Electron transport driven by a chemical potential difference

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Based on Bhatnagar-Gross-Krook equation coupled with Maxwell equation, we investigate the spatial dependence of a chemical, an electrostatic and an electrochemical potentials inside a specimen connected with reservoirs. We also confirm that a gap of the chemical potential between at a connection point is negligible.

KEYWORDS: electron transport, BGK equation, chemical potential

Study of the electron transport has a long history and is one of the typical problems in the nonequilibrium statistical physics. In these days there has been an increasing interest in understanding the electron transport by the successful fabricated devices. In the nonequilibrium transport theory, it is noted that electron currents and heat currents are related with the temperature gradient, the chemical potential gradient and the electric field. For these thermoelectric relations, Wiedemann-Franz law and Seebeck effect are well known. On the other hand, it is interesting to investigate how the local thermodynamical quantities are distributed in the conductor. In this letter, we focus on the spatial dependence of the thermodynamical quantities in the steady electric current which is driven by the chemical potential difference.

Let us consider the electronic device which is composed of a specimen connected through reservoirs. The electric current is driven by the difference of the chemical potential in both sides of the reservoirs. We assume that the system is at the isothermal low temperature and any effects of the heat current do not exist. Furthermore, Joule heat caused by the electric current assumed to be negligible. At the connection point between the specimen and the reservoir, we need to be careful about the discontinuity of the thermodynamical quantities.

Joule heat caused by the electric current is given by the successful fabricated devices. Here, we do not consider the magnetic field induced electric current. When the distribution function is slightly different from the equilibrium Fermi distribution function, we obtain the solution

\[ f = f^0 - f^0(1 - f^0) e^{\beta(\epsilon(p) - \mu - \nu_x (E + \frac{1}{e} \frac{d\mu}{dx})}. \]

The most relevant processes to determine the relaxation time \( \tau \) in electric conduction at low temperature are electron-impurity scatterings. Employing Born approximation, we can evaluate \( \tau \) by the chemical potential \( \mu \) in the low temperature limit:

\[ \tau^{-1} = \frac{16\sqrt{2}\pi^3 m^{3/2}}{h^4} u_0^2 n_{\text{imp}} \mu^{1/2}, \]

where \( n_{\text{imp}} = N_{\text{imp}}/V \) is the impurity density, \( m \) is the electron mass, \( h \) is Planck constant and \( u_0 \) is connected to the scattering potential \( V(r) \) as \( V(r) = u_0 \delta(r - R_i) \) with the position of the random impurity \( \mathbf{R}_i \).
From eqs. (3) and (4), the current density is given by

$$ j = -2e \int \frac{dp}{\hbar^2} v_x f, $$

where factor 2 is the spin degeneracy. Furthermore, we have to take into account the charge imbalances that appear in the specimen. The electric field arises due to the local deviation of the electron density from its equilibrium value and satisfies the Maxwell equation

$$ \frac{dE}{dx} = -\frac{e}{\epsilon} [2 \int \frac{dp}{\hbar^2} f - \rho(x)], $$

where $\epsilon$ is the permittivity and the unperturbed electron density $\rho(x)$ is

$$ \rho(x) = 2 \int \frac{dp}{\hbar^2} f^0. $$

Now, we nondimensionalize the physical quantities (atomic units) as $j \leftarrow j \hbar^7(4\pi\epsilon_0)^{1/4}/m^3e^9$, $v_x \leftarrow v_x \hbar \pi \epsilon_0/e^2$, $x \leftarrow \hbar m^2/\hbar^2 4\pi\epsilon_0$, $\mu \leftarrow \mu^2(4\pi\epsilon_0)^{1/2}/me^4$, $E \leftarrow E \hbar^3(4\pi\epsilon_0)^{1/3}/m^2e^5$, $n_{imp} \leftarrow n_{imp} \hbar^6(4\pi\epsilon_0)^{2/3}/m^3e^6$, $u_0 \leftarrow \hbar^2 m^2/\hbar^2 4\pi\epsilon_0$. Applying Sommerfeld expansion\(^\text{11}\) to eq. (5), the dimensionless steady current density is given by

$$ j = \frac{2}{3\pi} \frac{1}{u_0^2 n_{imp}} \mu(E + \frac{d\mu}{dx}), $$

where we notice that $j$ is the negative value. Similarly, from eqs. (6) and (7), dimensionless Maxwell equation becomes

$$ \frac{dE}{dx} = \frac{8}{\sqrt{6}} \frac{1}{\epsilon_r u_0^2 n_{imp}} \sqrt{\mu(E + \frac{d\mu}{dx})}, $$

with the relative permittivity $\epsilon_r = \epsilon/\epsilon_0$.

Let us consider the chemical potential inside the specimen. From eqs. (8) and (9), we obtain the ordinary differential equation of the chemical potential:

$$ \frac{d^2\mu}{dx^2} + a \frac{1}{\mu^2} \frac{d\mu}{dx} + b \mu^{-1/2} = 0, $$

where $a = 10^{-8}$ and $b = 2 \times 10^{-10}$, and $a = 10^{-6}$ and $b = 10^{-10}$. The length of the specimen is $L = 2000$. The ratio of the chemical potential $\mu_L/\mu_R$ is 1.1.
where dimensionless coefficients \(a\) and \(b\) are given by

\[
\begin{align*}
    a &= \frac{3\pi}{2} n_0^2 n_{\text{imp}} j \\
    b &= \frac{12\pi}{\sqrt{6}\epsilon_r j}.
\end{align*}
\]

We now solve eq. (10) subject to the boundary conditions at \(\mu(0) = \mu_L\) and \(\mu(L) = \mu_R\). If we know the details of the material properties, the amount of the current density under the chemical potential difference can be determined. However, since the impurity potential \(u_0\) is hard to be measured in the experiment, we do not know the amount of the current density precisely. In this letter, we determine the spatial dependence of the chemical potential as a function of \(a\) and \(b\).

Let us set the ratio \(\mu_L/\mu_R=1.1\) with its normalized chemical potential \(\mu_L=0.0407\), \(\mu_R=0.0370\) and the normalized length \(L=2000\) (\(\mu_L=1.1\text{eV}, \mu_R=1.0\text{eV}, L=100\text{nm}\)). Figure 2 shows the spatial dependence of the chemical potential for the different coefficients \(a\) and \(b\). In the finite current density, the chemical potential profiles exhibit the strong nonlinearity. When the coefficient \((a, b) = (-10^{-8}, -2 \times 10^{-10})\), the spatial variation of the chemical potential has a concave profile, while the chemical potential profile with the coefficient \((-10^{-6}, -10^{-10})\) shows a convex one. There exists the solutions of eq. (10) only when the value of \(b\) is smaller than \(10^{-8}\) for any coefficients \(a\).

The spatial dependence of the electrostatic potential in the specimen is of interest. The electrostatic potential is related to the electric field: \(\phi = -\int E dx\). Using the electric field \(E = \mu u^{-1} - d\phi/dx\) from eq. (8), the spatial dependence of the electrostatic potential can be determined. In Fig. 3(A), the electrostatic potential profile with the coefficient \((-10^{-8}, -2 \times 10^{-10})\) shows a concave one. On the other hand, in Fig. 3(B), the electrostatic potential profile with the coefficient \((-10^{-6}, -10^{-10})\) almost increases linearly and shows a larger spatial variation compared with the corresponding chemical potential profile in Fig. 2.

If we treat the system with the electric filed, the electrostatic potential must be added to the chemical potential for the potential of the electron. Now, we consider the dimensionless electrochemical potential \(\bar{\mu} = \mu - \phi\) in the specimen. We have shown that the chemical potential and the electrostatic potential have a strong nonlinearity for the finite current density, but the electrochemical potential profiles decrease almost linearly for any \(a\) and \(b\) in Fig. 4(A) and 4(B). If the gradient of the chemical potential causes the electric current, it is reasonable that no electric current with the coefficient \((0, 0)\) shows the constant electrochemical potential profile in Fig. 4(A). Under the small external field, the linearity of the electrochemical potential profile corresponds the explanation of the electron transport by Ohmic law.

These spatial dependence are reproducible by the perturbation expansion. Now, we expand \(\bar{\mu}, \phi\) and \(\mu\) by the coefficient \(a\): \(\bar{\mu} = \bar{\mu}_0 + a\bar{\mu}_1 + \cdots, \phi = \phi_0 + a\phi_1 + \cdots\) and \(\mu = \mu_0 + a\mu_1 + \cdots\). Substituting these \(\bar{\mu}, \phi\) and \(\mu\) into eqs. (8) and (9), we obtain the zeroth order of \(a\) as \(\bar{\mu}_0 = c_1, \phi_0 = c_2x + c_3\) and \(\mu_0 = \bar{\mu}_0 + \phi_0\) where the value of the each coefficient is given by \(c_1 = 0, c_2 = -1.85 \times 10^{-6}\) and \(c_3 = 0.0407\) to recover the profile at \((a, b) = (0, 0)\). Expanding until the first order of \(a\), we obtain the electrochemical potential as

\[
\bar{\mu} = \frac{a}{c_2} \log(1 + \frac{c_2}{c_3} x).
\]

Similarly, the electrostatic potential is given by

\[
\phi = c_2 x + c_3 + a \left[ -\frac{4}{3} \frac{b}{ac_2} (c_2 x + c_3)^{3/2} + (d_1 x + d_2) \right],
\]

where the coefficients \(d_1\) and \(d_2\) are given by

\[
d_1 = \frac{1}{L} \left[ \frac{4}{3} \frac{b}{ac_2} (c_2 L + c_3)^{3/2} - c_3^{3/2} \right] - \frac{1}{c_2} \log(1 + \frac{c_2}{c_3} L),
\]

and

\[
d_2 = \frac{4}{3} \frac{b}{ac_2} c_3^{3/2}.
\]

Fig. 4. Top(A): Electrochemical potential profile for the coefficient \((a,b) = (-10^{-8}, -2 \times 10^{-10})\) and \((0, 0)\). Bottom(B): Electrochemical potential profile for the coefficient \((-10^{-6}, -10^{-10})\). Line 1st are the electrochemical potential profile for the first order perturbative solution in eq. (12). All the remaining parameters are the same as in Fig. 2.
in Fig. 2, the electrostatic potential profile in Fig. 3 and the electrochemical potential profile in Fig. 4.

Now, let us estimate the gap of the chemical potential based on the approach by Nishino and Hayakawa. We first consider the distribution function at the connection point. On the left reservoir side of the connection point, electrons with $p_x > 0$ obeying the equilibrium distribution function $f_{eq}$ go through the connection point ballistically. In the same way, on the specimen side of the connection point, electrons with $p_x \leq 0$ obeying the nonequilibrium distribution function $f_{ne}$ go through the connection point ballistically. Therefore the dimensionless distribution function at the connection point is approximately given by

$$f_{cp}(p) = \begin{cases} f_{eq}(p, \mu_{eq}) & p_x > 0 \\ f_{ne}(p, \mu_{ne}) & p_x \leq 0, \end{cases} \quad (14)$$

where the equilibrium distribution function is

$$f_{eq} = \frac{1}{e^{\beta(\epsilon-\mu_{eq})}+1}, \quad (15)$$

and the nonequilibrium distribution function as the first order of the current density is

$$f_{ne} = f_{ne}^0 - \frac{3\pi^2}{2\sqrt{2}f_{ne}^0}(1-f_{ne}^0)^2\beta v_x\mu_{ne}^{-3/2}j, \quad (16)$$

with $f_{ne}^0 = 1/(e^{\beta(\epsilon-\mu_{ne})}+1)$. The expansion of the chemical potential in terms of the dimensionless current density becomes

$$\mu_{ne} = \mu_{eq}(1+ dj), \quad (17)$$

where $d$ is the gap parameter to be determined. Using eq. (14), we define the dimensionless current density at the connection point given by

$$J = -2\int \frac{dp}{(2\pi)^3} v_x f_{cp}. \quad (18)$$

Since the electric current exists continuously at the connection point, we assume that $J$ is equal to $j$ in eq. (5). From these equations, the gap parameter is given by $d = \sqrt{3}\pi^2/2\mu_{eq}^2$. Now, we consider the maximum amount of the gap at the left connection point. We have the solution of eq. (10), only when the coefficient $b$ in eq. (11) is less than $10^{-6}$. If the specimen has the unit relative permittivity, the maximum amount of the gap is given by $dj = 3.3 \times 10^{-4}$. Therefore, we confirm that the gap of the chemical potential at the connection point is negligible.

Now, let us discuss our result. Although we are interested in the quantum effects of the electron transport, the essence of electrons is believed to be described by semi-classical treatments as we have discussed. Quantum effect may not be important for simple electron transports, while such effects are essentially important in localization problems. We have treated the system at the isothermal low temperature, but, it is straightforward to extend our analysis to the transport at high temperature cases, where the heat conduction is as important as the electron transport. In such a system, the gap of the thermodynamical quantities at the connection point needs to be considered. The discussion of this effect is the subject of a subsequence paper.

In summary, we have examined the electron transport processes which is driven by the chemical potential difference based on BGK equation coupled with Maxwell equation at the isothermal low temperature. We determine the spatial dependence of the chemical, electrostatic and electrochemical potential as functions of the current and the impurity potential. While the spatial dependence of the chemical potential and the electrostatic potential show the strong nonlinearity, the electrochemical potential decreases almost linearly for any coefficient. The behaviors of these thermodynamical quantities can be understood by the simple perturbation theory. We also confirm that the gap of the chemical potential at the connection point between the reservoir and the specimen is negligible.

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