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Thermoelectric properties of the interacting two dimensional electron gas in the diffusion regime

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We demonstrate that kinetic coefficients related to thermoelectric properties of the two dimensional electron gas in the diffusive regime are strongly influenced by electron-electron interaction. As an example we consider the thermoelectric coefficients of the diluted two-dimensional electron gas in Si(100) MOSFET's in the presence of charged-impurity scattering. We find that the screening anomaly at $q = 2k_{\mathrm{F}}$, also responsible for Friedel oscillations, leads at low electron densities to a large change in the thermoelectric coefficient for the thermopower.

Since a long time thermoelectric effects in metals are considered in textbooks, see for instance the book by Ashcroft and Mermin [1]. Nevertheless, all known results of explicit calculations for two dimensional metals are made within the random-phase approximation and are, therefore, only valid for weak electron-electron interaction, which means for very high electron densities [2]. In a number of publications [3–7] the attempt was made to describe real experiments and these results were extrapolated down to low electron density where the Coulomb interaction is strong. We argue in this paper that an important term for the calculation of thermoelectric coefficients was neglected in this extrapolation.

The present calculation demonstrates that the interaction leads to a strong change in the kinetic characteristics of the two dimensional electron gas, such that all textbook predictions for the Seebeck and the Peltier effect became invalid in the limit of low electron densities. From experiment [8–10] and the theory [11–13] it is well known that electron-electron interaction is the origin of a significant change in the electron dispersion law. The influence of interaction on kinetic coefficients is an additional effect which is not related to a change of the dispersion law of electrons.

The presence of temperature T and electric potential gradients (electric field $\mathbf{E}$) in the metallic system is accompanied by the flow of an electric current $\mathbf{I}$ and a heat current $\mathbf{J}$:

$$\begin{gathered}\mathbf{I} = L^{11}\mathbf{E} + L^{12}(-\nabla T),\\ \mathbf{J} = L^{21}\mathbf{E} + L^{22}(-\nabla T),\\ L^{21} = TL^{12}.\end{gathered} \tag{1}$$

In the heat transfer phonons prevail at high temperatures and thermoelectric effects are caused by the electron-phonon interaction. In the low temperature limit electrons give the main contribution to the heat flow and the thermoelectric effects at low temperatures are caused by the diffusion of electrons.

Below we discuss thermoelectric effects due to diffusion in the two dimensional electron gas in the presence of electron-electron interaction. At low electron densities n the interaction effects become very large. In the best two dimensional electron systems [14] the value of dimensionless Wigner–Seitz parameter $r_s = 1/(\pi n a_{\mathrm{B}}^2)^{1/2}$, describing the importance of the interaction effects, is about 10. Here a_{B} is the effective Bohr radius.

Parameter $r_s = 10$ means that the potential energy exceeds the Fermi energy (kinetic energy) by about one order of magnitude. Recently very clear expressed evidences of the strong electron-electron interaction were experimentally observed in Si-MOSFETs (see e.g. Refs. [8–10]). Having this fact in mind we will apply our consideration to (100) Si-MOSFET with high mobility. Of course our results will be valid for other two dimensional electron and hole system.

To the best of our knowledge thermopower calculations in the low density range with strong electron-electron interaction were never realized, despite the fact that the experimental activity in two-dimensional electron systems is directed in lowering the electron density. We restrict our consideration to the region of low electron densities, where the system is still chacterized by a metallic conductivity $\sigma \gg e^2/h$. We consider a simple model of a two-dimensional electron system in the metallic regime and we use the relaxation-time approximation. A gas of Landau quasiparticles has, renormalized by interaction effects, a mass m and a thermodynamic density of states ρ_{F} [15]. In our calculation the heat transfer due to the contribution of low energy collective modes [16] is neglected. Having in mind a low electron density system we suppose charged-impurity scattering by impurities randomly distributed at the $\mathrm{Si/SiO_2}$ interface with an impurity concentration n_i. The extension effects of the electron wave function into the silicon are described by the formfactor $F_i(q)$ for the electron-impurity interaction and by $F(q)$ for the electron-electron interaction.

The appearance of thermoelectric effects is caused by the fact that the diffusion coefficient near the Fermi level is a function of the energy. A temperature gradient produces two diffusion streams of electrons: "cold" electrons moves along the temperature gradient and "hot" ones in the opposite direction. If the diffusion coefficient is independent of energy, charge transfer is absent. In the case of an energy independent transport scattering time the diffusion coefficient increases with energy, which leads to a charge flow opposite to the temperature gradient, i.e., to the appearance of a charge flow typical for ideal electron system. The contribution from an energy dependent transport scattering time should be added to this term.

For a strong electron-electron interaction the screening function and the transport scattering time show a peculiar behavior at the Fermi energy. Scattering processes for electrons below and above the Fermi level are different due to the difference in the screening properties [17, 18] which can be also interpreted as additional scattering due to Friedel oscillations for high energy electrons [19]. On the first glance this peculiar behavior of the screening function gives only small contributions to the transport scattering time and can be omitted for zero temperature [17, 18]. However, the contribution to the energy dependence of the diffusion coefficient has the same order of magnitude as other terms and is therefore very important. This effect was never considered in the past and will be shown in the following.

Below we show that the "ideal electron system" contribution to the energy dependence of the diffusion coefficient for a strong electron-electron interaction is compensated in part by the energy dependence of the transport scattering time. As a result the Seebeck effect and Peltier effect at low electron densities are expected to be significantly smaller than those for a non-interacting electron gas and even might change the sign [20].

Thermoelectric coefficients are sensitive to the energy dependence of the transport scattering time and are equal to

$$L_d^{12}=\frac{L_d^{21}}{T}=\frac{g_v e}{2\pi^2}\iint \mathbf{v}_k\mathbf{v}_k\tau_0(\varepsilon)\frac{\varepsilon-\varepsilon_{\mathrm{F}}}{T}\frac{dS}{|v_k|}\left(-\frac{\partial f^0}{\partial\varepsilon}\right)d\varepsilon, \tag{2}$$

where v_k is the electron velocity, $dS=|k|d\phi$, f^0 is the Fermi–Dirac distribution function, and g_v is the valley degeneracy.

The transport scattering time $\tau_0(\varepsilon)$ for a particle of energy ε in lowest order of the random potential $\langle|U(q)|^2\rangle$ is given by [17, 21]

$$\frac{1}{\tau_0(\varepsilon)}=\frac{1}{2\pi\hbar\varepsilon}\int_0^{2k}dq\frac{q^2}{(4k^2-q^2)^{1/2}}\frac{\langle|U(q)|^2\rangle}{\epsilon(q)^2}, \tag{3}$$

where $\langle|U(q)|^2\rangle=n_iV(q)^2F_i(q)^2$ with $V(q)=2\pi e^2/\epsilon_L q$, and $\epsilon_L=\frac{1}{2}(\epsilon_{sc}+\epsilon_{ins})$ is the dielectric constant of the background material [21].

For a non-interacting electron gas with a short-range random potential as disorder the time τ_0 is independent of energy and only the "ideal electron system" contribution to the thermoelectric coefficients exists. In this case the thermopower is given by the well known expression

$$S_{d0}=-\frac{L^{12}}{L^{11}}=-\frac{L^{12}}{\sigma_0}=-\frac{\pi g_v k_{\mathrm{B}}^2 mT}{3en},\quad k_{\mathrm{B}}T\ll\varepsilon_{\mathrm{F}}. \tag{4}$$

Here m is effective electron mass.

With the aim to take into account the screening of impurities and especially the anomalous screening for $q>2k_{\mathrm{F}}$ we write

$$\epsilon(q)=\epsilon_1(q)\left\{1-\frac{V(q)[1-G(q)]\rho_{\mathrm{F}}F(q)}{\epsilon_1(q)}\left(1-\frac{4k_{\mathrm{F}}^2}{q^2}\right)^{1/2}\Theta(q^2-4k_{\mathrm{F}}^2)\right\}, \tag{5}$$

where $\epsilon(q)$ is the screeing function of the two dimensional electron system, $G(q)$ describes the local-field correction for exchange and correlations effects not taken into account in the random-phase approximation [22], $\Theta(x)$ is the step function with $\Theta(x)=1$ for $x\geq 0$ and $\Theta(x)=0$ for $x<0$, $\epsilon_1(q)$ is defined by

$$\epsilon_1(q)=1+V(q)F(q)[1-G(q)]\rho_{\mathrm{F}}. \tag{6}$$

We use for the explicit calculation the local-field corrections in the Hubbard (H) approximation $G(q)=G_{\mathrm{H}}(q)$ where an analytical expression is available as

$$G_{\mathrm{H}}(q)=\frac{1}{2g_v}\frac{q}{(q^2+k_{\mathrm{F}}^2)^{1/2}}. \tag{7}$$

For Si(100) MOSFET structures the valley degeneracy factor is $g_v = 2$.

With Eqs. (5), (6) we can write inverse transport scattering time as

$$\frac{1}{\tau_0(\varepsilon)} = \frac{1}{\tau_0(\varepsilon_{\rm F})} + \frac{1}{\tau_1(\varepsilon)}. \qquad (8)$$

For low temperatures only terms proportional to $(\varepsilon - \varepsilon_{\rm F})/\varepsilon_F$ need to be taken into account in the energy development of the transport scattering time in Eq. (8). Only these terms will be important for the calculation of L^{ij} for low temperatures.

We evaluate the energy independent part as

$$\frac{1}{\tau_0(\varepsilon_{\rm F})} \simeq \frac{4m}{\pi\hbar^3}\frac{\langle|U(2k_{\rm F})|^2\rangle}{[\epsilon_1(2k_{\rm F})]^2}\int_0^1 \frac{x^2dx}{(1-x^2)^{1/2}} = \frac{m}{\hbar^3}\frac{\langle|U(2k_{\rm F})|^2\rangle}{[\epsilon_1(2k_{\rm F})]^2}. \qquad (9)$$

The contributions to $1/\tau_1(\varepsilon)$ consist of two terms:

$$\frac{1}{\tau_1(\varepsilon)} \simeq (\varepsilon - \varepsilon_{\rm F})\frac{m}{\hbar^3}\frac{\partial}{\partial\varepsilon}\left[\frac{\langle|U(2k)|^2\rangle}{[\epsilon_1(2k)]^2}\right]_{\varepsilon=\varepsilon_{\rm F}} + \frac{\varepsilon-\varepsilon_{\rm F}}{\varepsilon_{\rm F}}\frac{2m}{\hbar^3} \Theta(\varepsilon-\varepsilon_{\rm F})V(2k_{\rm F})F(2k_{\rm F})[1-G(2k_{\rm F})]\rho_{\rm F}\frac{\langle|U(2k_{\rm F})|^2\rangle}{\epsilon_1^3(2k_{\rm F})}. \qquad (10)$$

As we will see, the first is the regular term of the expansion and gives only a small contribution to thermoelectric coefficients at low electron densities. More important is the second non-analytic term in the energy expansion of the transport scattering time.

From Eq. (9) and Eq. (10) it follows

$$\frac{1}{\tau_1(\varepsilon)} = \frac{1}{\tau_0(\varepsilon_{\rm F})}\frac{\varepsilon-\varepsilon_{\rm F}}{\varepsilon_{\rm F}}[B(\varepsilon_{\rm F}) + 2C(\varepsilon_{\rm F})\Theta(\varepsilon-\varepsilon_{\rm F})], \qquad (11)$$

where $B(\varepsilon_{\rm F}) = B_1(\varepsilon_{\rm F}) + B_2$ is the sum of two terms. One of the terms in square brackets describes the contribution of form factors and is equal to

$$B_1(\varepsilon_{\rm F}) = \frac{1}{8}(15 - 33\frac{\epsilon_{\rm ins}}{\epsilon_{\rm sc}})\frac{k_{\rm F}}{b} - \frac{1}{\epsilon_1(2k_{\rm F})}, \qquad (12)$$

where $b = (48\pi m_\perp e^2 N^*/\epsilon_{\rm sc})^{1/3}$, $N^* = N_{\rm depl} + \frac{11}{32}n$, and $k_F/b \ll 1$.

The second term B_2 is caused by the local-field correction and is independent of electron density and equal to

$$B_2 \simeq \frac{1}{5^{3/2}g_v - 5}. \qquad (13)$$

For $g_v = 2$ we have $B_2 \simeq 0.06$ and for $g_v = 1$ we have $B_2 \simeq 0.16$. The function $C(\varepsilon_{\rm F})$ is expressed by:

$$C(\varepsilon_{\rm F}) \simeq 1 - \frac{1}{\epsilon_1(2k_{\rm F})}. \qquad (14)$$

This $C(\varepsilon_{\rm F})$ term describes the non-analytical behavior of the energy expansion of the transport scattering time and will be the origin of anomalous temperature dependencies. The transport scattering time is then given by

$$\tau_0(\varepsilon) = \tau_0(\varepsilon_F)\left\{1 - \frac{\varepsilon-\varepsilon_{\rm F}}{\varepsilon_{\rm F}}[B(\varepsilon_{\rm F}) + 2C(\varepsilon_{\rm F})\Theta(\varepsilon-\varepsilon_{\rm F})]\right\}. \qquad (15)$$

After substitution of Eq. (15) into Eq. (2) we obtain the final result for $g_v = 2$

$$L_d^{12} \simeq \left[-0.06 + \frac{2}{\epsilon_1(2k_{\rm F})} - \frac{15 - 33\epsilon_{\rm ins}/\epsilon_{\rm sc}}{8}\frac{k_{\rm F}}{b}\right]\frac{\pi e\tau_0(\varepsilon_{\rm F})}{3}k_{\rm B}^2 T. \qquad (16)$$

Note that the "ideal electron system" contribution and the main term in the non-analytical energy dependence of the transport scattering time cancel each other. In the limit of very small electron density Eq. (16) reads

$$L_d^{12} \simeq \left[-0.06 + \frac{2}{g_v r_s \frac{m}{m_b}\left(\frac{g_v}{2}\right)^{1/2}\left(1 - \frac{0.45}{g_v}\right)} - 0.47\left(\frac{k_{\rm F}}{b}\right)\right]\frac{\pi e\tau_0(\varepsilon_{\rm F})}{3}k_{\rm B}^2 T. \qquad (17)$$

Here effective mass m is renormalized by interaction effects and m_b is the value for the band mass.

Eqs. (16), (17) show us that within the accuracy of our calculations the diffusion thermoelectric coefficients in the regime of strong electron-electron interaction are significantly lower than the values expected for the case of a normal metal with weak interaction. A similar behavior is observed in experiment [23]. Moreover, there is a contribution which leads to the sign change of the thermoelectric coefficient L_d^{12} at very low electron densities, reachable in remote doped Si/SiGe heterostructures, where the Coulomb interaction is strong.

In our model the thermopower at low temperatures is given by the following expression

$$S_d = -\frac{\pi^2 k_{\rm B}^2 T}{3e\varepsilon_{\rm F}}[1 - B(\varepsilon_{\rm F}) - C(\varepsilon_{\rm F})], \quad k_{\rm B}T \ll \varepsilon_{\rm F}. \qquad (18)$$

It clearly shows the importance of the Coulomb interaction by the factor $C(\varepsilon_{\rm F})$ containing explicitly and in analytical form the interaction potential including exchange and correlation. The appearance of this factor $C(\varepsilon_{\rm F})$ in the formula for the thermoelectric power of an interacting 2DEG is the new result of our paper. This factor does not appear in three-dimensional systems because there the non-analytical term in the scattering time is much smaller. But we expect that a similar term should exist in the one-dimensional interacting electron gas.

The parameter $B(\varepsilon_{\rm F})$ also can be written as

$$B(\varepsilon_{\rm F}) = -\frac{\varepsilon_{\rm F}}{\tau_0(\varepsilon_{\rm F})}\left[\frac{d\tau_0(\varepsilon)}{d\varepsilon}\right]_{\varepsilon=\varepsilon_{\rm F}^-}. \qquad (19)$$

We stress that the derivative must be taken at an energy from below the Fermi energy $\varepsilon = \varepsilon_{\rm F}^-$ in order to avoid the non-analytic behavior of the transport scattering time. This term $B(\varepsilon_{\rm F})$ is in agreement with earlier results on the thermopower [3–5, 7].

For (100)Si MOSFET systems with intermediate electron density $(3-10)\cdot 10^{11}\,{\rm cm}^{-2}$ we evaluate the thermopower as

$$S_d \simeq -\frac{r_s^2 a_{\rm B}^2 m}{3e\hbar^2} k_{\rm B}^2 T\left[1.3\frac{m_b}{m r_s} - 0.47\frac{k_{\rm F}}{b} - 0.06\right]. \qquad (20)$$

It is interesting to compare Eq. (20) and Eq. (4). At low density ($r_s \gg 1$) the absolute value of thermopower is strongly decreased and the dependence on the electron density is expected to be rather weak, because $S_d \propto r_s$.

Until now we have discussed only the low temperature behavior of the thermoelectric coefficients. In experiment the temperature interval for the diffusion regime conventionally is defined as the interval in which the thermopower is proportional to the temperature. For the thermopower in the diffusive regime we get linear corrections, which are anomalous due to the anomalous screening in two dimensions. We conclude that $S_d/T = c_1 + c_2 T$; c_1 was calculated in the present paper.

For more realistic calculations and the comparison with real experimental results one needs all disorder parameters such as the density of impurities, the parameters for the interface-roughness scattering and a realistic form of confinement potential (depletion density) [24]. Moreover, for the comparison between theory and experiment it would be useful to measure for the same sample as function of density and temperature the conductivity and the thermopower.

The main message of our calculation consist in the result that the anomalous screening in two dimensions has a much larger impact for the Seebeck and the Peltier effect than on the conductivity. The effect is such large that at low carrier density all calculations, not taking into account this contribution, are unable to predict correctly even the order of magnitude for the Seebeck and the Peltier effect. The corresponding contributions to the conductivity (L^{11} in Eq. (1)) and the thermoconductivity (L^{22} in Eq. (1)) are only small corrections, linear in temperature [17, 18], and disappear at very low temperature.

Our theory generalizes earlier theoretical results obtained for the diffusion thermoelectric coefficients in the interacting two-dimensional electron gas. The additional contribution we obtain depends strongly on the strength of the Coulomb interaction including exchange-correlation effects via the local-field correction.

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