Self-Consistent Higher-Order Corrections to the Dielectric Screening Function

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An evaluation is carried out for the dielectric screening function of a free-electron gas. We include selfenergy and exchange ladder diagrams, taking an effective Yukawa interaction as a model. It is shown that using a self-consistent interaction instead of a random-phase-approximation interaction gives an appreciable correction to the dielectric function.

HE Lindhard¹ random-phase approximation (RPA) for the frequency- and wave-number-dependent dielectric function $\epsilon(q,\omega)$ provides a good description of many properties of the degenerate electron gas. However, there has been much effort expended toward obtaining the dielectric function in approximations beyond the (RPA). Du Bois² incorporated some exchange terms into $\epsilon(q,\omega)$ in the limit $q \rightarrow 0$. Osaka³ calculated the contribution of all possible combinations of ladder interactions and exchange self-energy. He used a Coulomb interaction screened with a static RPA dielectric function and worked in the limit $\omega = 0$, $q \rightarrow 0$. Recently, Kleinman⁴ developed an approximate method for summing the same set of diagrams as Osaka to obtain the dielectric function for all values of q and ω . A more complete list of references is given in his paper.

In all these calculations the interaction is taken in the RPA or some approximation of the RPA. A selfconsistent calculation would have to include an interaction which is screened by the complete dielectric function. Such a calculation is prohibitive because of the size of the enterprise for the general case. Therefore, it seems to be of some interest to investigate the effect of the self-consistency for a simple model in the limit $\omega = 0, q \rightarrow 0.$

We make the following ansatz for the static dielectric function:

$$\epsilon_i(q) = 1 + (q_s/q)^2 / \zeta_i. \tag{1}$$

This represents a Yukawa-type interaction.

Here q_s is given by

$$(q_s/2k_F)^2 = \rho = 0.52r_s/\pi = me^2/k_F\pi$$
, (2)

where $\frac{4}{3}\pi r_s^3$ is the volume per electron measured in units of Bohr radii, and k_F is the Fermi vector.

 ζ_i is a function of either r_s or ρ . It is the aim of this work to calculate ζ_i for the following approximations: i = HF (Hartree-Fock approximation), i = RPA, $i = SE^*$ [exchange self-energy corrections (with a RPA interaction)], i = SE [exchange self-energy corrections (with a self-consistent interaction)], $i = LSE^*$ [ladder-selfenergy corrections (with a RPA interaction)], and,

finally, i = LSE [ladder-self-energy corrections (with a self-consistent interaction).

In Fig. 1 we show the diagrams included for the various dielectric functions ϵ_i . Following the usual rules,⁵ we have from Fig. 1

$$\frac{1}{\zeta_{\text{RPA}}} = -\lim_{\omega=0, q \to 0} \frac{4\pi e^2}{q_s^2} \frac{-2}{2\pi i}$$

$$\times \int d\omega_1 \sum_{\mathbf{k}} G^0(\mathbf{k}, \omega) G^0(\mathbf{k} - \mathbf{q}, \omega - \omega_1), \quad (3)$$
where

where

$$G^{0}(\omega,q) = i/(\omega - q^{2}/2m + i\delta), \quad \delta = \mp 0 \quad \text{for} \quad k \geq k_{F}.$$
 (4)

The ansatz in Eq. (2) for $\epsilon_i(q)$ is not completely consistent because

$$\boldsymbol{\epsilon}_{\mathbf{RPA}} = 1 + (q_s/q)^2 [1 + F(q/2k_F)], \qquad (5)$$

FIG. 1. Diagrams included in the various approximations in calculating the dielectric function. The dashed line represents the unscreened Coulomb interaction and the solid line the zerothorder electron propagator.

 ¹ J. Lindhard, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. 28, 8 (1954).
 ² D. F. Du Bois, Ann. Phys. (N. Y.) 7, 174 (1959).
 ³ Y. Osaka, J. Phys. Soc. Japan 17, 547 (1962).
 ⁴ L. Kleinman, Phys. Rev. 172, 383 (1968).

⁶ J. R. Schrieffer, *Theory of Superconductivity* (W. A. Benjamin, Inc., New York, 1964), Secs. 5-9.

where

$$F(x) = \left[\frac{(1-x^2)}{4x} \right] \ln \left| \frac{(1+x)}{(1-x)} \right| - \frac{1}{2}.$$
 (6)

But in this paper we will not discuss the effect of correlation on F, which would be difficult to do in a selfconsistent way. Because we are not interested in calculating actual values but only want to compare different approximations, we feel justified in neglecting F(x). Then Eq. (3) follows immediately.

$$\frac{1}{\zeta_{\rm HF}} = \left(1 + \lim_{\omega=0, q \to 0} \frac{4\pi e^2}{q_s^2} \frac{-2}{2\pi i} \times \int d\omega_1 \sum_{\mathbf{k}} G^0(\mathbf{k}, \omega) G^0(\mathbf{k} - \mathbf{q}, \omega - \omega_1)\right)^{-1}.$$
 (7)

In this formulation, the HF approximation looks more complicated than the RPA because the geometric sum is already included in the definition of the dielectric function.

$$\frac{1}{\zeta_{SE^*}} = -\lim_{\omega=0, q\to 0} \frac{4\pi e^2}{q_s^2} \frac{-2}{2\pi i}$$

$$\times \int d\omega_1 \sum_{\mathbf{k}} G(\mathbf{k}, \omega) G(\mathbf{k} - \mathbf{q}, \omega - \omega_1), \quad (8)$$
with

$$G(q,\omega) = i/[\omega - q^2/2m - i\sum (q,\omega) + i\delta], \qquad (9)$$

where the equation for the self-energy is

$$\sum(q,\omega) = \sum_{\mathbf{k}} \int d\omega_{\mathbf{1}} \frac{v_{\mathbf{RPA}}(\mathbf{k}-\mathbf{q})}{2\pi i} G(\mathbf{k},\omega_{\mathbf{1}}) . \quad (10)$$

The expression for ζ_{SE} is identical to the one given for ζ_{SE^*} , except that v_{RPA} is replaced by

$$v_{\mathbf{SE}}(q) = 4\pi e^2/q^2 \epsilon_{\mathbf{SE}}(q) \tag{11}$$

in Eq. (10).

$$\frac{1}{\zeta_{\text{LS E}^*}} = -\lim_{\omega \to 0, q \to 0} \frac{4\pi e^2}{q_s^2} \frac{-2}{2\pi i} \int d\omega_1 \sum_{\mathbf{k}} \cdots G(\mathbf{k}, \omega) G(\mathbf{k} - \mathbf{q}, \omega - \omega_1) H(\mathbf{k}, \mathbf{k} - \mathbf{q}, \omega, \omega - \omega_1).$$
(12)

The equation for the ladder interaction H becomes

$$H(\mathbf{k}_{1},\mathbf{k}_{1}',\omega_{1},\omega_{1}')$$

$$=1+\sum_{\mathbf{k}_{2}}\int d\omega_{2} \frac{v_{\mathrm{RPA}}(\mathbf{k}_{2}-\mathbf{k}_{1})}{2\pi i}$$

$$\cdots H(\mathbf{k}_{2},\mathbf{k}_{2}',\omega_{2},\omega_{2}')G(\mathbf{k}_{2},\omega_{2})G(\mathbf{k}_{2}',\omega_{2}'), \quad (13)$$

where $\mathbf{k}_{1,2} - \mathbf{k}_{1,2}' = \mathbf{q}$ and $\omega_{1,2} - \omega_{1,2}' = \omega$. The self-energy is given by Eq. (10).

The expression for ζ_{LSE} is identical with the one given for ζ_{LSE^*} except that v_{RPA} is replaced by

$$v_{\rm LSE}(q) = 4\pi e^2/q^2 \epsilon_{\rm LSE}(q) \tag{14}$$

in Eqs. (10) and (13).

All the integrals appearing in Eqs. (3)-(13) can be performed analytically. The results can be written as follows:

$$\zeta_{\rm HF} = 1 - \rho, \qquad (15)$$

$$\zeta_{\mathbf{RPA}} = 1, \qquad (16)$$

$$\zeta_{SE^*} = 1 - \rho + \rho(\rho + \frac{1}{2}) \ln(1/\rho + 1), \qquad (17)$$

$$\zeta_{SE} = \lfloor 1 + \eta - \eta (\eta + \frac{1}{2}) \ln(1/\eta + 1) \rfloor^{-1}, \quad (18)$$

$$p = \eta \zeta_{\rm SE},$$
 (19)

$$\zeta_{\rm LSE^*} = 1 - \rho + \rho^2 \ln(1/\rho + 1), \qquad (20)$$

and, finally,

where

with

$$\zeta_{\rm LSE} = [1 + \eta - \eta^2 \ln(1/\eta + 1)]^{-1}, \qquad (21)$$

$$\rho = \eta \zeta_{\text{LSE}}.$$
 (22)

The various approximations ζ_i are represented graphically in Fig. 2. First, note that the long-wavelength zero-frequency polarizability

 $\alpha = 4\pi e^2/q_s^2\zeta$

of an electron gas diverges in the HF approximation $(\zeta_{\rm HF}=0)$ for $\rho=1$; i.e., for $r_s=\pi/0.52$. This instability is the same found by Sawada,⁶ by Wolff,⁷ and by Gartenhaus and Stranahan.8 If correlation effects are included in the RPA, the instability vanishes $(\zeta_{RPA} \equiv 1)$. It is known, however, that the RPA screening overestimates correlation effects. Garrison et al.9 have suggested a method of computing the screening parameter in a self-consistent way. Their calculation corresponds to ours for ζ_{SE} . We see from Fig. 2 that in



Fig. 2. ζ_i as function of $1/\rho$ for different approximations; 5SE and 5SE* almost coincide and have not been drawn separately.

⁶ F. Iwamoto and K. Sawada, Phys. Rev. 126, 887 (1961).
⁷ P. A. Wolff, Phys. Rev. 120, 814 (1960).
⁸ S. Gartenhaus and G. Stranahan, Phys. Rev. Letters 14, 34

⁹ J. C. Garrison et al., Nuovo Cimento 47B, 200 (1967).

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this case the correlation effect is overestimated even more, although the result is not very different from the RPA result. Furthermore, the self-consistency condition is not important for this approximation. The correlation effects are reduced drastically (see Fig. 2) by including the ladder diagrams (Fig. 1). As mentioned at the beginning, a recent calculation of the dielectric screening function in this approximation has been done by Kleinman⁴ for all values of q and ω .

For $\omega = 0$, $q \rightarrow 0$, his result corresponds to ours for ζ_{LSE^*} . We are now able to estimate the importance of doing a self-consistent calculation by comparing ζ_{LSE^*} with ζ_{LSE} (see Fig. 2). At $\rho = \infty$ the correction amounts to 50% of the difference between the RPA and the LSE approximation. At $\rho = \frac{1}{3}$ ($r_s \simeq 2$) the correction has decreased to approximately 10%.

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Electron Tunneling in Superconducting Cd-Al₂O₃-Al Junctions*

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Studies were performed of the superconducting tunneling characteristics of Cd-Al₂O₃-Al junctions. The superconducting energy gap $2\Delta_{Cd}(0)$ was found to be 0.130 mV. Its variation with temperature was studied and has been compared with the predictions of the BCS theory. Measurements were also made in the presence of magnetic fields, and an effort was made to compare measurements with the Ginzburg-Landau theory. Extra structure in the first derivative of the tunneling characteristics (dV/dI versus V) was observed, and experiments were undertaken to ascertain whether this structure was caused by edge effects in the films or was a more basic feature of the films.

I. INTRODUCTION

 $\mathbf{E}^{\mathrm{XPERIMENTAL}}_{\mathrm{neling}}$ in superconducting Cd-Al₂O₃-Al junctions have been performed by us. Most superconductors studied by this technique¹ have transition temperatures $T_c > 1^{\circ}$ K. Cadmium, on the other hand, was reported to have a transition temperature² $T_c \simeq 0.5^{\circ}$ K and had not been studied previously by this method. We hoped to compare the superconducting properties of Cd metal in the form of evaporated metal films with the predictions of the Bardeen-Cooper-Schrieffer (BCS) theory.³ Hence, experiments were initiated to investigate the magnitude of the superconducting energy gap 2Δ and its variation with temperature and magnetic field. Measurements of the I-V curves were supplemented by studies of the differential resistance dV/dI. This permitted the observation of structure in the tunneling characteristics.

Since these experiments involved working in the temperature range below 1°K, they presented two main

Massachusetts Institute of Technology, Cambridge, Mass. 02139, ¹G. I. Giaever and K. Megerle, Phys. Rev. **122**, 1101 (1961). ²J. R. Clement, Phys. Rev. **92**, 1578 (1953).

problems. First, because the samples could not be immersed in a uniform temperature helium bath, the problem of maintaining thermal equilibrium between the sample and the temperature-measuring resistors was more difficult. Second, the low transition temperature of Cd implies a small superconducting energy gap, necessitating measurements of voltages considerably smaller than those of the superconductors having higher transition temperatures.

II. APPARATUS

The cryostat used in these experiments was a standard adiabatic demagnetization apparatus and He³ refrigerator, as shown in Fig. 1. The general features shown in this figure from top to bottom are the He³ refrigerator pot, the sample holder, the cerium magnesium nitrate Ce₂Mg₃(NO₃)₁₂·24H₂O (hereafter referred to as CMN) thermometric salt, the lead heat switch, and potassium chrome alum $KCr(SO_4)_2 \cdot 12H_2O$ (hereafter referred to as KCr alum) cooling salt.

The sample holder is shown in more detail in Fig. 2. Samples were evaporated on 1×3 -in. glass or quartz substrates and were held in place by the Teflon holder shown in Fig. 2.

Each half of the Teflon holder had two $1 \times \frac{1}{32}$ -in. slots cut into it. About 300 No. 40 AWG Cu wires were varnished together to form a foil (referred to as coil foil) which was threaded through the slot in the Teflon holder to the left in Fig. 2 and was in contact with the entire back surface of the substrate. This coil foil served

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³ J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. 108, 1175 (1957).