Some Surface Effects in an Electron Gas*

PETER A. FEDDERS
Palmer Physical Laboratory, Princeton University, Princeton, New Jersey
(Received 7 July 1966)

The effects of various external probes on a gas of interacting electrons confined to a foil are examined in an approximation for the response functions which reduces to the random-phase approximation for a bulk sample. Some band effects are included in a phenomenological manner. Surface corrections to the bulk properties are found which cannot be obtained in a wave-number-independent treatment nor in the Born approximation. The momentum dependence of the surface plasmon's resonant frequency is found and the response of the system to fast incident electrons and electromagnetic radiation is calculated.

I. INTRODUCTION

IN this paper a formalism is developed to treat a gas of interacting electrons confined to a slab of finite thickness. The boundary condition of specular reflection is applied directly to the electronic wave functions. The response functions for this system to various external disturbances are calculated from a unified point of view in a well-defined approximation. The basic approximation to the response functions is identical to the random-phase approximation (RPA) in a bulk sample. Using the response functions obtained from this formalism, some properties of metals due to surfaces and finite size are investigated.

In addition to the usual resonance at the plasma frequency, a surface resonance is found. This is the surface-plasma mode first predicted by Ritchie[1] and further elucidated by Ferrell,[2,3] Stern,[3] and others. It is shown that the resonant frequency of this mode depends linearly on its momentum parallel to the sides of the slab in a thick sample. There are some minor corrections to Ritchie's expression for the energy loss of a fast electron passing through the sample. These corrections are due to further wave-number dependence of the response function. A calculation is also made for the energy loss in a reflection[4] experiment where the Born approximation cannot be used. A crude calculation indicates that surface effects may alter the electromagnetic reflectivity in a thick sample if lifetime effects due to other processes are small.

The model consists of a gas of electrons interacting via the Coulomb potential in a slab confined to $0\leq z\leq d$ with infinite lateral extent in the x-y plane. An infinitely high potential barrier is assumed to exist at the boundaries. This boundary condition of specular reflection is valid only for metals with a smooth surface and no oxide[5] coating. The effects of bands and phonons will be inserted phenomenologically.

Since the slab is infinite in the x-y plane, periodic boundary conditions are applied on a square of side L in this plane. The wave numbers in this plane are denoted by $\mathbf{p}$ and those in the z direction by k. The letter $\mathbf{q}$ will be reserved for the pair $(\mathbf{p},k)$. The treatment is restricted to zero temperature and $q_Fd\gg1$, where q_F is the Fermi momentum. Further, $\hbar$ is set equal to 1. The noninteracting wave functions for this model are

$$\phi(\mathbf{r})=(2/L^2d)^{1/2}\exp i\mathbf{p}\cdot\boldsymbol{\rho}\sin kz \tag{1}$$

for $0\leq z\leq d$ and zero outside this region. The cylindrical coordinates $\mathbf{r}=(\boldsymbol{\rho},z)$ have been used. The components of $\mathbf{p}$ are $2\pi n/L$ and k is restricted to $\pi n/d$ where n is an integer. The noninteracting single-particle energies are

$$E(\mathbf{q})=E(\mathbf{p},k)=(\mathbf{p}^2+k^2-q_F{}^2)/2m \tag{2}$$

as measured from the Fermi surface. It is assumed that the background of positive charge does not appreciably alter ϕ or E.

The response functions are calculated in the Appendix using Green's-function techniques. In terms of these techniques the approximation used is identical to the RPA in a bulk sample. The structure of the surface corrections, and in particular the surface plasmon, are discussed in Sec. II. The formalism is used to discuss the energy loss of fast incident electrons and the interaction of the sample with electromagnetic waves in Secs. III and IV, respectively.

II. STRUCTURE OF THE SURFACE PLASMON

The linear response or correlation functions $L_{\mu\nu}$ are given in the Appendix by Eqs. (A16) through (A24). We note that $L_{\mu\nu}(\mathbf{p},k',k'',\omega)$ contains two distinct types of terms. One type, consisting of the first term in Eq. (A17) and $S_\mu{}^0$, is proportional to $\delta(k'\pm k'')$. These terms are those which are equivalent to applying specular reflecting boundary conditions to the system after calculating the bulk response as is done in calculating the anomalous skin effect.[6] These terms contain the bulk plasma resonance but not the surface plasma resonance which is contained in R_μ. In the second type of term k' and k'' are unrestricted except that $n'+n''$

* Work supported by the U. S. Air Force Office of Research, Air Research and Development Command under Contract No. AF 49(638)-1545.

[1] R. H. Ritchie, Phys. Rev. **106**, 874 (1957).
[2] R. A. Ferrell, Phys. Rev. **111**, 1214 (1958).
[3] E. A. Stern and R. A. Ferrell, Phys. Rev. **120**, 130 (1960).
[4] See, for example, C. J. Powell and J. B. Swan, Phys. Rev. **115**, 869 (1959).
[5] For effects of an oxide layer see Ref. 3.
[6] See, for example C. Kittel, *Quantum Theory of Solids* (John Wiley & Sons, Inc., New York, 1963), Chap. 16.

must be even. Although in the Born approximation only contributions from $k'=k''$ enter for large d, the other contributions are important in general.

For the purposes of this paper only wave numbers small compared to q_F and frequencies of the order of the plasma frequency, $\omega_p=4\pi ne^2/m$, are considered. In this limit the last two terms in Eq. (A17) and the last term in Eq. (A18) may be neglected. The remaining quantities in Eq. (A17) are easily evaluated with the exception of R_μ which will be studied in this section. Before obtaining R_μ, however, a short discussion of $\epsilon(\mathbf{p}k\omega)$ defined by Eq. (A24) is necessary. In the limit as d approaches infinity all sums can be viewed as integrals and ϵ is identical to the RPA dielectric constant. However, Im $\epsilon(\mathbf{p}k\omega)=0$ if $pd<1$ except for special values of ω. This arises since contributions to Im ϵ come from points where the energy denominator of B vanishes [see Eq. (A10)]. For discrete k and $pd<1$ this occurs only for select ω. Further Im$\epsilon(\mathbf{q}\omega)=0$ for large ω of $q\ll q_F$ even in a bulk sample. This property of the model is not shared by real metals because of band effects, phonons, etc. In order to obviate these difficulties and render our results more physical, Imϵ will be given a small imaginary part g independent of wave number. B is altered accordingly. Except under exceptional circumstances g will be greater than $(q_Fd)^{-1}$.

The plasma mode manifests itself as a resonance in L through the functions S and R which are proportional to ϵ^{-1}. Similarly, the surface-plasma mode manifests itself as a pole in R. From Eqs. (A12) and (A18) one sees that R_μ is the solution to the equations

$$R_\mu(\mathbf{p}k\omega)=d^{-1}\sum_{n'}\mathcal{R}_\mu(\mathbf{p},k',k,\omega)\{n+n'\}\,, \tag{3}$$

$$\begin{aligned}\mathcal{R}_\mu(\mathbf{p},k',k,\omega)=&\mathcal{R}_\mu{}^0(\mathbf{p},k',k,\omega)\\&-R_\mu(\mathbf{p}k\omega)C_0(\mathbf{p}k'\omega)v(\mathbf{p}k')\epsilon^{-1}(\mathbf{p}k'\omega)\\&-(2d)^{-1}\sum_{\bar{n}}\mathcal{R}_\mu(\mathbf{p},\bar{k},k,\omega)B(\mathbf{p},\tfrac{1}{2}(k'+\bar{k}),\tfrac{1}{2}(k'-\bar{k}),\omega)\\&\times v(\mathbf{p}k')\{\bar{n}+n'\}\epsilon^{-1}(\mathbf{p}k')\,,\end{aligned} \tag{4}$$

where $\{n+n'\}$ indicates that the summation is taken only over even values of $n+n'$ and $\mathcal{R}_\mu{}^0(\mathbf{p},k',k,\omega)$ is given by $S_\mu{}^0(\mathbf{p},k',k,\omega)v(\mathbf{p}k')$. The rest of the quantities are defined in the Appendix. Since Eq. (4) is linear it can be split into two separate equations, each with the same kernel. These equations, for $\mathcal{R}'_\mu$ and $\mathcal{R}''_\mu$, have $\mathcal{R}_\mu{}^0$ and $-C_0v\mathcal{R}_\mu\epsilon^{-1}$ for inhomogeneous terms. The sum of the solutions equals $\mathcal{R}_\mu$. $\mathcal{R}'_\mu$ contributes only to the numerator of $\mathcal{R}_\mu$ so it is sufficient to obtain its lowest order contribution. To this order it is given by $\mathcal{R}_\mu{}^0$ and contributes

$$N_\mu=d^{-1}\sum_{\bar{n}}\mathcal{R}_\mu{}^0(\mathbf{p},k'k,\omega)\{n+\bar{n}\} \tag{5}$$

to the right side of Eq. (3).

$\mathcal{R}''_\mu$ is proportional to R_μ and will determine the resonant frequency and lifetime of the surface mode. The most important contribution to it is the inhomogeneous term. Using the expansion

$$\epsilon(\mathbf{q}\omega)=1-(\omega_p/\omega)^2[1-(v_Fq/\omega)^2]+ig$$

for $q\ll q_F$ and large ω, one finds that the most important contribution to Eq. (3) from $\mathcal{R}''_\mu$ is

$$\begin{aligned}-R_\mu[\omega^2-\omega_p{}^2+ig\omega^2]^{-1}\\\times\tfrac{1}{2}\{\omega_p{}^2(1+\epsilon_ne^{-pd})-\omega^2(1-\epsilon_ne^{-pd})p/\tilde{p}\}\,,\end{aligned} \tag{6}$$

where $\epsilon_n=(-1)^n$, v_F is the Fermi velocity, and

$$\tilde{p}^2=p^2+(\omega_p{}^2-\omega^2-ig\omega^2)(\omega/v_F\omega_p)^2. \tag{7}$$

The $\tilde{p}$ term would be absent if the wave-number dependence of ϵ were neglected in the summation. By iterating Eq. (4) and summing to find R_μ one can see that the remaining terms in $\mathcal{R}''_\mu$ contribute only to order $p[1-\epsilon_n\exp(-pd)]$ and are independent of k. Thus R_μ can be written as the quotient N_μ/D where

$$\begin{aligned}D=1+[\omega^2-\omega_p{}^2+ig\omega^2]^{-1}\tfrac{1}{2}\{\omega_p{}^2(1+\epsilon_ne^{-pd})\\-\omega^2(1-\epsilon_ne^{-pd})p/\tilde{p}\}-\gamma(1-\epsilon_ne^{-pd})\,,\end{aligned} \tag{8}$$

and N_μ is given by Eq. (5). The symbol γ is used to denote real and imaginary terms of order p/q_F.[7]

The real part of ω when $D=0$ gives the resonant frequency of the surface plasmon and the imaginary part gives the decay rate. If g, γ, and $\tilde{p}$ are neglected this resonant frequency is in agreement with previous determinations. For $pd\gg1$ the resonant frequency of the surface plasmon is $\omega_p/\sqrt{2}+$ terms of order ω_pp/q_F.[8,9] The decay rate contains terms of order ω_pp/q_F and ω_pg. For $pd\ll1$ the surface resonance takes place at $\omega=\omega_p(1-pd/4)$ plus corrections of order $(pd)\omega_pp/q_F$ if n is odd. The decay rate contains terms of order (pd) ω_pp/q_F and $g\omega_p$. For even n the resonant frequency approaches zero if $pd\ll1$ and is not considered here. In order to find γ exactly, an integral equation must be solved. This has not been done since its actual value is not important. Obviously other phenomenological additions can be inserted to reflect the fact that the surface-plasma frequency is not $\omega_p/\sqrt{2}$ for all metals. (e.g., silver.) This was not done in the present paper. The importance of inserting g is especially evident in Sec. IV.

III. ELECTRON ENERGY LOSS

In this section the probability of a fast incident electron creating a bulk or surface-plasma oscillation is calculated.[10] The volume of the slab is L^2d and the incident electron is quantized in a cube of side L. To start with the Born approximation is used. The initial momentum $\mathbf{Q}$ of the incident electron is much greater than

[7] For our purposes here, the plasma and Fermi energies are of the same magnitude.

[8] This is not in agreement with the work of Hideo Kanazawa [Progr. Theoret. Phys. (Kyoto) **26**, 851 (1961)]. The difference is attributed to different approximations. Kanazawa's results for the probability of energy loss from fast electrons also differs from ours and those in Refs. 1 and 3.

[9] R. H. Ritchie, Progr. Theoret. Phys. (Kyoto) **29**, 607 (1963); R. H. Ritchie and A. L. Marusak, Surface Sci. **4**, 234 (1966).

[10] For a treatment of the bulk case and further references, see David Pines, *Elementary Excitations in Solids* (W. A. Benjamin, Inc., New York, 1963).

the momentum transfer $\mathbf{q}$ and the energy transfer ω is much less than $Q^2/2m$. The interaction between the incident electron and the slab is given by $\sum v(r-r_i)$, where r_i is the position of the ith electron in the slab.

The total transition probability can be calculated as in Kadanoff and Martin's[11] paper yielding

$$W=|v(\mathbf{q})|^2\int_{-\infty}^{t}dt'\int_{-\infty}^{t}dt''\int d^3r'd^3r''\frac{1}{L^6}\times\langle n(\mathbf{r}'t')n(\mathbf{r}''t'')\rangle e^{i\mathbf{q}\cdot\mathbf{r}'}e^{-i\mathbf{q}\cdot\mathbf{r}''}e^{-i\omega(t'-t'')},\quad(9)$$

where n is the density operator and $\langle\ \rangle$ denotes expectation value. After dividing by the incident flux, relating $\langle nn\rangle$ to the time-ordered product L_{00} and shifting to wave-number space through Eq. (A16), one obtains P, the differential probability of an electron losing an energy $\omega=\mathbf{q}\cdot\mathbf{V}_0$ and a momentum $\mathbf{q}=(\mathbf{p},k)$.

$$P=\frac{v(q)}{V_0\cos\theta_0}\delta(\omega-\mathbf{q}\cdot V_0)F\frac{d^3q}{(2\pi)^3},\quad(10)$$

$$F=-\int_0^\infty d\omega\frac{1}{d^2}\sum_{n'+n''}\{n'+n''\}\times v(q)L_{00}''(\mathbf{p},k',k'',\omega)\frac{1-\epsilon_n\cos kd}{(k-k')(k-k'')},\quad(11)$$

where L_{00}'' is the imaginary part of L_{00}, $\mathbf{V}_0$ is the velocity of the incident electron, and θ_0 is the angle that the incident electron makes with the z axis. k is used to denote the z component of the momentum transfer in this section while k' and k'' refer to the quantized wave numbers. As mentioned earlier, the last two terms in Eq. (A17) for L_{00} and the last term in Eq. (A18) for S_0 may be neglected. The same is true for the second term in Eq. (A19) for $S_0{}^0$. When the remaining terms are combined one obtains

$$v(q)L_{00}(k',k'')=\frac{p^2+k'^2}{p^2+k^2}\frac{d}{2}[\delta(k'-k'')+\delta(k'+k'')]\times\frac{1-\epsilon(k')}{\epsilon(k')}\frac{p(1-\epsilon(k'))(1-\epsilon(k''))(1-\epsilon_{n'}e^{-pd})}{(p^2+k^2)\epsilon(k')\epsilon(k'')D},\quad(12)$$

where D is given by Eq. (8). The p and ω dependence of D and ϵ has been suppressed.

The first term in Eq. (12) contributes to F only near ω_p. By first integrating over ω and then summing one finds that this term contributes

$$F_p=\pi\omega_p d\quad(13)$$

to F near ω_p. This is exactly the result one obtains from a bulk sample as expected from the discussion in Sec. II. Almost the total contribution to F_p comes from $k'=k'\simeq k$. In order to observe the discreteness of the wave numbers one would have to measure q to order π/d and ω to order $qv_F{}^2/\omega_p d$. This would be incredible accuracy within the limitation $q_F d\gg1$.

The second term in Eq. (12) gives the surface corrections. In the present case, the Born approximation, only terms with $k'=k''$ contribute to F. For $pd>1$ the surface-plasma resonance contributes

$$F_{\text{sp}}=2\sqrt{2}\omega_p p/(p^2+k^2)\quad(14)$$

to F. At this frequency $|p/\tilde{p}|\ll1$ and the wave-number dependence of ϵ is unimportant. It is conceivable that the wave-number dependence of the surface-plasma frequency could be measured. The contribution to F from the surface term near ω_p is given approximately by

$$\delta F_p=-(2\pi\omega_p p/p^2+k^2)\max\{k^2/(p^2+k^2),\ g\omega_p{}^2/(v_F{}^2p^2+g\omega_p{}^2\}.\quad(15)$$

These last two equations are in agreement with Ritchie's[1] results except for the factor in the curly brackets in Eq. (15). This factor would be 1 if the wave-number dependence of ϵ were neglected in calculating D.

For $pd\ll1$ the surface correction to F at ω_p for even k' and k'' is small, of order $(pd)F_{\text{sp}}$. For odd k' and k'' the frequencies of the bulk and surface plasmons are very close together in this limit. Unless g is very small or k is quite large the two resonances overlap each other and the energy loss due to them separately cannot be obtained. It also appears to be impossible to measure momentum losses $p\ll d^{-1}$ using electrons fast enough to satisfy the Born approximation. Thus we shall only state that the contribution to F in this limit is positive, and is proportional to F_{sp} modulated by a factor $(\sin\frac{1}{2}kd)^2$ due to the discreteness of allowed wave numbers.

In reflection experiments measurements are made only on those incident electrons which emerge from the same side of the sample as they entered. The surface-plasma mode has more weight relative to the plasma mode for electrons of lower incident energy in this type of experiment.[4] This happens because lower energy electrons will not penetrate as far into the sample and will excite fewer plasmons. On the other hand, the surface plasmons are primarily excited near the surfaces. This effect can be taken into account in a semi-quantitative manner by using a modified Born approximation in which the wave function of the incident electron decreases as $\exp(-z/l)$ in the slab. F has been calculated with this modification under the assumptions that $d\gg l^{-1}$. It is found that in Eq. (13) for F_p that d is replaced by $\frac{1}{2}l$ and that δF_p and F_{sp} given by Eqs. (14) and (15) are reduced by $\frac{1}{2}$. This is exactly what is expected. It is because of the terms with $k'\neq k''$ that F_{sp} and δF_p are not reduced as much as F_p is.

IV. INTERACTION WITH LIGHT

Some aspects of the response of a thick sample to an incident electromagnetic field are now discussed in the

[11] L. Kadanoff and P. C. Martin, Ann. Phys. (N. Y.) 24, 419 (1963), Appendix A.

gauge $\nabla\cdot\mathbf{A}=\phi=0$. From Maxwell's equations and Eq. (A7) one obtains

$$\left(\epsilon_0\omega^2-c^2p^2+c^2\frac{d^2}{dz^2}\right)E_i(z)=-\frac{\pi e^2}{m^2}\int dz L_{ij}(p,z,\bar{z},\omega)E_j(\bar{z}) \quad (16)$$

for the z dependence of an electric field which varies in $\boldsymbol{\rho}$ and t as $\exp(-i\omega t+i\mathbf{p}\cdot\boldsymbol{\rho})$. The quantity ϵ_0 is $1-(\omega_p/\omega)^2$. The response function L_{ij} is given in the Appendix. Because of the way that it is Fourier transformed, it is most convenient to expand $E(z)$ as

$$E_i(z)=d^{-1}\sum_{n'}E_i(k')\,\mathrm{trig}_i(k'z)\,, \quad (17)$$

where trig_i is the sine for $i=3$ and cosine otherwise. One can verify by direct substitution that

$$E_i(k')=E_{0i}\frac{i(k+i\alpha)}{k^2+k'^2}\left\{(1-\delta_{i,z})+\frac{i(k+i\alpha)}{k'}\delta_{i,z}\right\} \quad (18)$$

describes the z dependence $\exp[iz(k+i\alpha)]$ in the limit as d approaches infinity. As in the last section, k is not discrete; k' and k'' are used to denote the quantized wave numbers.

The transform of E_z given by Eq. (18) is not the one obtained by inverting Eq. (17). In the limit of large d the result may be verified by direct substitution as previously mentioned. It may also be obtained by expanding $\partial E_z/\partial z$ in a cosine series and integrating to find E_z. The reason for the above procedure is that $\nabla\cdot\mathbf{E}$ does not converge if E_z is obtained by inverting Eq. (17).

Using Eq. (18), it is easily seen that terms in $L_{ij}(k'k'')$ which equal some constant times ip_j for $j=1$, 2 and the same constant times k'' for $j=3$, will not contribute to Eq. (16) in the present gauge. All terms which originate from the first term of S_j^0 in Eq. (A19) fall into this category. The terms which do contribute are the first term of Eq. (A17), which is temporarily neglected, and terms due to the second part of S_j^0. The lowest order nonvanishing contribution to L_{ij} is

$$-Z_{ij}pT_i(\mathbf{p}k'\omega)\tilde{R}_j(\mathbf{p}k''\omega)\epsilon^{-1}(\mathbf{p}k'\omega)(p^2+k'^2)^{-1}\,,$$

where $\tilde{R}_j$ is the part of R_j due to the second term of S_j^0. The denominator of R_j is given by Eq. (8) and the numerator by

$$-(2d)^{-1}\sum_{\bar{n}}\bar{T}_j(\mathbf{p},k'',\bar{k},\omega)v(\mathbf{p}\bar{k})\epsilon^{-1}(\mathbf{p}\bar{k}\omega)$$

which is larger for $j=1$, 2, than for $j=3$ by a factor of approximately q/k_F. T and $\bar{T}$ are given in the Appendix. For small wave numbers $T_i(\mathbf{p},k,\omega)$ is given approximately by $2q_iq_F^3/3\pi^2\omega$ and $\bar{T}_j$ by $p_jq_F/\pi\omega$ for $j\neq3$. Thus, to lowest order in the wave numbers L_{ij} is given by

$$\frac{\pi e^2}{m^2}L_{ij}(\mathbf{p},k',k'',\omega)=-Z_{ij}\frac{3\pi}{8q_f}\omega_p^4\frac{q_i'q_j''}{p^2+k'^2}\frac{1}{\epsilon}(\mathbf{p}k'\omega)\left[1-\frac{p}{\tilde{p}}\right]$$
$$[\omega^2-\tfrac{1}{2}\omega_p^2(1-\gamma-ig)-\tfrac{1}{2}p\omega_p^2/\tilde{p}]^{-1}(1-\delta_{j,z})\,, \quad (19)$$

where $\mathbf{q}'=(\mathbf{p},k')$ and $\mathbf{q}''=(\mathbf{p},k'')$.

Now consider the reflection of incident radiation from the $z=0$ surface of the sample. Let the radiation be directed in the x-z plane. If E is perpendicular to the plane of incidence, L_{ij} will contribute nothing. On the other hand, L_{ij} will contribute if E is contained in the plane of incidence. In order to estimate the effect of the surface term E is assumed to be proportional to $\exp[-i\omega t+i\mathbf{p}\cdot\boldsymbol{\rho}+iz(k+i\alpha)]$. Equation (18) and (17) are substituted into Eq. (16) for E_x. A crude equation can be obtained for k and α by multiplying Eq. (16) by $\exp(ikz-\alpha z)$ and integrating over z. This yields the equation

$$\epsilon_0\omega^2+4\pi i\omega\sigma_0-c^2(p^2+k^2-\alpha^2+2ik\alpha)=-4\pi i\omega\sigma_s\,, \quad (20)$$

where

$$\sigma_s=-3i\omega_p^4 2^{-5}[1-p/\tilde{p}][\omega^2-\omega_p^2+ig\omega^2]^{-1}p\alpha$$
$$\times(p+\alpha-ik)^{-1}[\omega^2-\tfrac{1}{2}\omega_p^2(1+\gamma-ig)-\tfrac{1}{2}p\omega_p^2/\tilde{p}]^{-1}. \quad (21)$$

σ_0 is the bulk conductivity and may be thought of as arising from the first term in Eq. (17).

Equation (20) can be solved for α and k. At the surface-plasma frequency σ_s effectively adds a term $+3\times2^{-1/2}\omega_pp/q_Fg$ to the real part of the conductivity. A positive term of this size is also added (subtracted) to the imaginary part of the conductivity for frequencies near and below (above) the resonant frequency. The situation at the plasma frequency is similar except that the contributions are of the opposite sign. If g is small enough a measurable difference in the reflectivities for E in and perpendicular to the plane of incidence could be observed. It has been assumed that $g\gg|\gamma|$.

This model has not been applied to the interaction with light in the limit $pd<1$, a case about which much has been written in the literature.[12] The reason for this is the complication which arises from the anisotropy of the conductivity predicted by this model. For this same reason the above calculation is not correct, although it does suggest that an effect can take place. This problem and a better treatment of band effects are being studied.

ACKNOWLEDGMENTS

The author would like to acknowledge many helpful discussions with J. J. Hopfield and to thank R. C. A. for their hospitality during the final stages of this paper.

[12] R. A. Ferrell (Ref. 2) was the first to discuss this aspect.

APPENDIX

A brief derivation for the response function is given in this Appendix using Green's-function techniques.[13] The single-particle Green's function is defined as

$$G(11') = -i\langle T(\psi(1)\psi^\dagger(1'))\rangle, \quad \text{(A1)}$$

whose arguments n stand for the space-time coordinates (r_n,t_n). The symbol T indicates time ordering and the angular bracket $\langle X\rangle$ means that the expectation value at zero temperature is to be taken. $\psi^\dagger$ and ψ are the electron creation and destruction operators. According to the model described in Sec. I, the noninteracting single-particle Green's function is

$$G(\mathbf{rr}',t-t') = \int \frac{d\omega}{2\pi}\int \frac{d^2p}{(2\pi)^2}\frac{1}{d}\sum_n \times \frac{e^{i\omega(t-t')}\exp i\mathbf{p}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}')\sin kz \sin kz'}{\omega - E(\mathbf{p},k)+i\delta\,\mathrm{sgn}(|q|-q_F)}, \quad \text{(A2)}$$

where δ is a vanishingly small positive quantity and $k=n\pi/d$. The summation over $\mathbf{p}$ has been converted to an integral. The starting point for the calculation is the RPA equation for a two-particle Green's function.[14]

$$L(11',22') = -2iG(12')G(21') - 2i\int d3d3'\, G(13)G(3'1')v(33')L(33',22'), \quad \text{(A3)}$$

where

$$L(11',22') = \sum_{\sigma,\sigma'}\{-i\langle(\psi_\sigma(1)\psi_{\sigma'}(2)\psi_{\sigma'}^\dagger(2')\psi_\sigma^\dagger(1'))\rangle + i\langle T(\psi_\sigma(1)\psi_\sigma^\dagger(1'))\rangle\langle T(\psi_{\sigma'}(2)\psi_{\sigma'}^\dagger(2'))\rangle\}, \quad \text{(A4)}$$

σ and σ' are spin indices, dn denotes the space-time integration $d^3r_n dt_n$, and $v(33')$ is the Coulomb potential multiplied by a delta function in time. G is approximated by the noninteracting Green's function. Results obtained in this Appendix will not be gauge-invariant because the approximation described by Eq. (A3) is not conserving.[15] The response functions may be obtained by first forming an equation for L_ν,

$$L_\nu(11',2) = (\partial/\partial x_2 - \partial/\partial x_{2'})_\nu L(11',22')|_{2'=2}, \quad \text{(A5)}$$

where ν is a four-index, (0, 1, 2, 3) whose last three components i correspond to the x, y, and z axes. $(\partial/\partial x_2 - \partial/\partial x_{2'})_0$ is equal to 1. After solving for L_ν, $L_{\mu\nu}$ is formed.

$$L_{\mu\nu}(1,2) = (\partial/\partial x_1 - \partial/\partial x_{1'})_\mu L_\nu(11',2)|_{1'=1}. \quad \text{(A6)}$$

L_{00} is the density-density correlation function and, except for multiplicative constants, L_{ij}, L_{0j}, and L_{i0} are the current-current, density-current, and current-density correlation functions. For example, in a gauge where the scalar potential is zero, the current induced by an electric field E is[16]

$$J_i(\mathbf{r}) = \frac{-ie^2}{4m^2\omega}\int d^3r' L_{ij}(\mathbf{r},\mathbf{r}')E_j(\mathbf{r}) - \frac{n(\mathbf{r})e^2}{im\omega}E_i(\mathbf{r}). \quad \text{(A7)}$$

In order to solve the equations, L_ν is Fourier-transformed according to the prescription

$$L_\nu(\mathbf{r}_1\mathbf{r}_{1'}\mathbf{r}_2,t_1-t_2) = \int \frac{d^2p}{(2\pi)^2}\frac{d^2p'}{(2\pi)^2}\frac{d\omega}{(2\pi)}\frac{1}{d^3}\sum_{n,n',n''}\{n+n'+n''\}L_\nu(\mathbf{p},\mathbf{p}',k,k',k'',\omega) \times \exp[-i\omega(t_1-t_2)+i\mathbf{p}\cdot(\boldsymbol{\rho}_1-\boldsymbol{\rho}_2)-i\mathbf{p}_1'(\boldsymbol{\rho}_2-\boldsymbol{\rho}_{1'})]\sin kz_1 \sin k'z_{1'}\,\mathrm{trig}_\nu k''z_2, \quad \text{(A8)}$$

after setting $t_1'=t_1$ and using the fact that the system is translationally invariant in t and ρ. Trig$_\nu$ is the sine function for $\nu=3$ and the cosine function for other ν, and $\{n+n'+n''\}$ restricts the summation to even values of the sum of the integers. Using this transform, an equation for L_ν is formed which is algebraic in the p and ω variables. For example, the equation for L_0 reads

$$L_0(\mathbf{p}'+\mathbf{p},\mathbf{p},k,k,'k'',\omega) = B(\mathbf{p}+\mathbf{p}',k;\mathbf{p}',k';\omega)\{\tfrac{1}{4}d[\delta(k-k'+k'')+\delta(k-k'-k'')-\delta(k+k'+k'')-\delta(k+k'-k'')] - \tfrac{1}{2}R_0(\mathbf{p}k''\omega)(1-\epsilon_n e^{-pd})p\{[p^2+(k-k')^2]^{-1}-[p^2(k+k')^2]^{-1}\} + \tfrac{1}{2}\{S_0(\mathbf{p},k-k',k'',\omega)v(\mathbf{p},k-k')-S_0(\mathbf{p},k+k',k'',\omega)v(\mathbf{p},k+k')\}, \quad \text{(A9)}$$

where ϵ_n is $(-1)^n$ and S, R, and $B(\mathbf{q}_1;\mathbf{q}_2;\omega)=B(\bar{n}_1,k_1;\mathbf{p}_2k_2;\omega)$ are defined as

$$B(\mathbf{q}_1\mathbf{q}_2\omega) = 2[f(\mathbf{q}_1)-f(\mathbf{q}_2)][E(\mathbf{q}_1)-E(\mathbf{q}_2)-\omega-i\delta]^{-1} \quad \text{(A10)}$$

if k_1, $k_2\neq 0$ and equals zero if k_1 or k_2 does. f is the Fermi (step) function.

[13] The definition of G and its Fourier transform in time is the same as that used for zero temperature in A. A. Abrikorov, L. P. Gorkov, and I. E. Dzaloshinski, *Methods of Quantum Field Theory in Statistical Mechanics*, translated by R. A. Silverman (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1963).

[14] See, for example, L. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W. A. Benjamin, Inc., New York, 1962), Chap. 8–2.

[15] Reference 12, Chap. 6–3.

[16] The electrical transport coefficients are related to the correlation function in P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959).

$$S_\mu(\mathbf{p},k,k',\omega)=d^{-1}\sum_{\bar{n}} L_\mu(\mathbf{p},\bar{k}+k,\bar{k},k',\omega)\{n+\bar{n}\}, \tag{A11}$$

$$R_\mu(\mathbf{p}k'\omega)=d^{-1}\sum_{\bar{n}} S_\mu(\mathbf{p},\bar{k},k',\omega)v(\mathbf{p}\bar{k})\{\bar{n}+n'\}. \tag{A12}$$

In the equations for L_i only the first term in Eq. (A9) is changed and S_0 and R_0 becomes S_i and R_i.

The derivation of Eq. (A9) is tedious but straightforward except for the Fourier transform of $v(r)$. Since the electrons are confined in the z direction, $v(r)$ can be transformed according to the algorithm

$$v(r)=\int\frac{d^2p}{(2\pi)}\frac{1}{2d}\sum_n \bar{v}(pk)\exp(i\mathbf{p}\cdot\boldsymbol{\varrho})e^{ikz}, \tag{A13}$$

$$\bar{v}(pk)=\int d^2\rho\int dz\, v(r)\exp(-i\mathbf{p}\cdot\boldsymbol{\varrho})e^{-ikz}, \tag{A14}$$

where the z integration runs from $-d$ to $+d$. In the last equation the ρ integration is done in polar coordinates with the angular integration performed first. The radial integral is then a limiting case of a tabulated integral.[17] The z integration is then trivial yielding

$$\bar{v}(pk)=v(pk)[1-\epsilon_n e^{-pd}], \tag{A15}$$

where $v(\mathbf{p},k)$ is $4\pi e^2/(p^2+k^2)$. The summations necessary in obtaining Eq. (A9) are straightforward if they are broken into partial fractions.

After more tedious labor, one obtains the following exact equation for $L_{\mu\nu}$.

$$L_{\mu\nu}(\mathbf{rr}',\omega)=\int\frac{d^2p}{(2\pi)^2}\frac{1}{d^2}\sum_{n,n'}\{n+n'\}L_{\mu\nu}(p,k,k',\omega)\exp i\mathbf{p}\cdot(\boldsymbol{\varrho}-\boldsymbol{\varrho}')\,\mathrm{trig}_\mu(kz)\,\mathrm{trig}_\nu(k'z'). \tag{A16}$$

$$\begin{aligned}L_{\mu\nu}(\mathbf{p},k,k',\omega)=Z_{\mu\nu}\Bigg\{&\int\frac{d^3\bar{q}}{(2\pi)^3}B(\bar{\mathbf{q}}+\mathbf{q},\bar{\mathbf{q}})(2\bar{\mathbf{q}}+\mathbf{q})_\mu(2\bar{\mathbf{q}}+\mathbf{q})_\nu\frac{d}{2}[\delta(k-k')+\epsilon_\mu(k+k')]+T_\mu(k)v(k)S_\nu(k,k')-C_\mu(\mathbf{p}k)R_\nu(k')\\&-\frac{1}{4}\int\frac{d^2\bar{p}}{(2\pi)^2}[B(\bar{\mathbf{p}}+\mathbf{p},\tfrac{1}{2}(k+k');\bar{\mathbf{p}},\tfrac{1}{2}(k-k'))+\epsilon_\mu\epsilon_\nu B(\bar{\mathbf{p}}+\mathbf{p},\tfrac{1}{2}(k-k');\bar{\mathbf{p}},\tfrac{1}{2}(k+k'))]\\&[(2\bar{\mathbf{q}}+\mathbf{q})_\mu(1-\delta_{\mu,3})+k'\delta_{\mu,3}][(2\bar{\mathbf{q}}+\mathbf{q})_\nu(1-\delta_{\nu,3})+k\delta_{\nu,3}][1-\delta(k+k')][1-\delta(k-k')]\\&-\int\frac{d^2\bar{q}}{(2\pi)^3}(2\bar{\mathbf{q}}+\mathbf{q})_\mu B(\bar{\mathbf{q}}+\mathbf{q},\bar{\mathbf{q}})v(2\bar{k}+k)S_\nu(2\bar{k}+k,k')\Bigg\}.\end{aligned} \tag{A17}$$

The p and ω dependence of functions in this equation has been suppressed where possible and $(2d)^{-1}\Sigma_{\bar{n}}$ has been denoted by $(2\pi)^{-1}\int dq_z$ for convenience. $(2\bar{\mathbf{q}}+\mathbf{q})_0$ is 1 and ϵ_μ is (-1) if $\mu=3$ and $+1$ otherwise. $Z_{\mu\nu}$ equals ϵ_μ times a factor of i for each μ and ν which is 1 or 2. S_μ is the solution to the equation

$$S_\mu(kk')=S_\mu^0(kk')-R_\mu(k')C_0(k)\epsilon^{-1}(k)-(2d)^{-1}\sum_{\bar{n}} B(\mathbf{p},\bar{k}+k,\bar{k})S_\mu(\bar{k}k')v(2\bar{k}+k), \tag{A18}$$

where

$$S_\mu^0(kk')=\tfrac{1}{2}d[\delta(k-k')+\epsilon_\mu\delta(k+k')]T_\mu(k)\epsilon^{-1}(k)-\epsilon^{-1}(k)\bar{T}_\mu(p,k,k')[1-\delta(k+k')][1-\delta(k-k')]. \tag{A19}$$

R_μ is given by Eq. (A11) and the rest of the functions are

$$B(\mathbf{p},\bar{k}+k,\bar{k},\omega)=\int\frac{d^2\bar{p}}{(2\pi)^2}B(\bar{\mathbf{q}}+\mathbf{q},\bar{\mathbf{q}},\omega), \tag{A20}$$

$$T_\mu(\mathbf{p}k\omega)=\int\frac{d^3\bar{q}}{(2\pi)^3}B(\bar{\mathbf{q}}+\mathbf{q},\bar{\mathbf{q}},\omega)(2\bar{\mathbf{q}}+\mathbf{q})_\mu, \tag{A21}$$

$$C_\mu(\mathbf{p}k\omega)=p(1-\epsilon_n e^{-pd})\left\{\frac{T_\mu(\mathbf{p}k\omega)}{p^2+k^2}-\int\frac{d^3\bar{q}}{(2\pi)^3}\frac{B(\bar{\mathbf{q}}+\mathbf{q},\bar{\mathbf{q}}\cdot\omega)(2\bar{\mathbf{q}}+\mathbf{q})_\mu}{p^2+(2\bar{k}+k)^2}\right\}, \tag{A22}$$

$$\bar{T}_\mu(\mathbf{p},k,k',\omega)=\frac{1}{2}\int\frac{d^2\bar{p}}{(2\pi)^2}[B(\bar{\mathbf{p}}+\mathbf{p},k;\bar{\mathbf{p}},k')+\epsilon_\mu B(\bar{\mathbf{p}}+\mathbf{p},k';\bar{\mathbf{p}},k)][(2\bar{\mathbf{q}}+\mathbf{q})_\mu(1-\delta_{\mu,z})+k\delta_{\mu,z}], \tag{A23}$$

and

$$\epsilon(\mathbf{p}k\omega)=1=T_0(\mathbf{p}k\omega)v(\mathbf{p}k). \tag{A24}$$

[17] A. Erdélyi, *Tables of Integral Transforms* (McGraw-Hill Book Company, Inc., New York, 1954), Vol. II.