Effective Fields in the Electron Gas*

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The effective fields acting on different probes are analyzed. Several formalisms are discussed. It is shown that the definition of an electron-test-charge dielectric function is compatible with all current approximations for the electron gas.

I. INTRODUCTION

The response of a many-particle system to an external perturbation can be found in two distinct ways, depending on the kind of information one desires. One may ask what is the behavior of the system as a whole, when acted on by the external perturbation, or inquire about the behavior of one particular subsystem when in the presence of the perturbing field. The subsystem can be of many different kinds, such as a particle occupying initially a state k, a wave packet, bound electron, etc. Depending on the response one is interested in, two effective fields are obtained: (a) that which an external probe would feel due to the external perturbation field. This defines the usual susceptibility or, in the case of charged particles, the usual dielectric function, which we shall call ϵ; (b) that which is felt by the subsystem under investigation. If this effective field does not depend on the specific subsystem chosen, a new susceptibility (or dielectric function κ) can be defined which is, in general, different from the usual one, defined in case a.

In order to investigate the relationship between the two responses we turn to the theory of the many-electron gas with a uniform background of positive charge with the same density as the average electron density. The system is known to represent to a certain extent the alkali metals, once the bare electron mass is replaced by an effective mass.

The usual dielectric function has been thoroughly investigated since, from knowledge of it, many thermodynamical quantities can be obtained, such as the free energy of the gas, the specified heat, collective modes, Landau parameters, etc.[1] This dielectric function is usually obtained by linear response theory supplemented by a decoupling ansatz.[2,3] Recently[4] some calculations took as a starting point the response of individual electrons to the external field, and from there the usual dielectric function was calculated.

The purpose of this paper is to study the relation between the two formalisms and discuss the approximations involved in the definition of the electron-test-charge dielectric constant.

II. ELECTRON-TEST-CHARGE DIELECTRIC FUNCTION

When an external potential is acting on the electron gas, the effective field felt by one particular electron is certainly different from that felt by an external probe. This difference is due to the fact that the two probes interact quite differently with the medium. Only in the simplest of the self-consistent approximations, the random-phase approximation (RPA), are the two fields identical. The reason for this is well known: The RPA corresponds to a macroscopic-field approximation and is the same no matter what probe one uses.

In the RPA the dielectric constant is given by

$$\epsilon(q) = 1 - \phi(\vec{q})\chi^0(q), \tag{1}$$

where $\phi(\vec{q}) = 4\pi e^2/|\vec{q}|^2$, q are four vectors $(\vec{q}, \omega)$, and $\chi^0(q)$ is the susceptibility of the noninteracting electron gas with the same density as the interacting one considered.

A useful approximation is to assume that the local field $\phi_l(q)$ acting on every quasiparticle is the same, and to define a new dielectric function $\kappa(q)$ as the ratio of the external to the local field:

$$\frac{\phi_l(q)}{\phi(q)} = \frac{1}{\kappa(q)}. \tag{2}$$

This dielectric function shields the external potential as seen from the quasiparticles, and therefore the collection of quasiparticle responds to this field as a system of noninteracting particles

$$\langle \rho(q) \rangle = \chi^0(q)\phi_l(q) = \frac{\chi_0(q)\phi(q)}{\kappa(q)}, \tag{3}$$

with the connection between $\epsilon(q)$ and $\kappa(q)$ trivially obtained as

$$\kappa(q) = \frac{\epsilon(q)\phi(q)\chi^0(q)}{1 - \epsilon(q)}. \tag{4}$$

It is instructive to rewrite the dielectric function κ in terms of the local-field corrections (over the macroscopic field) $J(q)$. If

$$\epsilon(q) = 1 - \frac{\phi(q)\chi^0(q)}{1 - J(q)\chi^0(q)}, \tag{5}$$

then

$$\kappa(q) = 1 - \phi(q)\chi^0(q) - J(q)\chi^0(q). \tag{6}$$

Notice that in the RPA $J(q) = 0$ and $\epsilon(q) = \kappa(q)$.

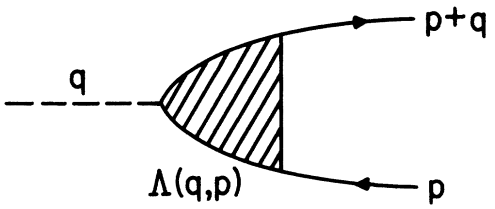

FIG. 1. Graphical representation of the function Λ.

III. GRAPHICAL INTERPRETATION

Let us start by defining, following the notation of Langreth,[5] the electron vertex function $\Lambda(q, p)$, which represents the full interaction of the electron with an external potential. The function Λ has the graphical representation shown in Fig. 1.

The effective potential acting on electron p is readily obtained from Λ:

$$\phi^{e}_{\mathrm{eff}}(q, p) = \phi(q)\Lambda(q, p)\,. \tag{7}$$

Equation (7) is not a macroscopic equation since the effective potential depends on the electron four-momentum p. In order to define a dielectric function electron test charge, which is our goal, we must make ϕ_{eff} independent of p; i.e., we must take some average value for Λ,

$$\bar{\Lambda}(q) = \langle \Lambda(qp) \rangle, \tag{8}$$

and then

$$1/\kappa(q) = \bar{\Lambda}(q)\,. \tag{9}$$

As $\bar{\Lambda}(q)$ depends only on the potential four-vector q it may be replaced by a point in Fig. 1.

In Fig. 2 we show the graphical representation for $\bar{\Lambda}(q)$, where the cross can be identified as the source strength $\rho_0(q)$. The dot $\bar{\Lambda}(q)$ may now be

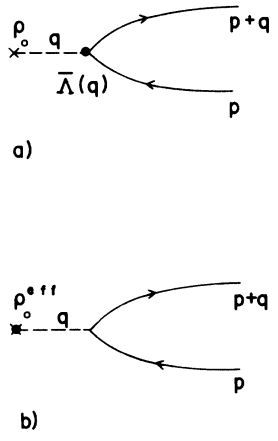

FIG. 2. Graphical representation of $\bar{\Lambda}(q)$ and the definition of the effective field strength.

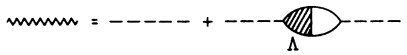

FIG. 3. Relation between the test-charge–test-charge effective potential and the function Λ.

multiplied by the cross $\rho_0(q)$, leading to Fig. 2, where the cross with a dot is the effective external-field strength. Figure 3 may be interpreted in a similar way.

An effective potential may be understood as a renormalization of an effective external charge density, interacting with the system via the bare potential line.

In order to write κ in terms of the bulk dielectric function we write the equation for ϵ in terms of Λ,

$$1/\epsilon(q) = 1 + \phi(q) \int_{p'} \Lambda(qp')G(p')G(p'+q)\,, \tag{10}$$

where $\int_{p'}$ includes spin summation and all GG products are diagonal in spin.

This equation can be represented graphically in a very simple way. Define the effective field acting on a test charge as $\phi^{t}_{\mathrm{eff}} = \phi/\epsilon$ and let it be represented by a wavy line; then Fig. 3 clarifies the meaning of Eq. (10).

If the approximation used in order to obtain κ is made, the bulk dielectric function becomes

$$1/\epsilon(q) = 1 + \phi(q)\bar{\Lambda}(q)\chi(q)\,, \tag{11}$$

where $\chi(q) = \int_{p'} G(p')G(p'+q)$ is the single-particle susceptibility.

Combining Eqs. (9) and (11), we obtain the desired relation between ϵ and κ, namely,

$$1/\epsilon = 1 + (\phi\chi/\kappa)\,, \tag{12}$$

identical to that derived in Sec. I, if χ and χ^0 are identified. This χ, calculated from the renormalized single-particle Green's function, is usually called the short-range susceptibility.

The replacement of $\Lambda(q, p)$ by $\bar{\Lambda}(q)$, necessary in order to define κ, is exactly the approximation made in the present theories of the linear response theory of the electron gas. We shall show that this is the case by writing an integral equation for the vertex function, in terms of the four-point function I, which represents the total electron-hole interaction:

$$\Lambda(q, p) = 1 + \int_{p'} I(q, p, p')G(p')G(p'+q)\Lambda(qp')\,, \tag{13}$$

which is represented graphically in Fig. 4.

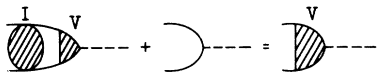

FIG. 4. Graphical representation of the integral equation for Λ.

In order to calculate the dielectric constant ϵ, all current approximations replace $I(q, p, p')$ by $\bar{I}(q)$, where p and p' have been averaged over the Fermi sphere. Replacing I by $\bar{I}$ in Eq. (13) we can solve for Λ, giving

$$\Lambda(qp) = \frac{1}{1 - \bar{I}(q)\chi(q)}, \tag{14}$$

independent of p, as we mentioned before.

In order to obtain a form similar to Eq. (3) we decompose I in two parts: the bare Coulomb interaction plus a new four-point function which we shall call J.

We may write the two dielectric functions as

$$\epsilon(q) = 1 - \frac{\phi(q)\chi(q)}{1 - \bar{J}(q)\chi(q)} \tag{15}$$

and

$$\kappa(q) = 1 - \bar{I}(q)\chi(q). \tag{16}$$

We must remark here that any approximations made in order to obtain $\bar{J}$ must be consistent with those made to obtain χ, so that no important sum rule is violated.[6]

$\bar{I}(q)$ is usually assumed to be only a function of the wave vector $\vec{q}$. This is an additional approximation which is certainly not correct for other systems, for example, an assembly of interacting permanent dipoles. In the RPA we have $\bar{J}(\vec{q}) = 0$.

Using Eq. (16) it is very simple to generalize some results obtained by Pines for the RPA, if we replace ϵ_{RPA} by κ. As an illustration, we may write for the structure factor[3]

$$S(\vec{q}) = (1/N)\langle 0 | [\rho^s(\vec{q})]^* [\rho^s(\vec{q})] | 0 \rangle,$$

where the matrix elements of ρ^s are

$$[\rho^s(\vec{q})]_{n0} = \frac{[\rho(\vec{q})]_{n0}}{\kappa(\vec{q}, \omega_{n0})},$$

the states under consideration being states of the noninteracting gas. The polarization cloud around the fluctuation is really related to the electron-test-charge dielectric function.

IV. COMPARISON WITH OTHER FORMULATIONS

Another way to analyze the linear response of the electron gas is to reduce the problem to the calculation of the irreducible polarization diagrams,[2,7,8] i.e., those which cannot be split by

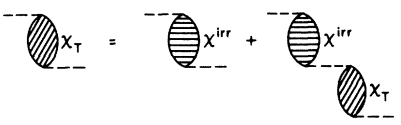

FIG. 5. Graphical representation of the integral equation for χ_T.

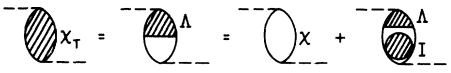

FIG. 6. Correspondence between χ_T and Λ shown here.

cutting a single internal potential line. The total susceptibility is written in the form of a Dyson equation in terms of the irreducible polarization χ^{irr},

$$\chi_T = \chi^{\mathrm{irr}} + \chi^{\mathrm{irr}}\phi\chi_T$$

or

$$\chi_T = \frac{\chi^{\mathrm{irr}}}{1 - \phi\chi^{\mathrm{irr}}}, \tag{17}$$

which is graphically represented in Fig. 5.

We have shown the graphs corresponding to Sec. II in Fig. 6.

It is straightforward to prove that

$$\chi^{\mathrm{irr}} = \chi/(1 - J\chi). \tag{18}$$

The simplest approximation for $\bar{J}$ is to average

$$\int \tfrac{1}{2} v(p - p')G(p')G(p' + q) \sim \int \langle v(p - p')\rangle_{p \text{ on FS}} G(p')G(p' + q)$$

over the Fermi sphere, as was done by Hubbard. The $\frac{1}{2}$ factor comes from the fact that v does not flip spins. In Kleinmann's approximation, the integral

$$\frac{1}{2}\int \frac{1}{\omega - \epsilon_{p'} + i\delta_{p'}} \left(\frac{v(p - p')}{\omega + \Omega - \epsilon_{p'+q} + i\delta_{p'+q}} \right) d\omega\, d^3p'$$

is performed by extending ω to the whole complex plane and closing the path with a semicircle in the lower part of the complex plane. $J(q)$ becomes

$$J(q) = \frac{1}{2}\int \frac{v(p - p')\, d^3p'}{\Omega + \epsilon_{p'} - \epsilon_{p'+q} + i\delta_{p'+q}} n_{p'} + \frac{1}{2}\int \frac{v(p - p')\, d^3p' n_{p'+q}}{-\Omega + \epsilon_{p'+q} - \epsilon_{p'} + i\delta_{p'}}.$$

The averaging process is performed at this point by averaging $v(p - p')$ inside the Fermi surface for p and p' in the first term on the right-hand side and, in the second term, averaging v over p inside the Fermi surface and over p' inside the surface centered on q. One then finds the two terms shown in Ref. 9.

The formalism of Singwi *et al.*[2] can also be understood as a very intuitive approximation for the electron-hole interaction inside the bubble. They assume that the electric field acting on an electron occupying point $\vec{r}$ at time t is of the form

$$\nabla\psi(\vec{r}, t) = \int \nabla\phi(\vec{r} - \vec{r}')n(\vec{r}', t)\, d^3r' + \int \nabla\phi(\vec{r} - \vec{r}')n(\vec{r}', t)[g(\vec{r} - \vec{r}') - 1]\, d^3\vec{r}'; \tag{19}$$

the second term of the right-hand side of Eq. (19) is the direct electron-hole interaction, if we put $(-\phi)$ instead of ϕ, since $-n(g-1)$ is the hole density around the particle at $\vec{r}$, and holes carry a positive charge. In Singwi *et al.*'s paper the interaction was changed to

$$\nabla\psi(\vec{r},\,t)=\int\nabla\phi(\vec{r}-\vec{r}\,')n(\vec{r}\,',\,t)\,d^3\vec{r}\,' + \int[(-\nabla\phi(\vec{r}-\vec{r}\,'')n_h(\vec{r},\,t') \times\frac{1}{\epsilon(\vec{r}\,'-\vec{r}\,'',\,t)}\,dt'\,d^3r'\,d^3r'',$$

assuming a shielded interaction between electrons and holds.

In Singwi's approximation [Eq. (19)] $J(q)$ is given by

$$J(q)=-\frac{\hbar}{v}\int\frac{d^3q'}{(2\pi)^3}[S(\vec{q}-\vec{q}\,')-1]\,\phi(\vec{q}\,')\frac{\vec{q}\cdot\vec{q}\,'}{q^2}\,.$$

It seems to be a very difficult task to put the above theory into a graphically simple expansion and, to the author's knowledge, no one has made any substantial progress in this direction.

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