R}^d} d\mathbf{v} \, \chi(\mathbf{r}, \mathbf{v}; \mathbf{k}, \omega) \tag{4.1}$$

This is achieved through a formal solution of the mean-field equation (3.15), which can be divided into the following steps. Defining $A(\mathbf{r}, \mathbf{v}; \mathbf{k}, \omega)$ through

$$\chi(\mathbf{r}, \mathbf{v}; \mathbf{k}, \omega) = \beta \rho(\mathbf{r}) \, \varphi(v) \, A(\mathbf{r}, \mathbf{v}; \mathbf{k}, \omega) \tag{4.2}$$

we first rewrite (3.15) as an integrodifferential equation for A. The latter is

then transformed into a purely integral equation. This integral equation for A leads to a linear inhomogeneous integral equation for

$$B(\mathbf{r}; \mathbf{k}, \omega) = \int d\mathbf{v}\, \varphi(v)\, A(\mathbf{r}, \mathbf{v}; \mathbf{k}, \omega) \tag{4.3}$$

which is solved in terms of an infinite series. The resulting expression for $\chi(\mathbf{k}, \omega)$ is obtained by using

$$\chi(\mathbf{k}, \omega) = \frac{\beta}{\Lambda_{\mathrm{WS}}} \int_{\mathrm{WS}} d\mathbf{r}\, \rho(\mathbf{r})\, B(\mathbf{r}; \mathbf{k}, \omega) \tag{4.4}$$

[Equation (4.4) is an obvious consequence of the definitions (4.1)–(4.3).] The method is given in Section 4.1; some comments are given in Section 4.2.

4.1. Formal Calculation of $\chi(\mathbf{k}, \omega)$

Replacing χ by (4.2) in (3.15), we obtain

$$\left[-i\omega + i\mathbf{k} \cdot \mathbf{v} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \frac{1}{m} \mathbf{F}(\mathbf{r}) \cdot \frac{\partial}{\partial \mathbf{v}} \right] A(\mathbf{r}, \mathbf{v}; \mathbf{k}, \omega) = -\mathbf{v} \cdot \mathbf{K}(\mathbf{r}; \mathbf{k}, \omega) \tag{4.5}$$

with

$$\mathbf{K}(\mathbf{r}; \mathbf{k}, \omega) = i\mathbf{k} - \int d\mathbf{r}'\, d\mathbf{v}'\, \chi(\mathbf{r}', \mathbf{v}'; \mathbf{k}, \omega)\, \mathbf{F}_C(\mathbf{r}' - \mathbf{r}) \exp[i\mathbf{k} \cdot (\mathbf{r}' - \mathbf{r})] \tag{4.6}$$

and where we have used the equilibrium mean-field equations (3.10).

Since $\mathbf{K}$ depends on A (through χ), (4.5) is an integrodifferential equation. The next step of the method consists in transforming (4.5) into an equation that does not involve partial derivatives of A with respect to $\mathbf{r}$ and $\mathbf{v}$. For this purpose, we introduce the trajectories of one electron in the potential $V(\mathbf{r})$. For each point $(\mathbf{r}, \mathbf{v})$ in the phase space, let $\mathscr{C}(\mathbf{r}, \mathbf{v})$ be the trajectory that goes through this point. The points $(\mathbf{s}, \mathbf{w})$ belonging to the curve $\mathscr{C}(\mathbf{r}, \mathbf{v})$ can be parametrized by a time t,

$$\mathbf{s} = \mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v}), \qquad \mathbf{w} = \mathbf{v}_{ce}(t; \mathbf{r}, \mathbf{v}) \tag{4.7}$$

where $\mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v})$ and $\mathbf{v}_{ce}(t; \mathbf{r}, \mathbf{v})$ are the position and the velocity of one electron at the time t moving in the potential $V(\mathbf{r})$ with the initial conditions

$r_{ce}(0; r, v) = r$ and $v_{ce}(0; r, v) = v$. Now we consider the restriction of (4.5) to the curve $\mathscr{C}(r, v)$. Using the equations of motion

$$\frac{\partial}{\partial t} r_{ce}(t; r, v) = v_{ce}(t; r, v), \qquad \frac{\partial}{\partial t} v_{ce}(t; r, v) = \frac{1}{m} F(r_{ce}(t; r, v)) \qquad (4.8)$$

we see that the differential operator

$$w \cdot \frac{\partial}{\partial s} + \frac{1}{m} F(s) \cdot \frac{\partial}{\partial w} \qquad (4.9)$$

merely reduces to $\partial/\partial t$ for (s, w) belonging to $\mathscr{C}(r, v)$. Along this curve, Eq. (4.5) then becomes

$$\left[\frac{\partial}{\partial t} + ik \cdot v_{ce}(t; r, v) - i\omega \right] A(r_{ce}(t; r, v), v_{ce}(t; r, v); k, \omega)$$

$$= -v_{ce}(t; r, v) \cdot K(r_{ce}(t; r, v); k, \omega) \qquad (4.10)$$

The point (r, v) being given, (4.10) is an ordinary differential equation with respect to t. This equation is easily solved by standard methods, as shown in Appendix A. We obtain

$$A(s, w; k, \omega)$$

$$= \left\{ 1 + \int dr' \, dv' \, \chi(r', v'; k, \omega) \, \phi_C(|r' - r|) \exp[ik \cdot (r' - r)] \right.$$

$$+ A(r, v; k, \omega) \bigg\} \exp[i\omega t - ik \cdot (s - r)]$$

$$- 1 - \int dr' \, dv' \, \chi(r', v'; k, \omega) \, \phi_C(|r' - s|) \exp[ik \cdot (r' - s)]$$

$$- i\omega \int_0^t dt' \left\{ \exp[i\omega(t - t') - ik \cdot (s - s')] \right.$$

$$+ \int dr' \, dv' \, \chi(r', v'; k, \omega) \, \phi_C(|r' - s'|)$$

$$\left. \times \exp[i\omega(t - t') - ik \cdot (s - r')] \right\} \qquad (4.11)$$

where (s, w) is given by the parametrization (4.7) as well as (s', w') with t' in place of t.

Equation (4.11) is the integrated form of Eq. (4.5) along the curve

$\mathscr{C}(\mathbf{r}, \mathbf{v})$. It gives a relation between $A(\mathbf{r}, \mathbf{v}; \mathbf{k}, \omega)$ and $A(\mathbf{s}, \mathbf{w}; \mathbf{k}, \omega)$, which can be rewritten as

$$
\begin{aligned}
A(\mathbf{r}, & \mathbf{v}; \mathbf{k}, \omega) \\
&= \left\{ 1 + \int d\mathbf{r}' \, d\mathbf{v}' \, \chi(\mathbf{r}', \mathbf{v}'; \mathbf{k}, \omega) \, \phi_C(|\mathbf{r}' - \mathbf{s}|) \exp[i\mathbf{k} \cdot (\mathbf{r}' - \mathbf{s})] \right. \\
&\quad \left. + A(\mathbf{s}, \mathbf{w}; \mathbf{k}, \omega) \right\} \exp[i\mathbf{k} \cdot (\mathbf{s} - \mathbf{r}) - i\omega t] \\
&\quad - 1 - \int d\mathbf{r}' \, d\mathbf{v}' \, \chi(\mathbf{r}', \mathbf{v}'; \mathbf{k}, \omega) \, \phi_C(|\mathbf{r}' - \mathbf{r}|) \exp[i\mathbf{k} \cdot (\mathbf{r}' - \mathbf{r})] \\
&\quad + i\omega \int_0^t dt' \left\{ \exp[i\mathbf{k} \cdot (\mathbf{s}' - \mathbf{r}) - i\omega t'] \right. \\
&\quad \left. + \int d\mathbf{r}' \, d\mathbf{v}' \, \chi(\mathbf{r}', \mathbf{v}'; \mathbf{k}, \omega) \, \phi_C(|\mathbf{r}' - \mathbf{s}'|) \right. \\
&\quad \left. \times \exp[i\mathbf{k} \cdot (\mathbf{r}' - \mathbf{r}) - i\omega t'] \right\}
\end{aligned} \tag{4.12}
$$

The point $(\mathbf{r}, \mathbf{v})$ being given, Eq. (4.12) is valid for any point $(\mathbf{s}, \mathbf{w})$ belonging to $\mathscr{C}(\mathbf{r}, \mathbf{v})$, i.e., for any time t. Thus, we can take the limit $t \to -\infty$ on the right-hand side of (4.12). Since the potential $V(\mathbf{s})$ is a continuous periodic function (with the periodicity of the lattice), $V(\mathbf{s})$ is bounded and the conservation of the energy implies that $|\mathbf{w}|$ is bounded along $\mathscr{C}(\mathbf{r}, \mathbf{v})$. Therefore, $A(\mathbf{s}, \mathbf{w}; \mathbf{k}, \omega)$, which is a continuous function of $(\mathbf{s}, \mathbf{w})$ and periodic in $\mathbf{s}$, is bounded along $\mathscr{C}(\mathbf{r}, \mathbf{v})$. The integral

$$
\int d\mathbf{r}' \, d\mathbf{v}' \, \chi(\mathbf{r}', \mathbf{v}'; \mathbf{k}, \omega) \, \phi_C(|\mathbf{r}' - \mathbf{s}|) \exp[i\mathbf{k} \cdot (\mathbf{r}' - \mathbf{s})] \tag{4.13}
$$

is a continuous periodic function of $\mathbf{s}$, and consequently is bounded along $\mathscr{C}(\mathbf{r}, \mathbf{v})$. Since ω has a finite, positive, imaginary part, the first term of the right-hand side of (4.12) then vanishes when $t \to -\infty$. In this limit, the time integral $\int_0^{-\infty} dt' \cdots$ is convergent and (4.12) reduces to

$$
\begin{aligned}
A(\mathbf{r}, & \mathbf{v}; \mathbf{k}, \omega) \\
&= -1 - \int d\mathbf{r}' \, d\mathbf{v}' \, \chi(\mathbf{r}', \mathbf{v}'; \mathbf{k}, \omega) \, \phi_C(|\mathbf{r}' - \mathbf{r}|) \exp[i\mathbf{k} \cdot (\mathbf{r}' - \mathbf{r})] \\
&\quad - i\omega \int_{-\infty}^0 dt' \left\{ \exp[i\mathbf{k} \cdot (\mathbf{s}' - \mathbf{r}) - i\omega t'] \right.
\end{aligned}
$$

$$+ \int d\mathbf{r}' \, d\mathbf{v}' \, \chi(\mathbf{r}', \mathbf{v}'; \mathbf{k}, \omega) \, \phi_\mathrm{C}(|\mathbf{r}' - \mathbf{s}'|)$$

$$\times \exp[i\mathbf{k} \cdot (\mathbf{r}' - \mathbf{r}) - i\omega t'] \bigg\} \qquad\qquad (4.14)$$

Taking into account the definition (4.2) of A, we see that (4.14) is a linear integral equation in the phase space for A. It is possible, and useful, to transform (4.14) into an integral equation in one Wigner–Seitz cell for $B(\mathbf{r}; \mathbf{k}, \omega)$. Multiplying (4.14) by $\varphi(v)$ and integrating upon $\mathbf{v}$, we obtain

$$B(\mathbf{r}; \mathbf{k}, \omega) = -1 - i\omega \int d\mathbf{v} \, \varphi(v) \int_{-\infty}^{0} dt' \exp[i\mathbf{k} \cdot (\mathbf{s}' - \mathbf{r}) - i\omega t']$$

$$- \beta \int d\mathbf{r}' \, \rho(\mathbf{r}') \, B(\mathbf{r}'; \mathbf{k}, \omega) \bigg\{ \phi_\mathrm{C}(|\mathbf{r}' - \mathbf{r}|) \exp[i\mathbf{k} \cdot (\mathbf{r}' - \mathbf{r})]$$

$$+ i\omega \int d\mathbf{v} \, \varphi(v) \int_{-\infty}^{0} dt' \exp(-i\omega t') \, \phi_\mathrm{C}(|\mathbf{r}' - \mathbf{s}'|)$$

$$\times \exp[i\mathbf{k} \cdot (\mathbf{r}' - \mathbf{r})] \bigg\} \qquad\qquad (4.15)$$

Furthermore, the integral upon $\mathbf{r}'$ can be restricted to WS by exploiting the periodicity of $\rho(\mathbf{r}')$ and of $B(\mathbf{r}'; \mathbf{k}, \omega)$. We have

$$\beta \int d\mathbf{r}' \, \rho(\mathbf{r}') \, B(\mathbf{r}'; \mathbf{k}, \omega) \, \phi_\mathrm{C}(|\mathbf{r}' - \mathbf{r}|) \exp[i\mathbf{k} \cdot (\mathbf{r}' - \mathbf{r})]$$

$$= \beta \int_{\mathrm{WS}} d\mathbf{r}' \, \rho(\mathbf{r}') \, B(\mathbf{r}'; \mathbf{k}, \omega) \sum_{\mathbf{R}_j} \phi_\mathrm{C}(|\mathbf{R}_j + \mathbf{r}' - \mathbf{r}|)$$

$$\times \exp[i\mathbf{k} \cdot (\mathbf{R}_j + \mathbf{r}' - \mathbf{r})] \qquad\qquad (4.16)$$

The sum $\sum_{\mathbf{R}_j} \cdots$ is a periodic function of the argument $(\mathbf{r}' - \mathbf{r})$ with the periodicity of the lattice. This function can be rewritten as the sum of its Fourier components upon the vectors $\mathbf{G}_j$ of the reciprocal lattice, with the result

$$\sum_{\mathbf{R}_j} \phi_\mathrm{C}(|\mathbf{R}_j + \mathbf{r}' - \mathbf{r}|) \exp[i\mathbf{k} \cdot \mathbf{R}_j + i\mathbf{k} \cdot (\mathbf{r}' - \mathbf{r})]$$

$$= \frac{1}{A_{\mathrm{WS}}} \sum_{\mathbf{G}_j} \tilde{\phi}_\mathrm{C}(|\mathbf{k} - \mathbf{G}_j|) \exp[i\mathbf{G}_j \cdot (\mathbf{r}' - \mathbf{r})]$$

$$= \frac{1}{\varLambda_{\mathrm{WS}}} \tilde{\phi}_{\mathrm{C}}(k) + \frac{1}{\varLambda_{\mathrm{WS}}} \sum_{\mathbf{G}_j \neq 0} \tilde{\phi}_{\mathrm{C}}(|\mathbf{k} - \mathbf{G}_j|) \exp[i\mathbf{G}_j \cdot (\mathbf{r}' - \mathbf{r})]$$

$$= \frac{1}{\varLambda_{\mathrm{WS}}} \tilde{\phi}_{\mathrm{C}}(k) + \psi_S(\mathbf{r}' - \mathbf{r}; \mathbf{k}) \tag{4.17}$$

[the last line of (4.17) is just the definition of $\psi_S(\mathbf{r}' - \mathbf{r}; \mathbf{k})$]. Replacing $\sum_{\mathbf{R}_j} \cdots$ by (4.17) in (4.16), we find

$$\beta \int d\mathbf{r}' \, \rho(\mathbf{r}') \, B(\mathbf{r}'; \mathbf{k}, \omega) \, \phi_{\mathrm{C}}(|\mathbf{r}' - \mathbf{r}|) \exp[i\mathbf{k} \cdot (\mathbf{r}' - \mathbf{r})]$$

$$= \tilde{\phi}_{\mathrm{C}}(k) \, \chi(\mathbf{k}, \omega) + \beta \int_{\mathrm{WS}} d\mathbf{r}' \, \rho(\mathbf{r}') \, B(\mathbf{r}'; \mathbf{k}, \omega) \, \psi_S(\mathbf{r}' - \mathbf{r}; \mathbf{k}) \tag{4.18}$$

Using (4.18), we finally rewrite (4.15) as

$$B(\mathbf{r}; \mathbf{k}, \omega) = -[1 + \tilde{\phi}_{\mathrm{C}}(k) \, \chi(\mathbf{k}, \omega)][1 + i\omega \mathcal{T}(\mathbf{r}; \mathbf{k}, \omega)]$$

$$- \beta \int_{\mathrm{WS}} d\mathbf{r}' \, B(\mathbf{r}'; \mathbf{k}, \omega) \, \rho(\mathbf{r}')[\psi_S(\mathbf{r}' - \mathbf{r}; \mathbf{k}) + i\omega \psi_D(\mathbf{r}', \mathbf{r}; \mathbf{k}, \omega)]$$

$$\tag{4.19}$$

with

$$\mathcal{T}(\mathbf{r}; \mathbf{k}, \omega) = \int d\mathbf{v} \, \varphi(v) \int_0^\infty dt \, \exp\{i\omega t + i\mathbf{k} \cdot [\mathbf{r}_{ce}(-t; \mathbf{r}, \mathbf{v}) - \mathbf{r}]\} \tag{4.20}$$

and

$$\psi_D(\mathbf{r}', \mathbf{r}; \mathbf{k}, \omega) = \int d\mathbf{v} \, \varphi(v) \int_0^\infty dt \, \exp\{i\omega t + i\mathbf{k} \cdot [\mathbf{r}_{ce}(-t; \mathbf{r}, \mathbf{v}) - \mathbf{r}]\}$$

$$\times \psi_S(\mathbf{r}' - \mathbf{r}_{ce}(-t; \mathbf{r}, \mathbf{v}); \mathbf{k}) \tag{4.21}$$

Equation (4.19) is an inhomogeneous linear integral equation in WS for $B(\mathbf{r}; \mathbf{k}, \omega)$. Its solution can be formally written in the form

$$B(\mathbf{r}; \mathbf{k}, \omega) = -[1 + \tilde{\phi}_{\mathrm{C}}(k) \, \chi(\mathbf{k}, \omega)] \, \Sigma(\mathbf{r}; \mathbf{k}, \omega) \tag{4.22}$$

where $\Sigma(\mathbf{r}; \mathbf{k}, \omega)$ is the infinite series

$$\Sigma(\mathbf{r}; \mathbf{k}, \omega) = \sum_{n=0}^\infty (-1)^n \beta^n \int_{(\mathrm{WS})^n} d\mathbf{r}_1 \cdots d\mathbf{r}_n$$

$$\times \prod_{j=0}^{n-1} \rho(\mathbf{r}_{j+1})[\psi_S(\mathbf{r}_{j+1} - \mathbf{r}_j; \mathbf{k}) + i\omega \psi_D(\mathbf{r}_{j+1}, \mathbf{r}_j; \mathbf{k}, \omega)]$$

$$\times [1 + i\omega \mathcal{T}(\mathbf{r}_n; \mathbf{k}, \omega)] \tag{4.23}$$

In $\sum_{n=0}^{\infty} \cdots$ the term $n = 0$ reduces to $[1 + i\omega \mathcal{T}(\mathbf{r}; \mathbf{k}, \omega)]$ and $\mathbf{r}_0$ is equal to $\mathbf{r}$. Replacing $B(\mathbf{r}; \mathbf{k}, \omega)$ by (4.22) in (4.4), we obtain a self-consistent equation for $\chi(\mathbf{k}, \omega)$ whose solution can be cast in the generic form

$$\chi(\mathbf{k}, \omega) = -\beta\rho \frac{k^2 T(\mathbf{k}, \omega)}{k^2 + \kappa_D^2 T(\mathbf{k}, \omega)} \tag{4.24}$$

with

$$T(\mathbf{k}, \omega) = \int_{WS} d\mathbf{r} \, \rho(\mathbf{r}) \, \Sigma(\mathbf{r}; \mathbf{k}, \omega)$$

$$= \sum_{n=0}^{\infty} (-1)^n \beta^n \int_{(WS)^{n+1}} d\mathbf{r} \, d\mathbf{r}_1 \cdots d\mathbf{r}_n \, \rho(\mathbf{r})$$

$$\times \prod_{j=0}^{n-1} \rho(\mathbf{r}_{j+1}) [\psi_S(\mathbf{r}_{j+1} - \mathbf{r}_j; \mathbf{k}) + i\omega\psi_D(\mathbf{r}_{j+1}, \mathbf{r}_j; \mathbf{k}, \omega)]$$

$$\times [1 + i\omega \mathcal{T}(\mathbf{r}_n; \mathbf{k}, \omega)] \tag{4.25}$$

4.2. Comments

The mean-field expression (4.24) is formal in the sense that $T(\mathbf{k}, \omega)$ is defined by the infinite series (4.25), whose convergence is not guaranteed at any temperature. Furthermore, the functions $\mathcal{T}$ and ψ_D are entirely determined by the trajectories in the mean-field equilibrium potential $V(\mathbf{r})$. For $d > 1$, these trajectories are rather complicated to study in detail, and it is hopeless to obtain closed analytic expressions for $\mathcal{T}$ and ψ_D, and consequently for $T(\mathbf{k}, \omega)$ and $\chi(\mathbf{k}, \omega)$. Although (4.24) is not completely explicit, this expression is particularly useful for establishing general properties of the static and dynamic structure factors (see Sections 5 and 6) and for studying particular cases or limits, such as the one-dimensional case or the high-temperature regime (see papers II and III).

The structure of the series (4.25), as well as its different ingredients, can be interpreted as follows. First, taking into account the definition (4.20) of $\mathcal{T}$, we note that the quantity

$$-\beta\rho(\mathbf{r})[1 + i\omega \mathcal{T}(\mathbf{r}; \mathbf{k}, \omega)] \tag{4.26}$$

is the local response function of independent electrons moving in the potential $V(\mathbf{r})$. In each term of (4.25) this local response function is coupled to the local electron density through the static and dynamic propagators ψ_S

and ψ_D, respectively. The series (4.25) represents a perturbative expansion to all orders with respect to this coupling mechanism.[5]

At finite temperatures, each term of (4.25) gives a contribution to $T(\mathbf{k}, \omega)$ whose magnitude depends on the inverse temperature β. In the high-temperature limit $(\beta \to 0)$, only the first term $(n = 0)$ contributes. Furthermore, the temperature-dependent potential $V(\mathbf{r})$ goes to $V_L(\mathbf{r})$ in this limit.[6] The high-temperature form of (4.24) then becomes

$$\chi(\mathbf{k}, \omega) = \frac{\chi_{V_L}^{(0)}(\mathbf{k}, \omega)}{1 - \tilde{\phi}_C(k)\,\chi_{V_L}^{(0)}(\mathbf{k}, \omega)} \qquad (4.27)$$

$\chi_{V_L}^{(0)}(\mathbf{k}, \omega)$ is the response function of independent electrons in the potential $V_L(\mathbf{r})$,

$$\chi_{V_L}^{(0)}(\mathbf{k}, \omega) = \frac{-1}{\varLambda_{\mathrm{WS}}} \int_{\mathrm{WS}} d\mathbf{r}\,\beta\rho(\mathbf{r})[1 + i\omega\mathcal{T}_L(\mathbf{r}; \mathbf{k}, \omega)] \qquad (4.28)$$

where $\mathcal{T}_L$ obviously is the dispersion function $\mathcal{T}$ corresponding to V_L. At finite temperatures, it is no longer possible to rewrite $\chi(\mathbf{k}, \omega)$ as (4.27) with V in place of V_L: the coupling mechanism described previously makes $T(\mathbf{k}, \omega)$ different from $-\chi_V^{(0)}(\mathbf{k}, \omega)/\beta\rho$.

Finally, note that the high-temperature form (4.27) appears as a natural extension of the man-field expression

$$\chi_0(k, \omega) = \frac{\chi_0^{(0)}(k, \omega)}{1 - \tilde{\phi}_C(k)\,\chi_0^{(0)}(k, \omega)} \qquad (4.29)$$

corresponding to the uniform background case,[17] i.e., to $\rho(\mathbf{r}) = \rho$ and $V(\mathbf{r}) = 0$. In (4.29), $\chi_0^{(0)}(k, \omega)$ is the response function of free electrons. Of course, (4.29) can be recovered from our general solution, as shown in Appendix B.

---

[5] The coupling mechanism between the local response function (4.26) and the local electron density is a particular aspect of the competition between the periodicities imposed by $\mathbf{k}$ and the lattice, respectively. This could be made more explicit in (4.25) by replacing the periodic functions ρ, $\mathcal{T}$, ψ_S, and ψ_D by their Fourier decomposition upon the wave vectors $\mathbf{G}_j$ of the reciprocal lattice.

[6] Here and in the forthcoming papers, $V_L(\mathbf{r})$ is the total potential created by the ionic lattice and the uniform charge distribution $-e\rho$. For the sake of simplicity, we keep the same notation for this total potential as for the ionic potential defined by (2.7) (the latter being in fact divergent, as mentioned in a previous footnote).

5. THE STATIC STRUCTURE FACTOR

In this section, we derive the formal mean-field expression of the static structure factor

$$S(\mathbf{k}) = \lim_{TL} \frac{1}{N} \left\langle \sum_{j=1}^{N} \exp(i\mathbf{k} \cdot \mathbf{r}_j) \sum_{j=1}^{N} \exp(-i\mathbf{k} \cdot \mathbf{r}_j) \right\rangle_{A,N} \qquad (5.1)$$

In the definition (5.1), $\langle \cdots \rangle_{A,N}$ means an equilibrium average for the finite system, and the subscript TL is used for the thermodynamic limit defined in Section 3. The small-k (long-wavelength) behavior of $S(\mathbf{k})$ is also investigated in order to determine the nature (plasma or dielectric) of the phase described by the mean-field theory.

5.1. Formal Calculation of $S(k)$

Let $\chi(\mathbf{k})$ be the static response function,

$$\chi(\mathbf{k}) = \chi(\mathbf{k}, \omega = 0) \qquad (5.2)$$

We immediately obtain from (4.24)

$$\chi(\mathbf{k}) = -\beta\rho \frac{k^2 T(\mathbf{k})}{k^2 + \kappa_D^2 T(\mathbf{k})} \qquad (5.3)$$

with

$$T(\mathbf{k}) = T(\mathbf{k}, \omega = 0) = \sum_{n=0}^{\infty} (-1)^n \beta^n \int_{(WS)^{n+1}} d\mathbf{r} \, d\mathbf{r}_1 \cdots d\mathbf{r}_n \, \rho(\mathbf{r})$$

$$\times \prod_{j=0}^{n-1} \rho(\mathbf{r}_{j+1}) \, \psi_S(\mathbf{r}_{j+1} - \mathbf{r}_j; \mathbf{k}) \qquad (5.4)$$

The static version of the fluctuation-dissipation theorem[18] reads

$$S(\mathbf{k}) = -\frac{1}{\beta\rho} \chi(\mathbf{k}) \qquad (5.5)$$

Replacing $\chi(\mathbf{k})$ by (5.3) in (5.5), we find

$$S(\mathbf{k}) = k^2 T(\mathbf{k})/[k^2 + \kappa_D^2 T(\mathbf{k})] \qquad (5.6)$$

The expression (5.6), with $T(\mathbf{k})$ given by (5.4), is the mean-field form of $S(\mathbf{k})$. In the high-temperature regime, $T(\mathbf{k})$ reduces to 1 [the first term

of the series (5.4)], and (5.6) becomes identical to the usual Debye–Hückel expression

$$k^2/(k^2 + \kappa_D^2) \qquad (5.7)$$

corresponding to the uniform background case. At finite temperatures all the terms of the series (5.4) contribute to $T(\mathbf{k})$, which then is different from 1. One can interpret $T(\mathbf{k})$ as a static form factor of the lattice, which takes into account all the nonlinear coupling effects between the local electron density at different points through the static propagator ψ_S.

5.2. The Static Dielectric Constant

The $\mathbf{k}$-dependent dielectric constant $\varepsilon(\mathbf{k})$ can be deduced from the knowledge of $S(\mathbf{k})$ through the standard relation

$$\frac{1}{\varepsilon(\mathbf{k})} = 1 - \frac{\kappa_D^2}{k^2} S(\mathbf{k}) \qquad (5.8)$$

In the long-wavelength limit $(k \to 0)$, $\varepsilon(\mathbf{k})$ goes to the static dielectric constant $\varepsilon = \varepsilon(0)$. If ε is infinite, the system is in a plasma phase (perfect screening), whereas if ε is finite, the system is in a dielectric phase (partial screening). The plasma-phase criterion is equivalent to the small-k behavior,

$$S(\mathbf{k}) \sim k^2/\kappa_D^2 \qquad \text{when} \quad k \to 0 \qquad (5.9)$$

which is known as the Stillinger–Lovett sum rule.[19] In the dielectric phase this sum rule is violated.

The mean-field expression (5.6) clearly satisfies the Stillinger–Lovett sum rule (5.9) if $T(0)$ is different from zero. We are going to show that $T(0)$ is always strictly positive, at any temperature and in any dimension. Thus, in the framework of the mean-field approach, the system is always in a plasma phase and there is no phase transition. This result is not *a priori* obvious, since $T(0)$ is a complicated object defined by the series

$$T(0) = \sum_{n=0}^{\infty} (-1)^n \beta^n \int_{(WS)^{n+1}} d\mathbf{r}\, d\mathbf{r}_1 \cdots d\mathbf{r}_n\, \rho(\mathbf{r})$$
$$\times \prod_{j=0}^{n-1} \rho(\mathbf{r}_{j+1})\, \psi_S(\mathbf{r}_{j+1} - \mathbf{r}_j) \qquad (5.10)$$

with

$$\psi_S(\mathbf{r}' - \mathbf{r}) = \psi_S(\mathbf{r}' - \mathbf{r}; \mathbf{k} = 0) = \frac{1}{A_{WS}} \sum_{\mathbf{G}_j \neq 0} \tilde{\phi}_C(G_j) \exp[i\mathbf{G}_j \cdot (\mathbf{r}' - \mathbf{r})] \qquad (5.11)$$

The remaining part of the section is devoted to the proof of the statement

$$T(0) > 0 \tag{5.12}$$

For proving the inequality (5.12) it is convenient to introduce the function $\xi(\mathbf{r})$ solution of the integral equation

$$\xi(\mathbf{r}) = 1 - \beta \int_{\mathrm{WS}} d\mathbf{r}' \, \xi(\mathbf{r}') \, \rho(\mathbf{r}') \, \rho(\mathbf{r}') \, \psi_s(\mathbf{r}' - \mathbf{r}) \tag{5.13}$$

Since $\xi(\mathbf{r})$ can be formally rewritten as

$$\xi(\mathbf{r}) = 1 + \sum_{n=1}^{\infty} (-1)^n \beta^n \int_{(\mathrm{WS})^n} d\mathbf{r}_1 \cdots d\mathbf{r}_n \prod_{j=0}^{n-1} \rho(\mathbf{r}_{j+1}) \, \psi_s(\mathbf{r}_{j+1} - \mathbf{r}_j) \tag{5.14}$$

$T(0)$ is nothing but

$$T(0) = \int_{\mathrm{WS}} d\mathbf{r} \, \rho(\mathbf{r}) \, \xi(\mathbf{r}) \tag{5.15}$$

First, we show that there exists a subdomain $\mathscr{D}_+$ of WS where $\xi(\mathbf{r})$ takes strictly positive values. For this purpose let us compute

$$\int_{\mathrm{WS}} d\mathbf{r} \, \xi(\mathbf{r}) \tag{5.16}$$

Using (5.13), we obtain

$$\int_{\mathrm{WS}} d\mathbf{r} \, \xi(\mathbf{r}) = \frac{1}{\rho} - \beta \int_{\mathrm{WS}} d\mathbf{r}' \, \xi(\mathbf{r}') \, \rho(\mathbf{r}') \int_{\mathrm{WS}} d\mathbf{r} \, \psi_s(\mathbf{r}' - \mathbf{r}) \tag{5.17}$$

Since ψ_s is a periodic function with the periodicity of the lattice, the integral

$$\int_{\mathrm{WS}} d\mathbf{r} \, \psi_s(\mathbf{r}' - \mathbf{r}) \tag{5.18}$$

is independent of $\mathbf{r}'$. Furthermore, according to the definition (5.11) of ψ_s, this integral is zero. The second term on the right-hand side of (5.17) then vanishes, and the integral (5.16) reduces to $1/\rho$, which is a strictly positive number. This implies that $\xi(\mathbf{r})$ takes strictly positive values in a nonempty subdomain $\mathscr{D}_+$ of WS. For the final part of the proof, we transform the

integral equation (5.13) into a differential equation. Taking the Laplacian with respect to $\mathbf{r}$ of each side of (5.13), we find

$$\nabla^2 \xi(\mathbf{r}) = \chi_D^2 \frac{\rho(\mathbf{r})}{\rho} \xi(\mathbf{r}) - \kappa_D^2 T(0) \tag{5.19}$$

For deriving (5.19) we have used the expression (5.15) of $T(0)$ in terms of $\xi(\mathbf{r})$, as well as the identity

$$\nabla^2 \psi_S(\mathbf{r}) = \frac{2\pi^{d/2}}{\Gamma(d/2)} e^2 \left[\rho - \sum_{\mathbf{R}_j} \delta(\mathbf{r} - \mathbf{R}_j) \right] \tag{5.20}$$

which is a direct consequence of the definition (5.11) of ψ_S. Since $\xi(\mathbf{r})$ is a continuous function, there exists at least one point $\mathbf{r}_{\max}$ belonging to $\mathcal{D}_+$ where $\xi(\mathbf{r})$ is maximum. At this point, one necessarily has

$$\nabla^2 \xi(\mathbf{r}_{\max}) \leqslant 0 \tag{5.21}$$

After having rewritten (5.19) for $\mathbf{r} = \mathbf{r}_{\max}$ as

$$T(0) = \frac{\rho(\mathbf{r}_{\max})}{\rho} \xi(\mathbf{r}_{\max}) - \frac{1}{\kappa_D^2} \nabla^2 \xi(\mathbf{r}_{\max}) \tag{5.22}$$

we finally obtain the inequality (5.12) by using (5.21) and the fact that $\xi(\mathbf{r}_{\max})$ and $\rho(\mathbf{r}_{\max})$ are strictly positive [$\rho(\mathbf{r})$ is strictly positive everywhere because $V(\mathbf{r})$ is bounded like any continuous periodic function].

6. THE DYNAMIC STRUCTURE FACTOR

In this section, we derive the formal mean-field expression of the dynamic structure factor

$$S(\mathbf{k}, \omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt\, e^{i\omega t}$$

$$\times \lim_{\mathrm{TL}} \frac{1}{N} \left\langle \sum_{j=1}^{N} \exp[i\mathbf{k} \cdot \mathbf{r}_j(t)] \sum_{j=1}^{N} \exp[-i\mathbf{k} \cdot \mathbf{r}_j(0)] \right\rangle_{A,N} \tag{6.1}$$

In (6.1), $\mathbf{r}_j(t)$ is the position of the electron j at time t moving in the N-body potential V_N, with the initial conditions $\mathbf{r}_j(0) = \mathbf{r}_j$ and $\mathbf{v}_j(0) = \mathbf{v}_j$; the equilibrium average $\langle \cdots \rangle_{A,N}$ is taken over the initial positions $\mathbf{r}_j$ and the initial velocities $\mathbf{v}_j$ of the electrons. We also give the mean-field expression of the function

$$s(\omega) = \lim_{k \to 0} \frac{S(\mathbf{k}, \omega)}{S(\mathbf{k})} \tag{6.2}$$

which characterizes the spectrum of the fluctuations in the long-wavelength limit. The nature (conducting or insulating) of the phase described by the mean-field theory then is determined by computing the dc conductivity σ, which can be expressed as[20,8]

$$\sigma = \frac{1}{4\pi^2 s(0)} \tag{6.3}$$

6.1. Formal Calculation of $S(k, \omega)$ and of $s(\omega)$

The fluctuation-dissipation theorem reads[18,17]

$$S(\mathbf{k}, \omega) = -\frac{1}{\pi\rho\beta\omega} \chi''(\mathbf{k}, \omega) \tag{6.4}$$

where $\chi''(\mathbf{k}, \omega)$ is the imaginary part of $\chi(\mathbf{k}, \omega)$. Let $T'(\mathbf{k}, \omega)$ and $T''(\mathbf{k}, \omega)$ be the real and imaginary parts, respectively, of $T(\mathbf{k}, \omega)$. Using the expression (4.24) of χ in (6.4), we obtain

$$S(\mathbf{k}, \omega) = \frac{k^4 T''(\mathbf{k}, \omega)}{\pi\omega\{[k^2 + \kappa_D^2 T'(\mathbf{k}, \omega)]^2 + \kappa_D^4 [T''(\mathbf{k}, \omega)]^2\}} \tag{6.5}$$

For computing $s(\omega)$, we have to investigate the small-k behavior of $T(\mathbf{k}, \omega)$. This is done in Appendix C, with the result

$$T(\mathbf{k}, \omega) = (k^2/\kappa_D^2)[W_1(\omega) + W_2(\omega)] + o(k^2) \tag{6.6}$$

when $k \to 0$. Here $W_1(\omega)$ and $W_2(\omega)$ are defined by

$$W_1(\omega) = -\frac{i\omega}{2d} \kappa_D^2 \int_{\mathrm{WS} \otimes \mathbb{R}^d} d\mathbf{r}\, d\mathbf{v}\, \rho(\mathbf{r})\, \varphi(v) \int_0^\infty dt\, \exp(i\omega t)[\mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v}) - \mathbf{r}]^2 \tag{6.7}$$

$$W_2(\omega) = -\frac{i\omega}{d} \kappa_D^2 \sum_{n=1}^\infty (-1)^n \beta^n \int_{(\mathrm{WS})^{n+1}} d\mathbf{r}\, d\mathbf{r}_1 \cdots d\mathbf{r}_n\, \rho(\mathbf{r})\, \rho(\mathbf{r}_1)$$

$$\times \boldsymbol{\alpha}(\mathbf{r}, \mathbf{r}_1; \omega) \cdot \boldsymbol{\gamma}(\mathbf{r}_n; \omega)$$

$$\times \prod_{j=1}^{n-1} \rho(\mathbf{r}_{j+1})[\psi_S(\mathbf{r}_{j+1} - \mathbf{r}_j) + i\omega\psi_D(\mathbf{r}_{j+1}, \mathbf{r}_j; \omega)] \tag{6.8}$$

with

$$\boldsymbol{\alpha}(\mathbf{r}, \mathbf{r}'; \omega) = i\omega \int_{\mathbb{R}^d} d\mathbf{v}\, \varphi(v) \int_0^\infty dt\, \exp(i\omega t)\, [\mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v}) - \mathbf{r}]$$

$$\times \psi_S(\mathbf{r}' - \mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v})) \tag{6.9}$$

and

$$\gamma(\mathbf{r}; \omega) = \int_{\mathbb{R}^d} d\mathbf{v}\, \varphi(v) \int_0^\infty dt\, \exp(i\omega t)\, [\mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v}) - \mathbf{r}] \qquad (6.10)$$

$\psi_S(\mathbf{r}' - \mathbf{r})$ and $\psi_D(\mathbf{r}', \mathbf{r}; \omega)$ are equal to $\psi_S(\mathbf{r}' - \mathbf{r}; \mathbf{k} = 0)$ and $\psi_D(\mathbf{r}', \mathbf{r}; \mathbf{k} = 0, \omega)$, respectively. From (6.6) we infer

$$T'(\mathbf{k}, \omega) = (k^2/\kappa_D^2)\, R(\omega) + o(k^2) \qquad (6.11)$$

$$T''(\mathbf{k}, \omega) = (k^2/\kappa_D^2)\, I(\omega) + o(k^2) \qquad (6.12)$$

when $k \to 0$, with

$$R(\omega) = \mathrm{Re}\{W_1(\omega) + W_2(\omega)\} \qquad (6.13)$$

$$I(\omega) = \mathrm{Im}\{W_1(\omega) + W_2(\omega)\} \qquad (6.14)$$

Replacing T' and T'' by their respective small-k expansions (6.11) and (6.12) in the mean-field expression (6.5), we obtain

$$S(\mathbf{k}, \omega) \sim \frac{k^2}{\kappa_D^2} \frac{I(\omega)}{\pi\omega\{[1 + R(\omega)]^2 + I^2(\omega)\}} \qquad (6.15)$$

when $k \to 0$. Using (6.15) and the fact that $S(\mathbf{k})$ always satisfies the Stillinger–Lovett sum rule (5.9) in the framework of the mean-field theory, we then find

$$s(\omega) = \frac{I(\omega)}{\pi\omega\{[1 + R(\omega)]^2 + I^2(\omega)\}} \qquad (6.16)$$

6.2. The DC Conductivity

The calculation of the dc conductivity through (6.3) requires the knowledge of the low-frequency behavior of $s(\omega)$. We are not able to study this behavior in a completely rigorous way, except for $d = 1$. This is due to the complexity of the classical trajectories $\mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v})$ for $d > 1$. However, in the next paragraph we give some intuitive and reasonable arguments that strongly suggest that $s(\omega)$ vanishes when ω goes to zero. According to the relation (6.3), this leads to an infinite dc conductivity: in the mean-field description, the system is always in a conducting phase.

The functions $W_1(\omega)$ and $W_2(\omega)$, which determine $s(\omega)$, depend on the time Laplace transforms of the quantities

$$\int_{WS \otimes \mathbb{R}^d} dr \, dv \, \rho(\mathbf{r}) \, \varphi(v) [\mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v}) - \mathbf{r}]^2 \tag{6.17}$$

$$\int_{\mathbb{R}^d} dv \, \varphi(v) [\mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v}) - \mathbf{r}] \tag{6.18}$$

and

$$\int_{\mathbb{R}^d} dv \, \varphi(v) [\mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v}) - \mathbf{r}] \, \psi_S(\mathbf{r}' - \mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v})) \tag{6.19}$$

The small-ω behavior of these Laplace transforms is related to the long-time behavior of (6.17)–(6.19). The latter can be studied by distinguishing three types of contributions, which arise, respectively, from the confined trajectories with a sufficiently small energy and from the unconfined ones with high and intermediate energies. The confined trajectories remain in the Wigner–Seitz cell (WS) and consequently $(\mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v}) - \mathbf{r})$ remains bounded when $t \to \infty$. Therefore the corresponding contributions to (6.17)–(6.19) are bounded for $0 \leqslant t \leqslant \infty$. For a sufficiently high energy, the unconfined trajectories go through an infinite number of cells. It is reasonable to assume that most of these trajectories deviate from the straight line going through $\mathbf{r}$ and colinear to $\mathbf{v}$ by a quantity that remains bounded when $t \to \infty$. The intuitive argument that sustains this assumption is the following one. When the energy is large enough, the deviation from the straight-line trajectory due to the crossing of one cell is small since the force $-\partial V/\partial \mathbf{r}$ is bounded. After a given time, many cells have been crossed and most of the previous deviations cancel out because the force is periodic and has a zero average upon WS. Therefore the contribution to (6.17) of the high-energy trajectories behaves as $\text{const} \times t^2$ when $t \to \infty$, whereas the corresponding contributions to (6.18) and (6.19) are bounded, respectively, by a constant and by $\text{const} \times t$ in this limit. For the unconfined trajectories with intermediate energies the contribution to (6.17) is clearly bounded by $\text{const} \times t^2$, and we assume that the contributions to (6.18) and (6.19) satisfy similar bounds to those obtained above for the high-energy trajectories. Summing the three types of contribution, we find

$$\int_{WS \otimes \mathbb{R}^d} dr \, dv \, \rho(\mathbf{r}) \, \varphi(v) [\mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v}) - \mathbf{r}]^2 \sim \text{const} \times t^2 \quad \text{when} \quad t \to \infty \tag{6.20}$$

$$\left| \int_{\mathbb{R}^d} dv \, \varphi(v) [\mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v}) - \mathbf{r}] \right| < \text{const}, \quad 0 \leqslant t \leqslant \infty \tag{6.21}$$

and

$$\left| \int_{\mathbb{R}^d} d\mathbf{v}\, \varphi(v) [\mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v}) - \mathbf{r}]\ \psi_S(\mathbf{r}' - \mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v})) \right| < \text{const} \times t, \qquad 0 \leqslant t \leqslant \infty$$

(6.22)

From the asymptotic behavior (6.20) and the definition (6.7), we infer

$$\text{Re}\{ W_1(\omega)\} \sim \text{const}/\omega^2 \tag{6.23}$$

$$\text{Im}\{ W_1(\omega)\} = o(1/\omega^2) \tag{6.24}$$

when $\omega \to 0$. Furthermore, the bounds (6.21), (6.22) imply that $\omega |\boldsymbol{\alpha}(\mathbf{r}, \mathbf{r}'; \omega)|$ and $\omega |\boldsymbol{\gamma}(\mathbf{r}; \omega)|$ remain bounded when $\omega \to 0$. Assuming the convergence of the series $\sum_{n=1}^{\infty} \cdots$ in (6.8), this leads to

$$\text{Re}\{ W_2(\omega)\} = o(1/\omega^2) \tag{6.25}$$

$$\text{Im}\{ W_2(\omega)\} = o(1/\omega^2) \tag{6.26}$$

when $\omega \to 0$. Using the expressions (6.13) and (6.14) of $R(\omega)$ and $I(\omega)$, respectively, we find

$$R(\omega) \sim \text{const}/\omega^2 \tag{6.27}$$

$$I(\omega) = o(1/\omega^2) \tag{6.28}$$

when $\omega \to 0$. Inserting these asymptotic behaviors in the mean-field expression (6.16), we finally obtain

$$\lim_{\omega \to 0} s(\omega) = 0 \tag{6.29}$$

which is the announced result. Let us point out that the previous semiheuristic derivation can be made completely rigorous in one dimension at all temperatures (see paper II) and in two dimensions at high temperatures (see paper III).

7. CONCLUSION AND COMMENTS

We have derived the formal mean-field expressions of $S(\mathbf{k})$ and of $S(\mathbf{k}, \omega)$ in terms of the *trajectories* of one electron in the mean-field equilibrium potential $V(\mathbf{r})$. The static and dynamic criteria, which characterize the nature (conducting or insulating) of the system, have been applied to these mean-field expressions. The mean-field theory predicts that the system is a conductor at all temperatures, independent of space dimension. In three dimensions, the system is indeed expected to be a conductor

at all temperatures. In two dimensions, the mean-field prediction is incompatible with the existence of the KT transition. The mean-field theory is, as usual, worse in one dimension, since the dielectric phase is stable at all temperatures in that case.[21]

It is not completely surprising that the mean-field theory does not predict any aspect (static or dynamic) of the KT transition in two dimensions. Indeed, the mean-field approximation is only a symptotically valid in the high-temperature limit, where the system is in its plasma (or conducting) phase; at low temperatures, where the system is in its dielectric (or insulating) phase, this approximation becomes uncontrollable. Furthermore, the failure of the mean-field theory regarding the dynamic aspect of the KT transition could be *a priori* expected. Since the electron–electron collisions are neglected, the Vlasov equation (3.6) does not contain any dissipative term in the zero-frequency limit. This necessary leads to the divergence of the mean-field dc conductivity at all temperatures (and for any dimension). The previous argument is corroborated by the explicit analysis of the mean-field solution done in Section 6.2. For the static aspect of the KT transition, no *a priori* argument predicts the failure of the mean-field theory. In fact, the latter is a bit subtle,[7] as illustrated by the proof in Section 5.2.

The absence of phase transition in the mean-field approach means that *correlations* (or electron–electron collisions) must play a crucial role in explaining the KT transition. The original argument of Kosterlitz and Thouless[2] appears then to be incomplete, especially for the present fixed-ion model, since it entirely ignores correlations. A more satisfactory argument[8] should include the cooperative effect between the ionic potential, which tends to localize each electron in one given cell, and the electron–electron repulsion, which tends to prevent two electrons from staying in the same cell (the mean-field theory only takes into account the first mechanism). The quantitative formulation of such an argument is an open and difficult problem, even for the statics. We believe this formulation to be essential to the derivation of an approximate theory describing *simultaneously* the plasma-conducting and dielectric-insulating phases.

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[7] Usually, mean-field theories are able to reproduce the static aspects of phase transitions, for instance, the paramagnetic–ferromagnetic transition of a system of spins.

[8] The deficiencies of the Kosterlitz–Thouless argument have been also noticed by Forrester,[22] who considers a one-dimensional system of charged rods in a periodic background with logarithmic interactions. This model has a KT-type transition. On the basis of exact results obtained for special values of the temperature, Forrester propounds a heuristic argument including correlation effects which predicts the phase diagram of the model. Unfortunately, this argument is specific to the logarithmic potential in one dimension: it does not work in two dimensions.

APPENDIX A

In this Appendix, we solve the linear, inhomogeneous, first-order differential equation (4.10) by the method of variation of parameters. First, the homogeneous equation reads

$$\{\partial/\partial t + i\mathbf{k}\cdot\mathbf{v}_{ce}(t;\mathbf{r},\mathbf{v}) - i\omega\}\, A(\mathbf{r}_{ce}(t;\mathbf{r},\mathbf{v}),\mathbf{v}_{ce}(t;\mathbf{r},\mathbf{v});\mathbf{k},\omega) = 0 \quad (A1)$$

whose general solution is

$$A(\mathbf{r}_{ce}(t;\mathbf{r},\mathbf{v}),\mathbf{v}_{ce}(t;\mathbf{r},\mathbf{v});\mathbf{k},\omega) = C\exp[i\omega t - i\mathbf{k}\cdot\mathbf{r}_{ce}(t;\mathbf{r},\mathbf{v})] \quad (A2)$$

In order to solve (4.10), we write A in the form (A2) with the constant C replaced by a time-dependent function $C(t;\mathbf{r},\mathbf{v};\mathbf{k},\omega)$. This gives

$$(\partial/\partial t)\, C(t;\mathbf{r},\mathbf{v};\mathbf{k},\omega) = -\mathbf{v}_{ce}(t;\mathbf{r},\mathbf{v})\cdot\mathbf{K}(\mathbf{r}_{ce}(t;\mathbf{r},\mathbf{v});\mathbf{k},\omega)$$

$$\times\exp[i\mathbf{k}\cdot\mathbf{r}_{ce}(t;\mathbf{r},\mathbf{v}) - i\omega t] \quad (A3)$$

which is integrated as

$$C(t;\mathbf{r},\mathbf{v};\mathbf{k},\omega)$$

$$= C(0;\mathbf{r},\mathbf{v};\mathbf{k},\omega) - \int_0^t dt'\, \mathbf{v}_{ce}(t';\mathbf{r},\mathbf{v})\cdot\mathbf{K}(\mathbf{r}_{ce}(t';\mathbf{r},\mathbf{v});\mathbf{k},\omega)$$

$$\times\exp[i\mathbf{k}\cdot\mathbf{r}_{ce}(t';\mathbf{r},\mathbf{v}) - i\omega t'] \quad (A4)$$

Noting that

$$\mathbf{v}_{ce}(t';\mathbf{r},\mathbf{v})\cdot\mathbf{K}(\mathbf{r}_{ce}(t';\mathbf{r},\mathbf{v});\mathbf{k},\omega)\exp[i\mathbf{k}\cdot\mathbf{r}_{ce}(t';\mathbf{r},\mathbf{v})]$$

$$= (\partial/\partial t')\{\exp[i\mathbf{k}\cdot\mathbf{r}_{ce}(t';\mathbf{r},\mathbf{v})]$$

$$+ \int d\mathbf{r}'\, d\mathbf{v}'\, \chi(\mathbf{r}',\mathbf{v}';\mathbf{k},\omega)\, \phi_C(|\mathbf{r}' - \mathbf{r}_{ce}(t';\mathbf{r},\mathbf{v})|)\exp(i\mathbf{k}\cdot\mathbf{r}')\} \quad (A5)$$

and integrating by parts the second term of the rhs of (A4), we rewrite $C(t;\mathbf{r},\mathbf{v};\mathbf{k},\omega)$ as

$$C(t;\mathbf{r},\mathbf{v};\mathbf{k},\omega)$$

$$= C(0;\mathbf{r},\mathbf{v};\mathbf{k},\omega) + \exp(i\mathbf{k}\cdot\mathbf{r})$$

$$+ \int d\mathbf{r}'\, d\mathbf{v}'\, \chi(\mathbf{r}',\mathbf{v}';\mathbf{k},\omega)\, \phi_C(|\mathbf{r}' - \mathbf{r}|)$$

$$\times\exp(i\mathbf{k}\cdot\mathbf{r}') - \exp[i\mathbf{k}\cdot\mathbf{r}_{ce}(t;\mathbf{r},\mathbf{v}) - i\omega t]$$

$$-\int d\mathbf{r}' \, d\mathbf{v}' \, \chi(\mathbf{r}', \mathbf{v}'; \mathbf{k}, \omega) \, \phi_C(|\mathbf{r}' - \mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v})|)$$

$$\times \exp(i\mathbf{k} \cdot \mathbf{r}' - i\omega t)$$

$$-i\omega \int_0^t dt' \left\{ \exp[i\mathbf{k} \cdot \mathbf{r}_{ce}(t'; \mathbf{r}, \mathbf{v}) - i\omega t'] \right.$$

$$+ \int d\mathbf{r}' \, d\mathbf{v}' \, \chi(\mathbf{r}', \mathbf{v}'; \mathbf{k}, \omega) \, \phi_C(|\mathbf{r}' - \mathbf{r}_{ce}(t'; \mathbf{r}, \mathbf{v})|)$$

$$\left. \times \exp(i\mathbf{k} \cdot \mathbf{r}' - i\omega t') \right\} \tag{A6}$$

The solution of (4.10) is obtained by multiplying $C(t; \mathbf{r}, \mathbf{v}; \mathbf{k}, \omega)$ by $\exp[i\omega t - i\mathbf{k} \cdot \mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v})]$. Taking into account the initial condition at $t = 0$, $C(0; \mathbf{r}, \mathbf{v}; \mathbf{k}, \omega)$ must be chosen equal to $A(\mathbf{r}, \mathbf{v}; \mathbf{k}, \omega) \exp(i\mathbf{k} \cdot \mathbf{r})$. This finally leads to the expression (4.11) given in the text.

APPENDIX B

In this Appendix, we check that the well-known expression (4.29) for a homogeneous electron gas can be recovered from our general solution (4.24).

The electron gas in a uniform background can be viewed as a particular case of the fixed-ion model, where the ions are smeared charges filling up the Wigner–Seitz cells with a charge density $e\rho$. The corresponding local electron density $\rho(\mathbf{r})$ then is constant (and equal to ρ), as well as the mean-field equilibrium potential $V(\mathbf{r})$. Therefore, the trajectories that determine the dispersion function $\mathscr{T}$ and the dynamic propagator ψ_D are the free trajectories

$$\mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v}) = \mathbf{r} + \mathbf{v}t \tag{B1}$$

Inserting (B1) into (4.20) and (4.21), we obtain

$$\mathscr{T}(\mathbf{r}; \mathbf{k}, \omega) = \mathscr{T}_0(k, \omega) = \frac{1}{i} \int d\mathbf{v} \, \varphi(v) \frac{1}{\mathbf{k} \cdot \mathbf{v} - \omega} \tag{B2}$$

and

$$\psi_D(\mathbf{r}'; \mathbf{r}; \mathbf{k}, \omega) = \psi_{D,0}(\mathbf{r}' - \mathbf{r}; \mathbf{k}, \omega) = \int d\mathbf{v} \, \varphi(v) \int_0^\infty dt \, \exp(i\omega t - i\mathbf{k} \cdot \mathbf{v}t)$$

$$\times \psi_S(\mathbf{r}' - \mathbf{r} + \mathbf{v}t; \mathbf{k}) \tag{B3}$$

According to (B2), the first term ($n = 0$) of the series (4.25) reduces to

$$1 + i\omega \mathcal{T}_0(k, \omega) = \int d\mathbf{v}\, \varphi(v) \frac{\mathbf{k} \cdot \mathbf{v}}{\mathbf{k} \cdot \mathbf{v} - \omega} = -\frac{\chi_0^{(0)}(k, \omega)}{\beta \rho} \qquad (B4)$$

In each term $n > 0$, one first computes the integral upon $\mathbf{r}$, which becomes

$$\rho \int_{WS} d\mathbf{r}\, [\psi_S(\mathbf{r}_1 - \mathbf{r}; \mathbf{k}) + i\omega \psi_{D,0}(\mathbf{r}_1 - \mathbf{r}; \mathbf{k}, \omega)] \qquad (B5)$$

Since both ψ_S and $\psi_{D,0}$ are periodic functions, the integral (B5) does not depend on $\mathbf{r}_1$. Furthermore, one has

$$\int_{WS} d\mathbf{s}\, \psi_S(\mathbf{s}; \mathbf{k}) = 0 \qquad (B6)$$

which is an obvious consequence of the definition of ψ_S [see the last line of Eq. (4.17)]. Using (B6), (B3), and the periodicity of ψ_S, we also find

$$\int_{WS} d\mathbf{s}\, \psi_{D,0}(\mathbf{s}; \mathbf{k}, \omega)$$

$$= \int d\mathbf{v}\, \varphi(v) \int_0^\infty dt\, \exp(i\omega t - i\mathbf{k} \cdot \mathbf{v}t) \int_{WS} d\mathbf{s}\, \psi_S(\mathbf{s} + \mathbf{v}t; \mathbf{k})$$

$$= \int d\mathbf{v}\, \varphi(v) \int_0^\infty dt\, \exp(i\omega t - i\mathbf{k} \cdot \mathbf{v}t) \int_{WS} d\mathbf{s}\, \psi_S(\mathbf{s}; \mathbf{k})$$

$$= 0 \qquad (B7)$$

From (B6) and (B7) we infer that the integral (B5) vanishes. All the terms $n > 0$ of the series (4.25) then do so, and $T_0(k, \omega)$ is just equal to the term $n = 0$, i.e.,

$$T_0(k, \omega) = -\chi_0^{(0)}(k, \omega)/\beta \rho \qquad (B8)$$

Replacing $T_0(k, \omega)$ by (B8) in (4.24), we finally obtain the expression (4.29) of $\chi_0(k, \omega)$, as it should.

APPENDIX C

In this Appendix, we study the small-k behavior of $T(\mathbf{k}, \omega)$. First, we prove the following lemma.

Lemma L1. If $\mathscr{F}(\mathbf{r}, \mathbf{v})$ is a periodic function of $\mathbf{r}$ with the periodicity of the lattice, then the average

$$\int_{\mathrm{WS} \otimes \mathbb{R}^d} d\mathbf{r} \, d\mathbf{v} \, \rho(\mathbf{r}) \, \varphi(v) \, \mathscr{F}(\mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v}), \mathbf{v}_{ce}(t; \mathbf{r}, \mathbf{v})) \tag{C1}$$

does not depend on the time t and reduces to the equilibrium average

$$\int_{\mathrm{WS} \otimes \mathbb{R}^d} d\mathbf{r} \, d\mathbf{v} \, \rho(\mathbf{r}) \, \varphi(v) \, \mathscr{F}(\mathbf{r}, \mathbf{v}) \tag{C2}$$

Proof. Let U_t be the evolution operator associated to the one-body Hamiltonian $H(\mathbf{p}, \mathbf{r}) = \mathbf{p}^2/2m + V(\mathbf{r})$. From Eqs. (3.9) and (3.10) we see that $\rho(\mathbf{r}) \, \varphi(v)$ is nothing but (apart from a normalization constant) the one-body Gibbs measure $\exp[-\beta H(\mathbf{p}, \mathbf{r})]$ with $\mathbf{p} = m\mathbf{v}$. Therefore $\rho(\mathbf{r}) \, \varphi(v)$ remains invariant under U_t, i.e.,

$$\rho(\mathbf{r}') \, \varphi(v') = \rho(\mathbf{r}) \, \varphi(v) \tag{C3}$$

with $\mathbf{r}' = U_t(\mathbf{r}) = \mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v})$ and $\mathbf{v}' = U_t(\mathbf{v}) = \mathbf{v}_{ce}(t; \mathbf{r}, \mathbf{v})$. Furthermore, according to Liouville's theorem,[23] the Jacobian of the transformation $(\mathbf{r}, \mathbf{v}) \to {}^{U_t}(\mathbf{r}', \mathbf{v}')$ is equal to 1, i.e.,

$$d\mathbf{r} \, d\mathbf{v} = d\mathbf{r}' \, d\mathbf{v}' \tag{C4}$$

By making the variable change $(\mathbf{r}, \mathbf{v}) \to (\mathbf{r}', \mathbf{v}')$ in the average (C1), we obtain

$$\int_{\mathrm{WS} \otimes \mathbb{R}^d} d\mathbf{r} \, d\mathbf{v} \, \rho(\mathbf{r}) \, \varphi(v) \, \mathscr{F}(\mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v}); \mathbf{v}_{ce}(t; \mathbf{r}, \mathbf{v}))$$

$$= \int_{U_t(\mathrm{WS} \otimes \mathbb{R}^d)} d\mathbf{r}' \, d\mathbf{v}' \, \rho(\mathbf{r}') \, \varphi(v') \, \mathscr{F}(\mathbf{r}', \mathbf{v}') \tag{C5}$$

with the help of the relations (C3) and (C4). Let $\Pi_{\mathbf{v}'}$ be the d-dimensional submanifold of the phase space in which the velocity is constant and equal to $\mathbf{v}'$. The integral on the right-hand side of (C5) can be rewritten as

$$\int_{\mathbb{R}^d} d\mathbf{v}' \, \varphi(v') \int_{\Pi_{\mathbf{v}'} \cap U_t(\mathrm{WS} \otimes \mathbb{R}^d)} d\mathbf{r}' \rho(\mathbf{r}') \, \mathscr{F}(\mathbf{r}', \mathbf{v}') \tag{C6}$$

Using the bijective and continuity properties of U_t, it is easy to check that $\Pi_{\mathbf{v}'} \cap U_t(\mathrm{WS} \otimes \mathbb{R}^d)$ is a compact domain[9] of $\mathbb{R}^d$, from which a complete

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[9] The shape of this domain is different from the one of WS and is very complicated (except for $d = 1$, where the latter reduces to an interval with the same length as WS).

tessellation of $\mathbb{R}^d$ can be generated by the translations belonging to the group of invariance of the lattice. Each nonempty intersection of this domain with a given Wigner–Seitz cell can be mapped to a subdomain of WS through a given translation belonging to this group; the previous tessellation property implies that all these subdomains do not intersect and their reunion is WS. Splitting the domain $\Pi_{\mathbf{v}'} \cap U_t(\text{WS} \otimes \mathbb{R}^d)$ into its intersections with the Wigner–Seitz cells, we then see that the integral of any periodic function of $\mathbf{r}$ upon this domain is just equal to the same integral upon WS. In particular, one has

$$\int_{\Pi_{\mathbf{v}'} \cap U_t(\text{WS} \otimes \mathbb{R}^d)} d\mathbf{r}'\, \rho(\mathbf{r}')\, \mathscr{F}(\mathbf{r}', \mathbf{v}') = \int_{\text{WS}} d\mathbf{r}\, \rho(\mathbf{r})\, \mathscr{F}(\mathbf{r}, \mathbf{v}') \qquad \text{(C7)}$$

since $\rho(\mathbf{r})\, \mathscr{F}(\mathbf{r}, \mathbf{v}')$ is periodic as the product of two periodic functions. Using (C7) in (C6), and taking into account (C5), we see that the *a priori* time-dependent average (C1) does reduce to the equilibrium average (C2). Now, we turn to the small-k expansion of $T(\mathbf{k}, \omega)$. The first term $(n = 0)$ of the series (4.25),

$$\int_{\text{WS}} d\mathbf{r}\, \rho(\mathbf{r})[1 + i\omega\mathscr{T}(\mathbf{r}; \mathbf{k}, \omega)]$$

$$= 1 + i\omega \int_0^\infty dt\, \exp(i\omega t) \int_{\text{WS} \otimes \mathbb{R}^d} d\mathbf{r}\, d\mathbf{v}\, \rho(\mathbf{r})\, \varphi(v)$$

$$\times \exp\{i\mathbf{k} \cdot [\mathbf{r}_{ce}(-t; \mathbf{r}, \mathbf{v}) - \mathbf{r}]\} \qquad \text{(C8)}$$

has to be treated separately, since its structure is different from that of the other terms $(n > 0)$ of (4.25). The small-k expansion of (C8) is obtained by replacing $\exp\{i\mathbf{k} \cdot [\mathbf{r}_{ce}(-t; \mathbf{r}, \mathbf{v}) - \mathbf{r}]\}$ by its Taylor series in $\mathbf{k}$. The zeroth-order term vanishes because of the neutrality sum rule (3.11) and of the normalization constraint $\int d\mathbf{v}\, \varphi(v) = 1$. The linear term in $\mathbf{k}$ also vanishes for symmetry reasons. It results from this that

$$\int_{\text{WS}} d\mathbf{r}\, \rho(\mathbf{r})[1 + i\omega\mathscr{T}(\mathbf{r}; \mathbf{k}, \omega)]$$

$$\sim -\tfrac{1}{2}i\omega \int_0^\infty dt\, \exp(i\omega t)$$

$$\times \int_{\text{WS} \otimes \mathbb{R}^d} d\mathbf{r}\, d\mathbf{v}\, \rho(\mathbf{r})\, \varphi(v)\{\mathbf{k} \cdot [\mathbf{r}_{ce}(-t; \mathbf{r}, \mathbf{v}) - \mathbf{r}]\}^2 \qquad \text{(C9)}$$

when $k \to 0$. The right-hand side of (C9) is a quadratic form of the

Cartesian components of $\mathbf{k}$, which must be invariant under the rotations belonging to the symmetry group of the lattice. Assuming the symmetry of the lattice to be high enough,[10] this quadratic form is then necessarily proportional to k^2. This property allows us to rewrite (C9) as

$$\int_{WS} d\mathbf{r}\, \rho(\mathbf{r})[1 + i\omega \mathcal{T}(\mathbf{r}; \mathbf{k}, \omega)] \sim \frac{k^2}{\kappa_D^2}\, W_1(\omega) \qquad \text{when} \quad k \to 0 \quad \text{(C10)}$$

with $W_1(\omega)$ given by the expression (6.7). For writing the latter in terms of $\mathbf{r}_{ec}(t; \mathbf{r}, \mathbf{v})$, we have used the symmetry properties $\mathbf{r}_{cc}(-t; -\mathbf{r}, \mathbf{v}) = -\mathbf{r}_{ce}(t; \mathbf{r}, \mathbf{v})$ and $\rho(-\mathbf{r}) = \rho(\mathbf{r})$.

Each term $n > 0$ of the series (4.25) can be rewritten as

$$(-1)^n \beta^n \int_{(WS)^n} d\mathbf{r}_n \cdots d\mathbf{r}_1\, \rho(\mathbf{r}_n)[1 + i\omega \mathcal{T}(\mathbf{r}_n; \mathbf{k}, \omega]$$

$$\times \rho(\mathbf{r}_{n-1})[\psi_S(\mathbf{r}_n - \mathbf{r}_{n-1}; \mathbf{k}) + i\omega \psi_D(\mathbf{r}_n, \mathbf{r}_{n-1}; \mathbf{k}, \omega)]$$

$$\times \cdots \times \rho(\mathbf{r}_1)[\psi_S(\mathbf{r}_2 - \mathbf{r}_1; \mathbf{k}) + i\omega \psi_D(\mathbf{r}_2, \mathbf{r}_1; \mathbf{k}, \omega)]$$

$$\times \int_{WS} d\mathbf{r}\, \rho(\mathbf{r})[\psi_S(\mathbf{r}_1 - \mathbf{r}; k) + i\omega \psi_D(\mathbf{r}_1; \mathbf{r}; \mathbf{k}, \omega)] \qquad \text{(C11)}$$

The small-k expansion of the integral

$$\int_{WS} d\mathbf{r}\, \rho(\mathbf{r})[\psi_S(\mathbf{r}_1 - \mathbf{r}; \mathbf{k}) + i\omega \psi_D(\mathbf{r}_1, \mathbf{r}; \mathbf{k}, \omega)] \qquad \text{(C12)}$$

reads

$$\int_{WS} d\mathbf{r}\, \rho(\mathbf{r})\, \psi_S(\mathbf{r}_1 - \mathbf{r}) + i\omega \int_0^\infty dt\, \exp(i\omega t)$$

$$\times \int_{WS \otimes \mathbb{R}^d} d\mathbf{r}\, d\mathbf{v}\, \rho(\mathbf{r})\, \varphi(v)\, \psi_S(\mathbf{r}_1 - \mathbf{r}_{ce}(-t; \mathbf{r}, \mathbf{v}))$$

$$+ \mathbf{k} \cdot \left\{ \int_{WS} d\mathbf{r}\, \rho(\mathbf{r}) \frac{\partial \psi_S}{\partial \mathbf{k}}(\mathbf{r}_1 - \mathbf{r}) + i\omega \int_0^\infty dt\, \exp(i\omega t) \int_{WS \otimes \mathbb{R}^d} d\mathbf{r}\, d\mathbf{v}\, \rho(\mathbf{r})\, \varphi(v) \right.$$

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[10] For instance, for $d = 2$, we shall consider a triangular lattice (see paper III). The rotations with angles $p\pi/3$ ($0 \leqslant p \leqslant 5$) belong to the symmetry group of the lattice, and the sole quadratic forms of $\mathbf{k}$ invariant under these rotations are indeed proportional to k^2. If we consider a rectangular lattice (which has a low symmetry), the right-hand side of (C9) is no longer proportional to k^2. This presence of anisotropic effects in the long-wavelength limit leads to anisotropic macroscopic behavior (in particular, the dc conductivity then depends on the direction of the applied external electric field).

$$\times \frac{\partial}{\partial \mathbf{k}} \psi_S(\mathbf{r}_1 - \mathbf{r}_{ce}(-t; \mathbf{r}, \mathbf{v})) \bigg\}$$

$$- \omega \mathbf{k} \cdot \int_0^\infty dt \, \exp(i\omega t) \int_{\text{WS} \otimes \mathbb{R}^d} d\mathbf{r} \, d\mathbf{v} \, \rho(\mathbf{r}) \, \varphi(v)$$

$$\times [\mathbf{r}_{ce}(-t; \mathbf{r}, \mathbf{v}) - \mathbf{r}] \, \psi_S(\mathbf{r}_1 - \mathbf{r}_{ce}(-t; \mathbf{r}, \mathbf{v})) + O(k^2) \qquad \text{(C13)}$$

with $\partial \psi_S/\partial \mathbf{k}(\mathbf{s}) = \partial \psi_S/\partial \mathbf{k}(\mathbf{s}; \mathbf{k} = 0)$. The vector $\mathbf{r}_1$ being given, $\psi_S(\mathbf{r}_1 - \mathbf{r})$ and $\partial \psi_S/\partial \mathbf{k}(\mathbf{r}_1 - \mathbf{r})$ are periodic functions of $\mathbf{r}$. We can then apply Lemma L1 to these periodic fuctions. This gives

$$\int_{\text{WS} \otimes \mathbb{R}^d} d\mathbf{r} \, d\mathbf{v} \, \rho(\mathbf{r}) \, \varphi(v) \, \psi_S(\mathbf{r}_1 - \mathbf{r}_{ce}(-t; \mathbf{r}, \mathbf{v}))$$

$$= \int_{\text{WS} \otimes \mathbb{R}^d} d\mathbf{r} \, d\mathbf{v} \, \rho(\mathbf{r}) \, \varphi(v) \, \psi_S(\mathbf{r}_1 - \mathbf{r})$$

$$= \int_{\text{WS}} d\mathbf{r} \, \rho(\mathbf{r}) \, \psi_S(\mathbf{r}_1 - \mathbf{r}) \qquad \text{(C14)}$$

and

$$\int_{\text{WS} \otimes \mathbb{R}^d} d\mathbf{r} \, d\mathbf{v} \, \rho(\mathbf{r}) \, \varphi(v) \frac{\partial \psi_S}{\partial \mathbf{k}} (\mathbf{r}_1 - \mathbf{r}_{ce}(-t; \mathbf{r}, \mathbf{v}))$$

$$= \int_{\text{WS} \otimes \mathbb{R}^d} d\mathbf{r} \, d\mathbf{v} \, \rho(\mathbf{r}) \, \varphi(v) \frac{\partial \psi_S}{\partial \mathbf{k}} (\mathbf{r}_1 - \mathbf{r})$$

$$= \int_{\text{WS}} d\mathbf{r} \, \rho(\mathbf{r}) \frac{\partial \psi_S}{\partial \mathbf{k}} (\mathbf{r}_1 - \mathbf{r}) \qquad \text{(C15)}$$

Taking into account (C14) and (C15), we see that the constant term (independent of $\mathbf{k}$) of (C13) vanishes, as well as the first linear term $\mathbf{k} \cdot \{\cdots\}$. This leads to

$$\int_{\text{WS}} d\mathbf{r} \, \rho(\mathbf{r}) [\psi_S(\mathbf{r}_1 - \mathbf{r}; \mathbf{k}) + i\omega \psi_D(\mathbf{r}_1, \mathbf{r}, \mathbf{k}, \omega)]$$

$$= -\omega \mathbf{k} \cdot \int_0^\infty dt \, \exp(i\omega t) \int_{\text{WS} \otimes \mathbb{R}^d} d\mathbf{r} \, d\mathbf{v} \, \rho(\mathbf{r}) \, \varphi(v)$$

$$\times [\mathbf{r}_{ce}(-t; \mathbf{r}, \mathbf{v}) - \mathbf{r}] \, \psi_S(\mathbf{r}_1 - \mathbf{r}_{ce}(-t; \mathbf{r}, \mathbf{v})) + O(k^2) \qquad \text{(C16)}$$

Using the definition (4.20) of $\mathcal{T}$, we easily obtain

$$1 + i\omega\mathcal{T}(\mathbf{r}_n; \mathbf{k}, \omega)$$

$$= -\omega\mathbf{k} \cdot \int_0^\infty dt \exp(i\omega t) \int_{\mathbb{R}^d} d\mathbf{v}_n \, \varphi(v_n)[\mathbf{r}_{ce}(-t; \mathbf{r}_n, \mathbf{v}_n) - \mathbf{r}_n] + O(k^2)$$

$$(C17)$$

Furthermore, one has

$$\psi_S(\mathbf{r}_{j+1} - \mathbf{r}_j; \mathbf{k}) + i\omega\psi_D(\mathbf{r}_{j+1}, \mathbf{r}_j; \mathbf{k}, \omega)$$

$$= \psi_S(\mathbf{r}_{j+1} - \mathbf{r}_j) + i\omega\psi_D(\mathbf{r}_{j+1}, \mathbf{r}_j, \omega) + O(k) \qquad (C18)$$

Using the small-k behavior (C16)–(C18) in (C11), and taking into account the symmetry properties of the lattice and of the trajectories, we find that the contribution of the terms $n > 0$ to $T(\mathbf{k}, \omega)$ is $O(k^2)$ and can be rewritten as

$$(k^2/\kappa_D^2) \, W_2(\omega) \qquad (C19)$$

with $W_2(\omega)$ given by the expression (6.8). The small-k behavior (6.6) of $T(\mathbf{k}, \omega)$ is finally obtained by adding to (C19) the contribution (C10) of the term $n = 0$.

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