Thermal vector potential theory of transport induced by temperature gradient

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A microscopic formalism to calculate thermal transport coefficients is presented based on a thermal vector potential, whose time-derivative is related to a thermal force. The formalism is free from unphysical divergences reported to arise when Luttinger’s formalism is applied naively, because the equilibrium (‘diamagnetic’) currents are treated consistently. The mathematical structure for thermal transport coefficients are shown to be identical with the electric ones if the electric charge is replaced by energy. The results indicates that the thermal vector potential couples to energy current via the minimal coupling.

Conversion of heat into electric and other currents and vice versa is of essential importance from the viewpoint of realizing devices with low energy consumption. Of recent particular interest is heat-induced spin transport in the field of spintronics, where spin current is expected to lead to novel mechanisms for information technology, and to devices with low-energy consumption due to the absence or weak Joule heating.

A hot issue in spintronics is to use magnetic insulators, which are suitable for fast magnetization switching and low-loss signal transmission. Insulators have, however, a clear disadvantage that electric current cannot be used for its manipulation. Instead, temperature gradients become the most important driving force in inducing spin transport. To study thermally-induced spin transport theoretically, a microscopic formulation is necessary for full understanding and for quantitative predictions. A microscopic description is, however, not straightforward; temperature gradients and thermal forces are macroscopic quantities arising after statistical averaging, and thus it is not obvious how to represent those effects in a microscopic quantum mechanical Hamiltonian.

In 1964, Luttinger proposed a solution [11]. To describe the effect of temperature gradient, he introduced a scalar potential \( \Psi \), which he called a ‘gravitational’ potential, which couples to energy density of the system, \( E \), via an interaction Hamiltonian,

\[
H_L = \int d^3r \nabla \Psi E.
\]

Although the microscopic origin of the potential has not been addressed, he argued that to satisfy the Einstein relation the potential adjusts itself to balance the thermal force, resulting in an identity \( \nabla \Psi = \frac{\nabla T}{T} \) in the thermal equilibrium. Owing to this trick, thermal transport coefficients can be calculated by linear response theory with respect to the field \( \Psi \) without introducing the temperature gradient in a microscopic Hamiltonian. Another approach, based on the Landauer-Blüttiker formalism, was presented by Butcher [12].

The Luttinger’s method has been applied to study various thermally-induced transports, and it turned out that naive application often leads to apparently wrong transport coefficients which diverge as \( T \to 0 \) [13, 14]. In the case of the thermal Hall effect, the divergence was identified to be due to a wrong treatment of the equilibrium diamagnetic current induced by the applied magnetic field, and it was found that the physical Hall coefficient is obtained if one subtracts the equilibrium contribution before applying linear response theory [14]. A similar problem was reported recently for thermally-driven spin-transfer torques [13].

In the case of electrically-driven transport, elimination of unphysical equilibrium contribution from transport coefficients is guaranteed by \( U(1) \) gauge invariance, which represents charge conservation. In the presence of an electromagnetic vector potential, \( A \), the physical electric current has two components, a paramagnetic current (the first term) and a diamagnetic current (the second term), as \( j = \frac{\hbar}{m} \langle p \rangle - \frac{e}{m} n_e A \), where \( \langle p \rangle \) is quantum average of the momentum operator, \( n_e \) is electron density and \( e \) and \( m \) are electron’s charge and mass. The paramagnetic current contains an equilibrium contribution arising from all the electrons below the Fermi level, which turns out to be \( \frac{e}{m} n_e A \). This equilibrium contribution thus cancels perfectly with the diamagnetic contribution, leaving only the contribution from excitations in the transport coefficients. Obviously, a consistent treatment of the two contributions is necessary for the cancellation of equilibrium contribution and for gauge-invariant physical results. If one uses, instead of a vector potential, a scalar potential to describe an conservative electric field, the role of the diamagnetic current is not clearly seen, and wrong results easily arise if an inconsistent treatment is employed.

From those experiences in electrically-induced transport, the divergence in the thermally-induced transport when the temperature gradient is described by Luttinger’s \( \Psi \) is expected to be due to an incorrect treatment of the ‘diamagnetic’ contribution [16]. If one could construct a microscopic vector potential representation of thermal effects, such problems would not occur, since the role of ‘diamagnetic’ current is clear and the calculation is straightforward. Temperature gradients exert a statistical force proportional to \( \nabla T \), which is conser-
The rate of the change of the entropy ($S$) due to an energy current is
\[ \dot{S} = - \int d^3r \frac{1}{T} \nabla \cdot \mathbf{j}_e = - \int d^3r \mathbf{j}_e \cdot \frac{\nabla T}{T^2}, \]
and this entropy change modifies the free energy, $F \equiv E - TS$ ($E$ is the internal energy). The effective Hamiltonian describing the effect of DC thermal force is therefore
\[ H_S = \frac{1}{T} \int d^3r \int_{-\infty}^t \mathbf{j}_e(t') dt' \cdot \nabla T. \]
This is equivalent to Eq. (4) after the replacement $\nabla \Psi \rightarrow \nabla T/T$.

We now apply the thermal vector potential interaction, Eq. (4), to study thermal transport and demonstrate that the formalism works perfectly. We consider free electrons with a quadratic dispersion, described by the Hamiltonian $H_0 = \int d^3r \mathcal{E}_0$, where $\mathcal{E}_0 = \frac{k^2}{2m}(\nabla c \cdot \nabla c) - \mu c \gamma_i c\gamma_i$ is the free electron energy density, $\mu$ is the chemical potential and $\gamma_i$ and $c\gamma_i$ are creation and annihilation operators of the electron, respectively. The energy current density is derived by use of the energy conservation law, Eq. (2). For free electrons, $\nabla \cdot \mathbf{j}_e^{(0)} = -\frac{1}{\hbar}[\mathcal{H}_0, \mathcal{E}_0(r)]$, and the result is
\[ \mathbf{j}_e^{(0)} = \frac{i\hbar^3}{(2m)^2} \left[ (\nabla^2 c \gamma_i) \nabla c - (\nabla c \gamma_i) (\nabla^2 c) \right] - \frac{\mu}{e} \mathbf{j}_e^{(0)}, \]
where $\mathbf{j}_e^{(0)} = \frac{\gamma_i}{\hbar} m c \gamma_i \nabla c$ is the paramagnetic part of the electric current density. We focus on the uniform component of the current considering the case of spatially uniform temperature gradient, which reads ($V$ is system volume)
\[ \mathbf{j}_e^{(0)} = \frac{\hbar}{m V} \sum_k k_i \epsilon_k \gamma_i \gamma_k, \]
where $\epsilon_k \equiv \frac{\hbar^2 k^2}{2m} - \mu$ is the energy measured from the Fermi energy.

We now apply this interaction to study thermally-driven longitudinal electron transport on a basis of diagrammatic (Green’s function) formalism. Besides the interaction Hamiltonian, we need to take account of the ‘diamagnetic’ current contribution proportional to $A_T$. We derive it by use of the charge conservation law, $\dot{\rho} + \nabla \cdot \mathbf{j} = 0$ ($\rho$ is electric charge density) taking account of thermal vector potential. Namely, we calculate a commutator, $-\frac{1}{\hbar}[\mathcal{H}_0^{(3)} \gamma_i, c\gamma_i] \equiv \nabla \cdot \mathbf{j}^{A_T}$, and derive the expression for $\mathbf{j}^{A_T}$. The result of the uniform component is
\[ j_i^{A_T} = -\frac{e}{m} A_T \frac{1}{V} \sum_k \gamma_k^{ij} \epsilon_k c\gamma_k, \]
where
\[ \gamma_k^{ij} \equiv \epsilon_k \delta_{ij} + \frac{\hbar^2}{m} k_i k_j. \]
As expected from Eq. (9), the diagrammatic calculation is carried out by a straightforward replacement of charge $e$ in the electric field driven case. By energy $\epsilon_k$. Including the interaction with the vector potential to the linear order, the DC paramagnetic current is

$$j_i^{(0)} = \frac{e\hbar}{mV} \sum_{k\omega} \epsilon_k^{ij} \left[ A_{T,i} f^{\prime}(\omega) (\phi_{k\omega})^2 - 2A_{T,j} f(\omega) \text{Im}[(g^0_{k\omega})^2] \right]$$

(12)

where $\epsilon_k^{ij} = \frac{\hbar^2}{m} k_i k_j \epsilon_k$, $\phi_{k\omega} = g^0_{k\omega} - g^0_{k\omega} + \sum_{\omega'} \equiv \int \frac{d\omega}{2\pi}$ and Im denotes the imaginary part. The retarded and advanced Green’s functions for free electron are denoted by $g^0_{k\omega} = \frac{1}{\epsilon_k + i\eta}$, and $g^0_{k\omega} = (g^0_{k\omega})^*$, where $\eta$ is the elastic lifetime. By use of $\frac{\hbar k_i}{m} (g^0_{k\omega})^2 = \partial_{k_i} g^0_{k\omega}$ and integration by parts with respect to $k$, we rewrite the last contribution using

$$\sum_k \epsilon_k^{ij} \left[ (g^0_{k\omega})^2 - (g^0_{k\omega})^2 \right] = - \sum_k \gamma_k^{ij} \phi_{k\omega},$$

(13)

to obtain

$$j_i^{(0)} = -\frac{e\hbar}{mV} \sum_{k\omega} A_{T,j} \epsilon_k^{ij} f^{\prime}(\omega) (\phi_{k\omega})^2 - j_i^{A_T}$$

(14)

where $j_i^{A_T} = i\frac{e\hbar}{mV} A_{T,i} \sum_k \gamma_k^{ij} f(\omega) \phi_{k\omega}$ agrees with the diamagnetic current (Eq. (10)). The equilibrium (diamagnetic) contribution is therefore eliminated from the physical thermally-induced electric current, obtaining $j_i = \sigma_T E_{T,i}$, where

$$E_T = -\frac{\partial A_T}{\partial t} = -\nabla T$$

(15)

is the thermal field, and $\sigma_T = \frac{e^2}{3mV r^2} \sum_k k^2 \epsilon_k f^{\prime}(\omega) |g^0_{k\omega}|^4$ (assuming rotational symmetry for $k$). The low temperature behavior is seen by a series expansion ($\Phi_k(\omega) = |g^0_{k\omega}|^4$)

$$\int_{-\infty}^{\infty} d\omega f^{\prime}(\omega) \Phi_k(\omega) = -\Phi_k(0) - \frac{\pi^2}{6} (k_B T)^2 \Phi_k(0),$$

(16)

where $O(T^4)$ is neglected. Since $\epsilon_k = 0$ on the Fermi surface, we have $\sum_k k^2 \epsilon_k \Phi_k(0) = 0$ (to the leading order of $\frac{\hbar}{k_B T}$). We therefore see that $\sigma_T = O(T^2)$ at $T \rightarrow 0$ and the thermally-induced current vanishes at $T = 0$.

We now study the thermally-driven Hall effect, where a problem of divergence due to a broken time reversal symmetry has been noted in a naive application of the Luttinger’s scheme [14]. We expect that no such unphysical result arises in the present vector potential formulation, since the ‘diamagnetic’ current cancels the unphysical equilibrium contribution in the ‘paramagnetic’ contribution owing to the relation $\gamma_k^{ij} = \partial_{k_i} (k_j \epsilon_k)$. Let us confirm this by an explicit calculation.

We introduce the interaction with an electromagnetic vector potential, $H_A = -\int d^3r A \cdot j$, to describe the effect of the applied magnetic field, where $j = j^{(0)} + j^A + j^{A_T}$, $j^A = -\frac{e}{m} A e c$ being the diamagnetic current of the electromagnetic origin. The electromagnetic vector potential is treated as static but has finite wave vector, since its role here is to represent a static magnetic field, $B = \nabla \times A$.

The thermal vector potential has an infinitesimal angular frequency (\Omega) and is spatially uniform. The Hall current is calculated to the lowest order, i.e., linear in both $A$ and $A_T$. It turns out that the leading contribution is linear both in the angular frequency $\Omega$ and in the wave vector $q$.

The contributions to the paramagnetic part of the current, $j_i^{(0)}$ are shown diagrammatically in Fig. 1(a). (‘Diamagnetic’ currents shown in Fig. 1(c), vanish, since $A$ and $A_T$ carry only either finite angular frequency or finite wave vector in the present description.) The contribution of Fig. 1(a) is

$$j_i^{(a)} = -\frac{e^2 \hbar^4}{m^3 V} (\nabla_m A_j) A_{T,i} \sum_{k\omega} k_i k_j \gamma_k^{lm} \Phi_k^{(H)}$$

(17)

where $\Phi_k^{(H)} = \text{Im}[f^{\prime}(\omega) (g^0_{k\omega})^2 g^0_{k\omega,\omega} + h f(\omega) (g^0_{k\omega})^4]$.

FIG. 1. Diagramatic representation of the contributions to the thermal Hall effect. Solid, wavy and dotted lines denote the electron, thermal vector potential $A_T$ and the electromagnetic vector potential $A$, respectively.

Because of ‘diamagnetic’ current due to the thermal vector potential, $j_i^{A_T}$, we have an interaction vertex, $-\int d^3r A \cdot j^{A_T}$, containing both $A$ and $A_T$. The contribution shown in Fig. 1(b) arises from this interaction vertex. It is

$$j_i^{(b)} = \frac{e^2 \hbar^4}{m^3 V} (\nabla_m A_j) A_{T,i} \sum_{k\omega} k_i k_m \gamma_k^{lj} \Phi_k^{(H),ij}$$

(18)

The total Hall current, $j_i^{(H)} = j_i^{(a)} + j_i^{(b)}$, is finally obtained as

$$j_i^{(H)} = \Theta_H (E_T \times B)$$

(19)

where $\Theta_H = \frac{e^2 \hbar^4}{3m^3 V} \sum_{k\omega} k^2 \epsilon_k \Phi_k^{(H)}$. We see that the Hall current vanishes at $T = 0$ (see Eq. (16)), as is physically required. The vector potential formalism applied straightforwardly therefore leads to the correct result, in sharp contrast to Luttinger’s ‘gravitational’ potential formalism.
For consistency of the vector potential formalism, we need to confirm that the same mechanism works also for the energy current density; in other words, we need to see that ‘diamagnetic’ current naturally arises also for the energy current. This is not a trivial question, since we cannot invoke a gauge invariance concerning the energy current, in contrast to the case of electric current. In our scheme, ‘diamagnetic’ contribution is explored again by looking into the energy conservation law. In fact, including the thermal vector potential interaction, Eq. (14), in the left-hand side of Eq. (22), we see that the energy current acquires a ‘diamagnetic’ contribution linear including the thermal vector potential interaction, Eq. (21), by looking into the energy conservation law. In fact, we might be understood as due to a ‘gauge invariance’ as a result of the energy conservation law. In fact, we have shown that the Luttinger’s $\Psi$ and the present $A_T$ have the identical effect concerning steady state properties. In other words, we may assign a part of thermal force to $\Psi$ and the rest to $A_T$, so that $\frac{\delta}{\delta \Psi} = \nabla \Psi + A_T$. Thus we have a ‘gauge invariance’ under a transformation $\Psi \to \Psi - \chi$ and $A_T \to A_T + \nabla \chi$ ($\chi$ is a scalar function). Such a gauge transformation is generally defined for a vector field coupling to a conserved current. One should note a difference between the thermal and the electric vector potentials: The former has no ‘magnetic’ component and the ‘Lorentz force’ for energy current does not exist. Besides, we expect that there are higher order terms with respect to $A_T$ in the Hamiltonian, which may make another difference from the electromagnetic case with an exact gauge invariance.

The thermal vector potential formalism applies to spin-polarized cases straightforwardly. It was recently pointed out by Kohno [13] that naive application of the Luttinger’s scheme to calculate thermal spin-transfer torque results in a wrong result which diverges at $T \to 0$. Such issue does not appear if we use the vector potential form. In fact, as is obvious from the above analysis, thermally driven torques can be obtained from the result of Ref. [20] for the electric field-induced torque simply by replacing the electric charge by energy. It is easy to check that the thermal torque vanishes at $T = 0$, as is physically required.

To conclude, we propose a vector potential form of a microscopic interaction describing the effect of temperature gradient. We have demonstrated that the calculation of transport coefficients such as thermal longitudinal and Hall conductivities, thermal spin-transfer torque, and thermal conductivity for the energy current, are straightforwardly carried out without encountering any unphysical divergences. This feature is due to particular relations between the ‘diamagnetic’ contribution to currents and the interaction vertex, and the relations indicates that the coupling to the thermal vector potential is the minimal coupling.

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