Generalization of the Lindhard dielectric function to include fluctuation effects

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The random-phase-approximation dielectric function for the homogeneous electron gas has been derived by Lindhard. Here, we generalize this work to include fluctuation effects, and we also study their influence on the Friedel oscillations. In particular, our generalized function is analytic for all wave vectors and frequencies, in contrast to the Lindhard function.

I. INTRODUCTION

The Lindhard dielectric function, which is derived using the random-phase approximation (RPA), serves as the basic ingredient of theories of the homogeneous electron gas.[1-13] However, it does not take account of interactions between electrons (beyond the RPA), impurities, and phonons.[3-13] Since the pioneering RPA work of Bohm and Pines,[1] and Lindhard,[2] much effort has gone into solving two main difficulties associated with applying the RPA to realistic systems. First of all, in the long-wavelength limit ($q \to 0$),[3-5] it fails to reduce to the well-known results of the classical Boltzmann theory or the Fermi-liquid theory. Secondly, in the short-wavelength region (large q),[6-13] the RPA is no longer a good approximation, and, in addition, it has the $q = 2k_F$ nonanalyticity problem. Two different approaches have been developed toward a solution of these problems.

In the *phenomenological approach* (Fermi-liquid theory or classical Boltzmann theory),[3-5] one is interested in the long-wavelength behavior of the electron gas. The focus of attention is on obtaining a modified Lindhard dielectric function which reduces to the correct *classical* behavior in the $q \to 0$ limit. This was first achieved by Mermin[4] by using a local equilibrium density matrix and the relaxation-time approximation. Obviously, the deficiency in the behavior of the original Lindhard function for large q never appears as a problem of interest in this approach, where one is only interested in the $q \to 0$ behavior. In what we shall call the *microscopic approach*,[6-13] one is more interested in the quantum-mechanical nature and the short-wavelength (large-q) behavior of the electron gas. Two typical examples are the electron gas in a strong magnetic field,[13] where one needs to study the electrons in quantized Landau levels, and the transport properties of a two-dimensional electron gas,[9] where mobility is known to be sensitive to the method used to round off the $q = 2k_F$ nonanalyticity of the Lindhard function. In the study of these kinds of systems one usually performs microscopic calculations[8,11] of the response function by using either the Kubo formula or the memory function in Mori's formalism, to obtain the conductivity $\sigma(\omega)$ and the dielectric function $\epsilon(\omega)$ for realistic systems under some approximations. In this microscopic approach one generally uses the Lindhard function as a starting point and then incorporates other interaction effects such as electron-electron (beyond RPA) interactions, and impurity or phonon effects as perturbations. In other words, in this approach the Lindhard dielectric function is not the dielectric function $\epsilon(\omega)$ of the real system. Rather, the final results for $\sigma(\omega)$ and $\epsilon(\omega)$ from the microscopic calculations are consistently checked with the Boltzmann theory and the Fermi-liquid theory. So the focus of attention in the microscopic approach is to deal with the large-q deficiency of the RPA and to develop a generalized Lindhard function that is valid for all wave vectors and frequencies, and which reduces to the RPA in the $q \to 0$ limit. The present work and related papers[11-13] represent another attempt to develop such a generalized Lindhard function along the lines of the microscopic approach stated above.

Previously, the generalization of the Lindhard dielectric function in the microscopic approach was mainly focused on the effect of the electron-electron interactions.[6-8] In the formulation of Singwi *et al.*,[7] the short-range exchange and correlation effects among electrons were included to obtain a modified Lindhard dielectric function, which has been successful in its application. Nevertheless, the Hubbard-Singwi form of the Lindhard function is rather complicated, and the $q = 2k_F$ nonanalyticity is not addressed. On the other hand, there have been indications[9,10] that the short-range electron-impurity interaction also has a strong effect on the dielectric properties of electrons and will remove the $q = 2k_F$ nonanalyticity. In Sec. II we generalize the Lindhard dielectric function to include fluctuation effects arising from such electron-electron and electron-impurity interactions. In particular, we find that our generalized function is analytic at $q = 2k_F$. In Sec. III we study the Friedel oscillations as an example of the application of our generalized version of the Lindhard function. Finally, in Sec. IV, we present a summary and discussion of our results.

II. FORMULATION

Recently, we have developed a new approach to quantum transport based on the use of a generalized quantum Langevin equation.[11-13] In our approach, the many-body memory function associated with the total momentum of the center of mass of the electron gas is expressed

as a function of the density-density response function of the relative electrons. Since we derive the memory function directly in the process of solving the Heisenberg equations for the center-of-mass and relative electrons, expressions for the response function and conductivity are obtained simply as a by-product. We found that when the fluctuation of the coordinates of the center-of-mass electrons is included, the structure of the response function is changed significantly.[12] In the linear case, our expression for the density-density response function of free electrons is[12]

$$\chi^0(\mathbf{q},\omega)=\sum_{\mathbf{k},\sigma}\frac{f(\mathbf{k})-f(\mathbf{k}+\mathbf{q})}{\hbar\omega-(\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}})+iDq^2}\ , \tag{1}$$

where $f(\mathbf{k})$ is the Fermi distribution function, $\varepsilon_{\mathbf{k}}=\hbar^2k^2/2m$ is the electron energy, $\mathbf{q}$ is the wave vector associated with the electron density, σ denotes the spin, D is the diffusion constant for the center-of-mass coordinate defined by

$$D=\lim_{t\to\infty}\frac{1}{2t}\overline{\delta\mathbf{R}^2(t)}\ ,$$

and $\delta\mathbf{R}(t)$ is the fluctuation of the center-of-mass coordinate, $\mathbf{R}(t)$. We stress that (1) is obtained from first principles without any restriction on ω or $\mathbf{q}$, and the diffusion constant D is, in principle, rigorously calculable. In other words, our approach is to be distinguished from the usual relaxation-time approximation (which is restricted to small q values). However, in this paper, D will be treated as a parameter.

The iDq^2 term in (1), which is new, introduces a damping effect in the electron response. In the original Lindhard function this term is replaced by an $i\delta$ term, where δ is infinitesimally small. Obviously, in the small-wave-vector limit ($q\to0$) our formula (1) reduces to the Lindhard result $\chi^0(q,\omega)\to Nq^2/m\omega^2$, which is different from a well-known result, $x_F(q,\omega)\to Nq^2/m\omega(\omega+i/\tau)$, obtained from the Landau theory of Fermi liquids in the relaxation-time approximation.[3-5] We recall that this $q\to0$ connection to the RPA result is a common feature of the generalized Lindhard function in the microscopic approach,[8] and the main correction to the original Lindhard function is the large-q contribution. In essence, we are generalizing the Lindhard function to include fluctuation effects, with emphasis on large-q effects. This approach is to be contrasted with the relaxation-time approximation in the phenomenological approach, where one is interested in the $q\to0$ behavior of the dielectric function and where one phenomenologically introduces in (1) an i/τ term (in contrast to our iDq^2 term).

We emphasize that our introduction of the iDq^2 term will manifest itself mainly for large-q values. In a previous paper we used a generalization of (1) to include the presence of a large magnetic field to successfully explain various cyclotron-resonance experiments on a two-dimensional electron gas.[13] Here we restrict ourself to the study of the analytic evaluation of (1) in the three-dimensional case. For arbitrary q, it is a nontrivial matter to generalize the longitudinal dielectric constant of Lindhard and simultaneously conserve local-electron number. In the phenomenological approach ($q\to0$), one simply cannot replace ω by $\omega+i/\tau$ in the collisionless result, as pointed out by Mermin,[5] who also obtained the correct result for $\epsilon(q,\omega)$:

$$\epsilon_M(\mathbf{q},\omega)=1-V(\mathbf{q})\chi_M(\mathbf{q},\omega)\ , \tag{2}$$

where $V(\mathbf{q})=4\pi e^2/q^2$ is the Fourier transform of the Coulomb energy and where the subscript M refers to Mermin. In addition, as $q\to0$, $\epsilon_M(\mathbf{q},\omega)\to\epsilon_F(\mathbf{q},\omega)$, where $\epsilon_F(\mathbf{q},\omega)$ is the Fermi-liquid result. Furthermore,[3]

$$\epsilon_F(\mathbf{q},\omega)=1-V(\mathbf{q})\chi_F(\mathbf{q},\omega) \tag{3}$$

and

$$\epsilon_F(\omega)=\lim_{q\to0}\epsilon_F(\mathbf{q},\omega)=1+\frac{4\pi i}{\omega}\sigma_F(\omega)\ . \tag{4}$$

Let us now return to (1) with a view toward calculating the dielectric function in the RPA approximation, but with fluctuation effects included. Analogous to (2), we have

$$\epsilon(\mathbf{q},\omega)=1-V(\mathbf{q})\chi^0(\mathbf{q},\omega)\ , \tag{5}$$

where $\chi^0(\mathbf{q},\omega)$ is defined by (1). However, *as distinct from the phenomenological* (Fermi-liquid) *theory* described above, in our theory (and, in fact, in *all* microscopic theories) there is no relation, analogous to that given by (4), between the $\epsilon(\mathbf{q},\omega)$ given in (5) and our calculated value of $\sigma(\omega)$. In other words, $\epsilon(\mathbf{q},\omega)$ is not a dielectric function in the phenomenological sense of the word. It *is fundamentally a microscopic quantity* that is used in the calculation of $\sigma(\omega)$, a *macroscopic* quantity.

We now turn to the question of how the conductivity is calculated in the case of arbitrary q. It is, in fact, obtained from first principles along the lines outlined in Ref. 11. Explicitly,

$$\sigma(\omega)=\frac{ine^2}{m}\frac{1}{\omega+M(\omega)}\ , \tag{6}$$

where n refers to the number of particles per unit volume and the memory function $M(\omega)$ is given in terms of $\chi^0(\mathbf{q},\omega)$—which is related to $\epsilon(\mathbf{q},\omega)$ by (5)—by (19) of Ref. 11. Of course, one may then use this result for $\sigma(\omega)$ to define a macroscopic dielectric function $\epsilon(\omega)=1+(4\pi i/\omega)\sigma(\omega)$, but this quantity is *not* the $q\to0$ limit of the quantity $\epsilon(\mathbf{q},\omega)$ given by (5). Thus, in the microscopic theory, whereas $q\to0$ implies that the imaginary part of $\epsilon(\mathbf{q},w)\to0$, it does *not* imply that the real part of the conductivity vanishes.

As a consequence of the above discussion, it is clear that there is no simple connection between the results from our microscopic theory and those from the phenomenological relaxation-time approximation. In a way this is not surprising since the latter theory is always an approximation even in the $q\to0$ limit. In other words, there is nothing to be gained by comparing χ_F to χ^0. On the other hand, it may be shown, in the limit $q\to0$, that $\sigma(\omega)$ is the same as $\sigma_F(\omega)$. Also, one can form a quantity $1+(4\pi i/\omega)\chi(\omega)$, which is, in fact, the *macroscopic* dielectric function, but it is not same as the $q\to0$ limit of $\epsilon(\mathbf{q},\omega)$.

III. GENERALIZED LINDHARD FUNCTION AND APPLICATION TO THE STUDY OF FRIEDEL OSCILLATIONS

By using (1) and (5), after some straightforward algebra we obtain a new version of the RPA dielectric function $\epsilon=\epsilon_1+i\epsilon_2$. The real part is

$$\epsilon_1(x,y)=1+\frac{q_{\rm TF}^2}{8k_F^2x^2}\left[1+\frac{1}{8x}\left[(1+b^2x^2-\nu_+^2)\ln\left[\frac{(1+\nu_+)^2+b^2x^2}{(1-\nu_+)^2+b^2x^2}\right]+(1+b^2x^2-\nu_-^2)\ln\left[\frac{(1+\nu_-)^2+b^2x^2}{(1-\nu_-)^2+b^2x^2}\right]\right]\right.$$
$$\left.-\frac{b}{2}\left\{\nu_+\left[\arctan\left[\frac{1-\nu_+}{bx}\right]+\arctan\left[\frac{1+\nu_+}{bx}\right]\right]+\nu_-\left[\arctan\left[\frac{1-\nu_-}{bx}\right]+\arctan\left[\frac{1+\nu_-}{bx}\right]\right]\right\}\right], \tag{7}$$

where

$$x=\frac{q}{2k_F},\quad y=\frac{\hbar\omega}{4\varepsilon_F},\quad q_{\rm TF}^2=\frac{4me^2k_F}{\pi\hbar^2},\quad b=\frac{2mD}{\hbar},\quad \nu_\pm=x\pm y/x\ , \tag{8}$$

and ε_F is the Fermi energy. The imaginary part is

$$\epsilon_2(x,y)=\frac{q_{\rm TF}^2}{32k_F^2x^3}\left\{(1+b^2x^2-\nu_-^2)\left[\arctan\left[\frac{1-\nu_-}{bx}\right]+\arctan\left[\frac{1+\nu_-}{bx}\right]\right]\right.$$
$$-(1+b^2x^2-\nu_+^2)\left[\arctan\left[\frac{1-\nu_+}{bx}\right]+\arctan\left[\frac{1+\nu_+}{bx}\right]\right]$$
$$\left.+bx\left[\nu_-\ln\left[\frac{(1+\nu_-)^2+b^2x^2}{(1-\nu_-)^2+b^2x^2}\right]-\nu_+\ln\left[\frac{(1+\nu_+)^2+b^2x^2}{(1-\nu_+)^2+b^2x^2}\right]\right]\right\}. \tag{9}$$

We note that the real and imaginary parts of ϵ are even and odd functions of ω, respectively. Although the dielectric functions (7) and (9) are quite complicated, it is straightforward to see that when $b\to0$ or $q\to0$ they reduce to the Lindhard dielectric function. As a first step, here we study the static behavior ($\omega=0$) of the dielectric function. The study of the dynamical behavior will be reported in a planned, forthcoming paper.

When $\omega=0$ it is easy to see from (9) that $\epsilon_2(x,y)=0$. In other words, ϵ is purely real for $\omega=0$, q finite, as any analytically acceptable form must be. Hence, from (7) we obtain

$$\epsilon(x)\equiv\epsilon_1(x,y=0)=1+\frac{q_{\rm TF}^2}{8k_F^2x^2}L(x)\ , \tag{10}$$

where

$$L(x)\equiv1+\frac{1}{4x}(1-x^2+b^2x^2)\ln\left[\frac{(1+x)^2+b^2x^2}{(1-x)^2+b^2x^2}\right]$$
$$-bx\left[\arctan\left[\frac{1-x}{bx}\right]+\arctan\left[\frac{1+x}{bx}\right]\right]. \tag{11}$$

Obviously, when $b=0$ the well-known Lindhard static dielectric constant is obtained from (10) and (11). As is well known, it is not analytic at $x=1$. By contrast, our dielectric function (10) supplemented by (11) is analytic. In the large-wave-vector limit, (11) is reduced to

$$L(x)=-\frac{1+5b^2-8b^4}{(1+b^2)^3}\frac{1}{3x^2}\ . \tag{12}$$

Thus, in the limit of $x\to\infty$ (i.e., $q\to\infty$), $L(x)\sim-q^{-2}$, in agreement with what one expects from general principles.[10] Also, the prefactor appearing in (12) is a correction due to the diffusion effect of the electrons. When the latter is neglected (i.e., $b=0$), the prefactor reduces to 1 and the usual Lindhard result reappears. To illustrate the general features of the function $\epsilon(x)$ and $L(x)$ of (10) and (11), we plot $\epsilon^{-1}(x)$ and $L(x)$ versus x in Fig. 1. The figure shows that the $b\neq0$ analytic function $\epsilon^{-1}(x)$ and $L(x)$ deviate from their Lindhard ($b=0$) counterparts mainly in the vicinity of $x=1$, and the deviation is not significant when b is less than about 0.1. For example, when $b=10^{-3}$ the deviation is not observable in the scale of the figure. Also, to show the essential difference between the $b=0$ and $b\neq0$ cases on the analyticity property, we plot $dL(x)/dx$ for $b=0$, 0.001, and 0.01 (see the inset of Fig. 1). We note that it is well behaved for all wave vectors, in contrast to the Lindhard case ($b=0$), which exhibits a divergence at $x=1$. Also, we note that the selection of the values b in our study is based on that fact that the parameter b [defined by (8)] should be much less than 1 for real materials. For example, in the classical limit the diffusion constant of the center of mass $D\approx v_F^2\tau/N$, with $N\gg1$, where N is the number of electrons forming the center of mass and v_F is the Fermi velocity. It follows that $b\approx\varepsilon_F\tau/\hbar N$. Then, for a typical metal with $\varepsilon_F=6$ eV, $\tau=10^{-12}$ s and $n=10^{22}$ cm^{-3} and for a small system with typical dimension 10^3 Å, say, one obtains $b\approx10^{-3}$. For larger systems, b is even smaller, which justifies our statement that b is much less than 1 in

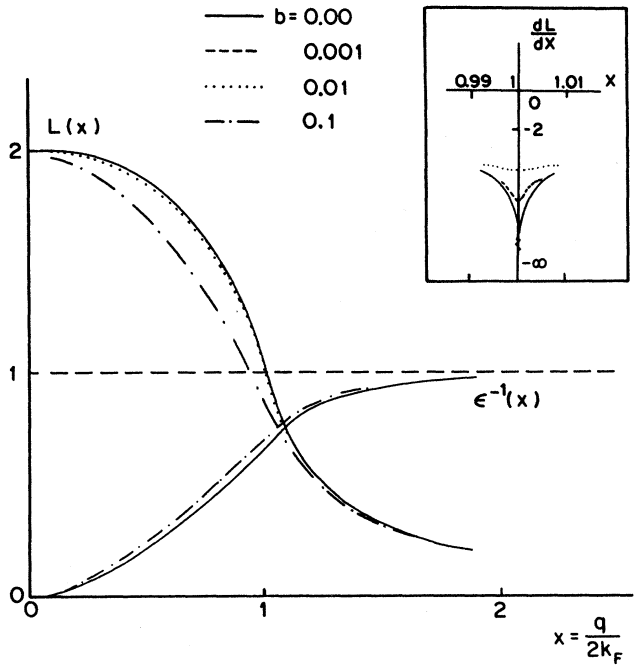

FIG. 1. The inverse of the static dielectric function $\epsilon^{-1}(x)$ and the generalized Lindhard function $L(x)$ at selected values of b. The insets describe the behavior of $dL(x)/dx$ near $q=2k_F$.

our formulation.

Next, as an application of Eq. (10), we study the screening charge density $n_s(r)$ for a static impurity of unit charge. The screening charge density at a distance r from a static unit charge is given by[8]

$$n_s(r)=\frac{1}{2\pi^2 r}\int_0^\infty q\sin(qr)\left[1-\frac{1}{\epsilon(q,0)}\right]dq\ . \tag{13}$$

The results obtained with the present dielectric function (10) at $r_s=3$, $b=0$, and other selected values of b are presented in Fig. 2. The solid line ($b=0$) represents

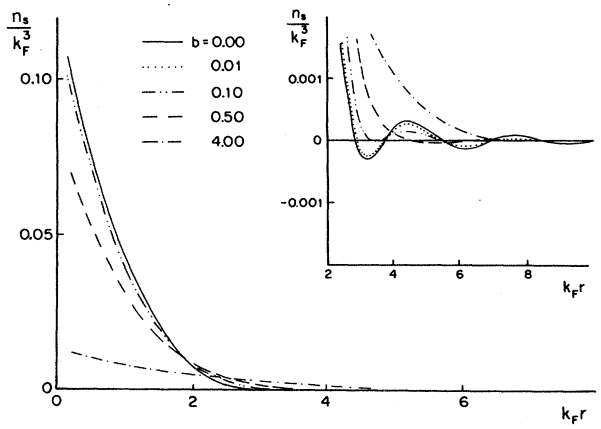

FIG. 2. The dimensionless screening charge density $n_s(k_Fr)/k_F^3$ vs k_Fr for $r_s=3$ at selected values of b.

Lindhard's RPA results, where one sees the well-known Friedel oscillation

$$n_s(r)\sim\frac{1}{r^3}\cos(2k_Fr)\ , \tag{14}$$

at large values of k_Fr. This behavior is generally recognized as the direct result of the nonanalyticity of the Lindhard function at $q=2k_F$. It is then of particular interest to see how it changes when we eliminate the nonanalyticity by using the dielectric function (10) at $b\neq 0$, i.e., by including the fluctuation effect. Our results show that, in general, the presence of fluctuations reduces the strength of the Friedel oscillation. When b is less than about 10^{-1}, the oscillation is still present, although the amplitude of the oscillation is reduced compared to the $b=0$ case. However, when b is greater than about 10^{-1}, the oscillation is almost not identifiable and the density decays by a power law. We will now make some comments on these results.

First, the conservation of the local electron number holds in our calculation, which can be easily seen by integrating the $n_s(r)$ of (13) over the whole r space. This is a different way of achieving the number conservation, compared to the phenomenological approach,[11] where the iDq^2 term does not appear. Our approach is basically from first principles and is rigorous, and thus the local electron number is conserved naturally in the calculation.

Secondly, in comparison with the RPA ($b=0$) results, after we consider the fluctuation effects ($b>0$) the screening charge density $n_s(r)$ in the region very close to the point impurity is reduced and compensated by an increase in the intermediate region where $k_Fr\geq 2$. Also, we find a reduction of the amplitude of the Friedel oscillations. We note that the behavior of this fluctuation contribution to the Friedel oscillations in the RPA calculation is different from some well-known results in the literature.[7,8] In the latter studies the short-range correlations arising from the Coulomb and exchange effects are added to the RPA calculation with the result that the screening charge density is increased for small r, compensated by the increase of the amplitude of the first oscillation peak of the negative charge, and for large r, the oscillation is unchanged.

Thirdly, the period of the Friedel oscillations is increased due to inclusion of the fluctuation effects. Using (10), (11), and (13), one can show that the Friedel-oscillation behavior of Eq. (14) should be replaced by

$$n_s(r)\sim\frac{1}{r^3}\cos\left[\frac{2k_Fr}{1+2b^2}\right]\ . \tag{15}$$

The above expression shows that when b increased (keeping $b<1$) the period of the Friedel oscillation becomes larger. This fact is indicated by the inset of Fig. 2.

IV. SUMMARY AND DISCUSSION

In summary, we have presented in (7) and (9) a well-behaved dielectric function for all wave vectors. In particular, our generalized Lindhard dielectric function improves the performance in the large-q region and is ana-

lytic at $q=2k_F$. The origin of the generalization is the inclusion of the fluctuations of the electrons. The study of $\epsilon(x,0)$ shows that at small b it does not change very much from the Lindhard function. The corresponding charge in the resulting screening charge density may be obtained by comparing (13) and (15), from which we deduce that the period of the oscillations is increased. There is also a small reduction in the amplitude of the oscillations.

Our conclusion that the Friedel oscillations are damped due to the inclusion of fluctuation effects is consistent with results of Pettifor and Ward,[14] who removed the nonanalyticity of the static Lindhard function by replacing it by a rational function. It should be noted that the removal of the nonanalyticity by Pettifor and Ward enables them to give a direct interpretation of the structural phase transitions of Na, Mg, and Al under pressure. However, the method used by these authors is not unique and is not based on a new physical effect, in contrast to the method used in our removal of the singularity. Thus, it would be of interest to apply our analytic function to the same problem as Pettifor and Ward,[14] a subject to which we hope to return at a future time.

Note added in proof. In the meantime, we have also solved the corresponding problem for the two-dimensional case[15] (generalization of Stern's result).

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