Effect of impurity scattering on the distribution function in two-dimensional Fermi systems

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Effects of impurity scattering on spectral properties of a two-dimensional electron gas are investigated within the Born approximation. In particular, the zero-temperature momentum distribution function is obtained and compared with the corresponding function at finite temperature without scattering. This enables one to conclude that impurity scattering can be as important as finite temperature in modifying electronic spectral properties. The importance of the dimension in such a calculation is pointed out, and the relevance of these results for silicon inversion layers is discussed.

I. INTRODUCTION

Recently it was shown by Stern[1] that the temperature dependence of the low temperature (1 – 50 K) resistivity of n-channel inversion layers on Si-SiO_2 metal-oxide–semiconductor structures can be quantitatively explained on the basis of a finite-temperature modification of the electron screening of charged impurity scattering at the Si-SiO_2 interface. This is significant, since earlier theoretical attempts[2] to understand the low-temperature mobility of these systems on the basis of phonon scattering alone gave results whose temperature-dependent parts are much smaller than those experimentally observed. The electronic polarizability function is mainly affected by finite temperature for wave vectors around $2k_F$, where k_F is the Fermi wave vector. This, as Stern explicitly demonstrates, gives rise to a significant temperature dependence in mobility even for low temperatures $T << T_F$, since the $2k_F$ scattering of electrons across the Fermi circle in two dimensions is a very effective Coulomb scattering process for transport properties.

Stern's calculation taking into account the finite wave vector, finite temperature screening of Coulomb, and surface roughness scattering (but no phonon scattering) is in good quantitative agreement with experimental results.[3] One effect not included in the calculation, however, is the modification of screening by impurity scattering itself. Impurity scattering acts somewhat like temperature by providing a broadening mechanism which smooths out the sharp discontinuity in the Fermi distribution function at $k = k_F$. This rounding is then responsible for modifying the screening function around $k = 2k_F$. Thus, scattering is likely to round the sharp corner in the two-dimensional screening parameter at very low temperatures in a way similar to the finite-temperature effect itself. It was already noted in Ref. 1 that this could modify the calculated temperature dependence of the resistivity, so in view of the excellent agreement between the calculation and the experimental results it becomes important to investigate the effect of impurity scattering on electronic spectral properties and to calculate the modification of screening produced by scattering.

In this paper we take the first step in that direction by calculating the effect of impurity scattering on the momentum distribution function $n(k)$ of a completely two-dimensional electron gas (2DEG) comparing the change in $n(k)$ particularly around $k = k_F$ produced by scattering and finite temperature individually. Thus we do not consider the realistic quasi-two-dimensional inversion layer as was done in Ref. 1. Our intention here is only to compare the relative importance of impurity broadening and thermal broadening in smoothing the Fermi distribution function of a 2DEG for realistic numbers

of electron and impurity density. We find that the impurity scattering has a rather significant effect on the distribution function, and its effect on screening probably should not be neglected in an accurate mobility calculation.

A calculation of the effect of impurity scattering on the electronic polarizability of a three-dimensional electron gas was carried out by de Gennes.[4] The difference between two and three dimensions makes a straightforward application of de Gennes' method impossible in two dimensions because of divergence difficulties. We shall indicate how a divergence-free calculation can be carried out in two dimensions. Even though this divergence problem is of a somewhat technical nature, it makes the study of the effect of scattering on screening a more difficult problem in two dimensions than in three. This is why we restrict ourselves in this paper to the effect on the single-particle distribution function and leave for future study the screening problem which involves calculating two-particle correlation functions.

II. THE DISTRIBUTION FUNCTION IN BORN APPROXIMATION

The self-energy of electrons in dimension d due to the electron-impurity interaction alone is given in Born approximation by

$$M(\vec{k},i\omega_n) = N_i \int \frac{d^d p}{(2\pi)^d} |u(\vec{k}-\vec{p})|^2 \times G_0(\vec{p},i\omega_n) \ , \tag{1}$$

where G_0 is the noninteracting electronic Green's function and u is the static electron-impurity interaction. N_i is the impurity concentration per unit d-dimensional volume. The impurities are assumed to be randomly distributed fixed point charges, and in Eq. (1) ensemble averaging over all configurations has been carried out. We take $\hbar = 1$ throughout this paper. The noninteracting Green's function G_0, defined at odd imaginary frequencies $i\omega_n = (2n+1)\pi i/\beta$, where $\beta = (k_B T)^{-1}$, is given by

$$G_0(\vec{k},i\omega_n) = \frac{1}{i\omega_n - k^2/2m + \mu} \ , \tag{2}$$

where μ is the chemical potential of the system and we have assumed a simple parabolic energy dispersion.

The electron-impurity interaction u should be the screened Coulomb interaction in d dimensions. Since impurity scattering affects the screening of the system, the problem should really be solved in such a way that screening and the scattering potential are determined self-consistently. Such calculations[5,6] have been carried out for a 2DEG under a strong magnetic field. For the problem under considerations this would be a difficult task. Here we only go to first order and follow de Gennes[4] in assuming a short-range model potential for the electron-impurity interaction. We shall establish that this model is rather good for the system we are investigating. A short-range delta-function potential in real space implies a wave-vector-independent u in reciprocal space: $u(q) = C$, where C is a constant parameter at this stage.

Using this interaction in Eq. (1), we get the following real and imaginary parts of the (retarded) self-energy:

$$M(\vec{k},i\omega_n \to \omega + i\eta) = \Delta(\omega) - i\Gamma(\omega) \tag{3}$$

$$\Gamma(\omega) = \begin{cases} \dfrac{mN_i|C|^2}{2\pi} H(\omega+\mu)[2m(\omega+\mu)]^{1/2} & \text{in 3D} \\ \dfrac{mN_i|C|^2}{2} H(\omega+\mu) & \text{in 2D} \end{cases} \tag{4}$$

and

$$\Delta(\omega) = \begin{cases} \dfrac{N_i|C|^2}{2\pi^2} \displaystyle\int_0^\infty dp \frac{p^2}{\omega+\mu-p^2/2m} & \text{in 3D} \\ \dfrac{N_i|C|^2}{2\pi} \displaystyle\int_0^\infty dp \frac{p}{\omega+\mu-p^2/2m} & \text{in 2D} \end{cases} \tag{5}$$

where $H(x)$ is the Heaviside step function.

The short-range model for the interaction makes the self-energy independent of wave vector. Two features of the self-energy are evident from Eqs. (3)–(5): (i) The imaginary part or broadening $\Gamma(\omega)$ is different in two and three dimensions. Γ is essentially constant in 2D whereas it increases as the square root of energy in 3D. (ii) The real part of the self-energy $\Delta(\omega)$ is "ultraviolet" divergent in both cases; the divergence is linear in 3D and logarithmic in 2D. This divergence is of course a result of the short-range model potential. For very large wave vectors screening must be ineffective and $u(q)$

must fall off as q^{1-d} for $q \to \infty$, thus making the integral for $\Delta(\omega) \sim \int dp\, p^{-d-1}$ convergent for both $d = 2$ and 3.

In 3D, de Gennes[4] circumvented this artificial divergence by subtracting and adding the $\Delta(\omega + \mu = 0)$ contribution to the self-energy. Clearly

$$\Delta_0 = \Delta(\omega + \mu = 0) \propto \int_0^\infty dp \frac{p^2}{p^2/2m}$$

is the linearly divergent term giving the shift of the whole band, and we have

$$\Delta(\omega) = \Delta_0 + \frac{mN_i |C|^2}{\pi^2} \times \int_0^\infty dp \frac{\omega + \mu}{\omega + \mu - p^2/2m} , \tag{6}$$

where the integral is now covergent and the divergence hidden in the physically irrelevant Δ_0 term can be neglected in further considerations. This is the crux of de Gennes' argument, and he could then solve the problem even for the polarizability.

However, this technique does not work in 2D, since subtraction of $\Delta_0 = \Delta(\omega + \mu = 0)$ in Eq. (5) introduces an "infrared" divergence:

$$\Delta(\omega) = \Delta_0 + \frac{mN_i |C|^2}{\pi} \times \int_0^\infty dp \frac{\omega + \mu}{p(\omega + \mu - p^2/2m)} , \tag{7}$$

where the integral is now logarithmically divergent for $p \to 0$. Instead we use a cutoff procedure to avoid the "ultraviolet" divergence in (5): We assume that $u(\vec{q})$ vanishes for wave vectors q larger than some (large) cutoff value q_c, i.e., $u(\vec{q}) = CH(q_c - q)$. For wave vectors $\vec{k}$ much smaller than q_c the self-energy is still independent of $\vec{k}$, and we get from Eq. (1)

$$\Delta(\omega) = \frac{N_i |C|^2}{2\pi^2} \times \left[-q_c + \int_0^{q_c} dp \frac{2m(\omega + \mu)}{\omega + \mu - p^2/2m} \right] \quad \text{for 3D,} \tag{8}$$

$$\Delta(\omega) = -\frac{mN_i |C|^2}{2\pi} \ln \left| \frac{\omega + \mu - q_c^2/2m}{\omega + \mu} \right| \quad \text{for 2D.} \tag{9}$$

Comparing Eqs. (6) and (8) we see that they are equivalent in the limit of $q_c \to \infty$ with $\Delta_0 = -q_c$, so that the cutoff procedure is completely equivalent to de Gennes' renormalization method as we expected on physical grounds. On the other hand, for two dimensions the cutoff gives a convergent result in contrast to the renormalization in Eq. (7).

We can now obtain the spectral weight function $\rho(\vec{k},\omega)$ for the 2DEG from the relation[7]

$$\rho(\vec{k},\omega) = -2\,\mathrm{Im}G(\vec{k}, i\omega_n \to \omega + i\eta), \quad \eta \to 0+ \tag{10}$$

where $G(\vec{k},i\omega_n)$ is the interacting Green's function. The latter can be obtained from Dyson's equation:

$$G(\vec{k},i\omega_n) = [G_0^{-1}(\vec{k},i\omega_n) - M(\vec{k},i\omega_n)]^{-1} . \tag{11}$$

From Eqs. (10), (11), and (3) we have

$$\rho(\vec{k},\omega) = \frac{2\Gamma(\omega)}{[\omega + \mu - k^2/2m - \Delta(\omega)]^2 + \Gamma(\omega)^2} . \tag{12}$$

Setting $A = mN_i |C|^2/2$ we obtain from Eqs. (4) and (9):

$$\rho(\vec{k},\omega) = 2AH(\omega + \mu) \Big/ \left[\left[\omega + \mu - \frac{k^2}{2m} + A \ln \left| \frac{\omega + \mu - q_c^2/2m}{\omega + \mu} \right| \right]^2 + A^2 \right] . \tag{13}$$

The momentum distribution function can be found by summing $\rho(\vec{k},\omega)$ over the energy:

$$n(k) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \rho(k,\omega) f(\omega) , \tag{14}$$

where $f(\omega) = (1 + e^{\beta\omega})^{-1}$ is the thermal weight factor for fermions. In the zero-temperature limit we finally get

$$n(k)=\frac{A}{\pi}\int_{-\infty}^{0}H(\omega+\mu)d\omega\Big/\left[\left[\omega+\mu-\frac{k^2}{2m}+\frac{A}{\pi}\ln\left|\frac{\omega+\mu-q_c^2/2m}{\omega+\mu}\right|\right]^2+A^2H(\omega+\mu)\right] . \quad (15)$$

The logarithmic singularity for $\omega=-\mu$ and the possible bound states for $\omega<-\mu$ suggest that for the numerical evaluation we calculate

$$n(k)=1-\frac{A}{\pi}\int_{0}^{\infty}d\omega\Big/\left[\left[\omega+\mu-\frac{k^2}{2m}+\frac{A}{\pi}\ln\left|\frac{\omega+\mu-q_c^2/2m}{\omega+\mu}\right|\right]^2+A^2\right] , \quad (16)$$

where we have used the relation[7]

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\rho(k,\omega)=1 .$$

III. RESULTS AND DISCUSSION

In order to evaluate $n(k)$ numerically from Eq. (16), we need to know μ, q_c, and $A=mN_i|C|^2/2$. The chemical potential μ is obtained by requiring that the total number of electrons

$$N_s=g\int\frac{d^2k}{(2\pi)^2}n(k)$$

be equal to the given density, where g is the degeneracy factor. The parameters C and q_c are obtained from the long-wavelength statically screened Coulomb interaction in two dimensions,[8]

$$u(\vec{q})=-\frac{ee_i}{2\bar{\epsilon}(q+q_{\rm TF})} , \quad (17)$$

where e_i is the impurity charge; $\bar{\epsilon}$ is the static background permittivity, and $q_{\rm TF}$, the two-dimensional Thomas-Fermi wave number, is given (for $q<2k_F$) by

$$q_{\rm TF}=g\frac{me^2}{4\pi\bar{\epsilon}} . \quad (18)$$

A typical wave vector q in Eq. (17) is of the order of the Fermi wave vector $k_F=(4\pi N_s/g)^{1/2}$. For an n-type inversion layer on Si(100) with $g=4$, $m=0.19m_e$, $\bar{\epsilon}=7.8\epsilon_0$, $q_{\rm TF}$ is much greater than k_F for normal values of N_s ($1-3\times10^{12}$ cm^{-2}) in the metallic regime. This enables us to neglect the q dependence in Eq. (17) and take the long-wavelength limit

$$u(\vec{q})\simeq-\frac{ee_i}{2\bar{\epsilon}q_{\rm TF}}=C . \quad (19)$$

Within this model a reasonable value for the cutoff wave vector q_c will be $q_{\rm TF}$. In the results presented below we have used these values, taking $e_i=e$ and evaluating $n(k)$ by numerical integration of Eq. (16).

In Fig. 1 we show our results for the distribution function $n(k)$ as a function of k/k_F for $N_s=10^{12}$ cm^{-2} and $N_i=10^{11}$ cm^{-2}. The curve $T=0$ shows the zero-temperature Fermi distribution, $n(k)=H(k_F-k)$. The curve denoted n_I is the result of Eq. (16), i.e., the zero-temperature distribution function in the presence of impurity scattering. For comparison, we also depict the finite-temperature Fermi function

$$n_T=1/\{1+\exp[(k^2/2m-\mu)/k_BT]\}$$

for a temperature T_I equivalent to the broadening produced by impurity scattering, i.e.,

$$k_BT_I\equiv\Gamma=mN_i|C|^2/2 . \quad (20)$$

For the parameters chosen $T_I=5.7$ K. This is a

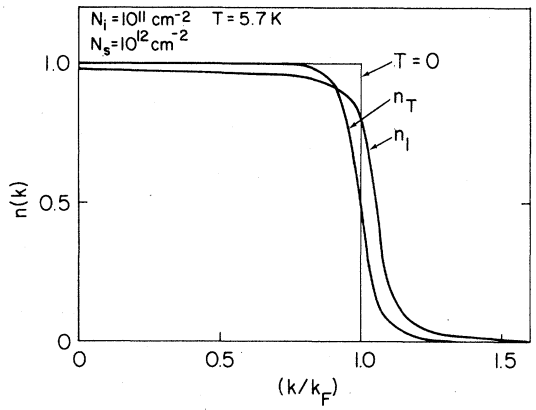

FIG. 1. Momentum distribution function $n(k)$ of a two-dimensional electron gas shown as a function of k/k_F, where k_F is the Fermi wave vector. The curve denoted $T=0$ is the zero-temperature no-scattering result; the one denoted n_I is the zero-temperature result with impurity scattering; the curve labeled n_T is the equivalent finite-temperature distribution function. $N_s=10^{12}$ cm^{-2} and $N_i=10^{11}$ cm^{-2}.

low temperature compared with the Fermi temperature T_F which is 73 K for $N_s = 10^{12}$ cm^{-2}, and it turns out that the chemical potential is not much different from the Fermi energy of the noninteracting system.

From the figure we conclude that the scattering effect on the single-particle distribution function is at least as important as the equivalent finite-temperature effect itself. We would therefore expect that the contribution of impurity scattering to rounding the sharp corner at $2k_F$ in the two-dimensional polarizability is as important as the finite temperature itself. Thus one should include scattering effects in screening along with the finite temperature in doing an accurate mobility calculation for inversion-layer carriers.

In this paper we have considered the simplest short-range model of electron-impurity scattering that is free from divergence and have shown that scattering effects are comparable with finite temperature in modifying the single-particle spectral properties of a 2DEG. We have pointed out the necessary difference between our two-dimensional calculation and the earlier work of de Gennes[4] on three-dimensional systems. An immediate improvement of our work would be the inclusion of the correct statistically screened interaction for $u(\vec{q})$ rather than the short-range model. This can be done without much difficulty within the random-phase approximation.[8] But in view of the large screening wave vector q_{TF} the result of such a calculation cannot differ much from the results reported here. We are presently investigating the more relevant question of the effect of scattering on screening itself in two dimensions.

Very recently Kawaguchi *et al.*[9] have measured the temperature dependence of mobility in silicon (100) n-channel inversion layers in the temperature range of 1.5 – 70 K. They report mobilities having a power law behavior closer to $1/T^2$ rather than the $1/T$ dependence predicted by Stern[1] and observed by Cham and Wheeler.[3] This discrepancy is suggestive of the role played by impurity scattering in modifying the screening and consequently in affecting experimental mobilities, providing additional incentive for studying the role of impurity scattering on spectral properties of 2DEG.

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