Topological current for transverse electrical and thermal conductivity in thermoelectric effect

Xuguang Shi
College of Science, Beijing Forestry University, Beijing, People’s Republic of China
E-mail: shixg@bjfu.edu.cn

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Abstract
Thermoelectric efficiency of the traditional thermoelectric material is low, which restricts the large scale applications. Recently, the developing of the topological insulator provides a new opportunity to get high thermoelectric efficiency material. There are two effects in topological insulator: anomalous Hall and Nernst effect, which have contribution to the transport properties. Because of anomalous Hall and Nernst effect the electrical thermal conductivity have transverse parts, which affect the Seebeck coefficient. However, the transverse parts can be expressed by Berry curvature. By using of \( \varphi \)-mapping topological theory, the Berry curvature is studied and we find there is topological vortex in the momentum space. The Bloch wave function is zero at the topological vortex. Finally, the relationships between the topological vortex and the transverse electrical and thermal conductivity is given and how the topology affects the Seebeck coefficient is researched in detail.

1. Introduction

Thermoelectric (TE) effect has inspired a lot of researches. To probe the TE material with high energy conversion is the main problem [1–3]. The energy conversion efficiency for TE devices is determined by the coefficient \( zT \) of TE materials, which is defined as \( zT = \frac{\alpha S T}{\sigma} \) [4], where \( \alpha, S, \sigma \) are longitudinal electrical conductivity, Seebeck coefficient, and thermal conductivity. \( T \) is the temperature. In the past few decades, the energy conversation efficiency has made a great progress. For example, the efficiency of \( \alpha = \text{MgAgSb} \) is \( \sim 1.1 \) from 300 K to 548 K [5]. The efficiency of SnSe is \( \sim 2.6 \) at 923 K [6]. The efficiency of Bromine doped \( n \)-type SnSe reaches \( \sim 2.8 \) at 773 K [7]. However, the \( zT \) of these materials is far from the large-scale commerce applications. Therefore, the main problem of TE material is how to improve the energy conversation efficiency. On the other hand, some thermal materials, such as PbTe, SnTe, HgTe and CdTe, demonstrate a topological insulator nature [8]. The recent important progresses in topological insulator offer a new opportunity for development of TE materials [9–13]. The reason lies in there is the topological vortex in momentum space. When the topological vortex does not exist in momentum space, the momentum space can be homeomorphism to the spherical manifold in 3-dimensional space. When one topological vortex exists, the momentum space can be homeomorphism to the toroidal manifold with one genus. In general, the anomalous Hall effect (AHE) and anomalous Nernst effect (ANE) play an important role in topological insulator. Moreover, AHE and ANE can directly affect the Seebeck coefficient. AHE and ANE can be explored in the frame of Berry connection and Berry curvature [14]. It is well known the Berry connection and Berry curvature are the concepts in coordinate space. When a particle moves through a closed contour around a point defect, the particle would acquire a geometric phase expressed by the winding number of the point defects.

In this paper, based on \( \varphi \)-mapping topological current theory [15, 16], we try to find the relations between the topological vortex in momentum space and the transport properties in materials. Furthermore, the topological expressions of the transverse electrical and thermal conductivities are given. These will help us understand how to improve \( zT \) in topological insulator. The contents are arranged as follows: In section 2, the efficiency of thermoelectric power of TE is reviewed. The Berry connection and Berry curvature in \( \mathbf{k} \)-momentum space are defined by using Bloch wave function. Then the transverse electrical and thermal
conductivity are introduced. In section 3, the topological expression of the Berry curvature is deduced in detail by using $\varphi_{\text{mapping}}$ topological current theory in $k$-momentum space. Then we find there is topological vortex when the Berry curvature is non-zero. The non-zero Berry curvature only exists at the zero points of the Bloch wave function. Finally, the relationships between the transverse electrical and thermal conductivity and the topological vortex in momentum space are given. In section 4, we give a conclusion.

2. The Seebeck coefficient, electrical and thermal conductivities

The efficiency produced by thermoelectric power is

$$zT = \frac{\partial S^2}{\partial T}.$$  \hspace{1cm} (1)

The Seebeck coefficient $S$ is the thermal power which describes the voltage generation owing to the temperature gradient. Let us consider the two-dimensional electron gas (2DEG) in topological insulator, in the frame of the semiclassical Boltzmann transport theory, the charge current can be expressed as

$$j = \sigma E + \alpha (\mathbf{\nabla} T),$$  \hspace{1cm} (2)

where $\sigma$ is electrical conductivity tensor and $\alpha$ is thermal conductivity tensor. $E$ is the electric field intensity. They are written as

$$\sigma = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix},$$  \hspace{1cm} (3)

$$\alpha = \begin{pmatrix} \alpha_{xx} & \alpha_{xy} \\ \alpha_{yx} & \alpha_{yy} \end{pmatrix}.$$  \hspace{1cm} (4)

In general, $\sigma_{xy}$ and $\alpha_{xy}$ are called the transverse electrical and thermal conductivity respectively, which originate from AHE and ANE. Here we only focus on the electronic contribution to the thermal conductivity. The transverse electrical and thermal conductivity can be expressed by Berry curvature. The formula for the Seebeck coefficient $S$ [4] is

$$S \equiv \frac{\partial E_i}{\partial T} = \frac{\alpha_{xx} \sigma_{xx} + \sigma_{xy} \alpha_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2},$$  \hspace{1cm} (5)

From (5), the contributions of the topological effects to Seebeck coefficient are nonnegligible. To find these in detail, the wave function in 2DEG with period potential is explored in detail. The wave function for a band in a crystal lattice are given as

$$\Psi_\eta(k, \mathbf{r}) = e^{ik \cdot \mathbf{r}} |u_\eta(k, \mathbf{r})|,$$  \hspace{1cm} (6)

where $k$ is the momentum of the electron and one has $k = (k^1, k^2, k^3) = (k^i)$. $|u_\eta(k, \mathbf{r})|$ is the Bloch wave function with the periodicity of the lattice, which is the period part of a Bloch state. The Berry connection $A_k$ in $k$-momentum space is defined by Bloch wave function, it is

$$A_k = \{u_\eta(k, \mathbf{r}), i \partial_k \} u_\eta(k, \mathbf{r}),$$  \hspace{1cm} (7)

which represents the geometric phase attached to the Bloch wave function. It is produced by the infinitesimal movement of the electron in $k$-momentum space. Then the Berry curvature $\Omega_{nk}$ in $k$-momentum space is defined as the curl of the Berry connection:

$$\Omega_{nk} = i \{ \partial_k u_\eta, \partial_\eta u_\eta \}. $$  \hspace{1cm} (8)

When the Berry curvature $\Omega_{nk} = 0$, the $k$-momentum space is flat. We say the topology is trivial. When the Berry curvature $\Omega_{nk} \neq 0$, the $k$-momentum space is not flat. We say the topology is non-trivial. It is well known the transverse conductivities are expressed as a function of Berry curvature. In anomalous transport case at low temperatures, we thus have [17, 18]

$$\sigma_{xy} = \frac{e^2}{h} \sum_n \int \frac{dk}{(2\pi)^3} f(\varepsilon_{kn}) \Omega_{nk},$$  \hspace{1cm} (9)

where $\varepsilon_{kn}$ is the energy of electron in a band and $e$ is the charge of the electron. $f(\varepsilon_{kn})$ is the equilibrium distribution function. The electrical conductivity $\sigma_{xx}$ is

$$\sigma_{xx} = \frac{e^2}{h} \sum_n \int d^2k v_n^x(k) \frac{\partial f(\varepsilon_{kn})}{\partial \varepsilon_{nk}},$$  \hspace{1cm} (10)

here, $v_n^x(k)$ is the group velocity of the electron. $\tau$ is the relaxation time. The transverse thermal conductivity $\alpha_{xy}$ is
\[ \alpha_{xy} = \frac{e}{\beta h} \sum \int \frac{dk^x dk^y}{(2\pi)^2} s_n(k) \Omega_{nk}, \]

where \( \beta = \frac{1}{k_B T}, k_B \) is Boltmann constant. \( s_n(k) \) is the entropy density of the electron gas, which can be given as

\[ s_n(k) = -f(\varepsilon_{k0}) \ln f(\varepsilon_{k0}) - (1 - f(\varepsilon_{k0})) \ln (1 - f(\varepsilon_{k0})). \]

### 3. Topology of the Berry curvature in k-momentum space of Bloch wave function

Geometry and topology have played an important role in mathematics and physics. A great deal of works have been done [19–23]. From the view of topology, The wave function in a crystal lattice provides a mapping from k-momentum space (base space) into the target manifold (filed) formed by Bloch wave function. However, the base space and field manifold, as well as mapping may possess some nontrivial topological feature. Then in this case, the generalization of the topological properties of the Bloch wave function is the theory of complex linear bundle. Let us consider a compact smooth differentiable manifold \( X \) with an open cover \( \{ U_a \} \). Locally the linear bundle is given by \( U_a \times \mathbb{C} \), where \( \mathbb{C} \) is a left group space. The local Cartesian products are put together by the transition function (gauge transformation) \( t_{ab} \) on each non-empty overlap \( U_a \cap U_b \). \( t_{ab} \) is complex-valued and no vanishing on the overlap. On a non-empty triple overlap \( U_a \cap U_b \cap U_c \), they satisfy the consistency condition \( t_{ab}t_{bc}t_{ca} = 1 \). The object that one constructed by putting together this collection of Cartesian products is called a complex linear bundle \( L \). The manifold \( X \) is called the base. A section of the linear bundle is given by a collection \( \{ \Psi_a \} \) of locally defined complex-valued function. Specially, let manifold \( K \) be the three-dimensional k-momentum space and \( C \) be a left \( U(1) \) group space. Then the complex linear bundle \( L \) discussed above can be described as an associated bundle \( K \times_{U(1)} C \). The wave function in a crystal lattice is just the section of the associated bundle \( K \times_{U(1)} C \). It is also a section of two-dimensional real vector bundle on the manifold \( K \). Then the Bloch wave function is given as

\[ u(k) = u^a(k) + i u^\beta(k). \]

From this expression, one unit vector is defined by

\[ n^a(k) = \frac{u^a(k)}{||u(k)||} a = 1, 2, \]

where \( ||u(k)|| = u^a(k) u^a(k) \). It is easy to see the unit vector satisfies the relation

\[ n^a n^a = 1. \]

The unit vector is just the mapping from the section of the real vector bundle to unit sphere in k-momentum space, which is called Gauss mapping. From the wave function, we give the Berry connection \( A \) in k-momentum space as

\[ A = \text{Im} \frac{\nabla_k u(k)}{u(k)}, \]

which is just the tangent vector on the section of the real vector bundle in k-momentum space. One can expand it as

\[ A = \frac{1}{u^a(k) u(k)} [u(k) \nabla_k u^a(k) - u^a(k) \nabla_k u(k)]. \]

From this expression, if the wave function has no zero points, the Berry connection is trivial. If the wave function has zero points, the Berry connection is non-trivial. That means there are some singularities in the k-momentum space. By using the unit vector, the Berry connection is rewritten as

\[ A_{ik} = \epsilon_{ik} n^a(k) \partial_k u^\beta(k). \]

Here, \( \epsilon_{ik} \) is the unit antisymmetry tensor. By use of the Berry connection, we deduce the Berry curvature \( \Omega_{ik} \) as

\[ \Omega_{ki} = e^{ik/k} \epsilon_{ab} \partial_k n^a(k) \partial_i n^b(k) = e^{ik/k} \epsilon_{ab} \frac{\partial}{\partial u^a(k)} \ln ||u(k)|| \partial_i u^b(k) \partial_k n^a u^\beta(k). \]

One can define the Jacobian vector of k-momentum wave function as

\[ e^{ab} D_{\mathbf{k}} \frac{\partial u}{\mathbf{k}} = e^{ik/k} \partial_k u^a(k) \partial_i n^b(k), \]

and it is well known the Green’s function is \( \nabla^2 \ln r = \delta(r) \) in coordinate space. Similarly, the Green’s function theory in k-momentum space is given by
\[
\frac{\partial}{\partial u^\mu(k)} \frac{\partial}{\partial u^\nu(k)} (\ln \|u(k)\|) = 2\pi \delta^2(u(k)).
\]  
(21)

Based on all the relations (19), (20) and (21), finally, the Berry curvature is rewritten as

\[
\Omega_{k_i} = 2\pi \delta^2(u) D_k \left( \frac{u}{k} \right).
\]  
(22)

Because of the Dirac function, the Berry curvature \(\Omega_{k_i} = 0\) when \(u(k) = 0\). Then the Bloch wave function should satisfy

\[
u^1(k^\ell) = 0, \quad \nu^2(k^\ell) = 0.
\]  
(23)

Let us assume there are \(l\) solutions satisfying the equations (23) and (24), \(l = 1, 2, \ldots, \ell\), which represents the isolated singular topological defects in \(k\)-momentum space. The defects are denoted by \(L_l (l = 1, 2, \ldots, \ell)\). Equation (23) decides one plane in \(k\)-momentum space and equation (24) decides the other plane. It is clear the topological defects in \(k\)-momentum space are made which is just the intersection of the two planes. These topological defects form a topological vortex in the \(k\)-momentum space. Let us assume that \(s\) is the parameter of the vortex. Given the two dimensional intersection \(\Sigma\) of the vortex and let us assume \(u = (k^\mu, k^\nu)\) is the coordinates on the intersection, where \(\mu, \nu = 1, 2\). It is obvious that there are some defects on the intersection. The topological defects on the intersection can be denoted as

\[k^\mu = k^\mu(s).\]
(25)

Then the solution of \(\delta^2(u)\) can be written as

\[
u^1(k^\mu, k^\nu, s) = 0, \quad \nu^2(k^\mu, k^\nu, s) = 0.
\]  
(26)

The zero points of Bloch wave function can be called point defects. From (25), (26) and (27), we find the topological vortex in momentum space appears with the point defect together. The Dirac function \(\delta^2(u)\) can be expanded at the solutions

\[
\delta^2(u) = \sum_{i=1}^{n} G_i \delta^2(k^\mu_i - k^\mu(s),
\]  
(28)

where \(G_i\) is the positive coefficients. The winding number of the \(lth\) topological vortex is

\[
W(u, k^\ell) = G_l \sum \delta^2(k^\mu - k^\mu(s)) D \left( \frac{u}{k} \right) dk^\mu dk^\nu
\]  
(29)

Here, Jacobian matrix \(D \left( \frac{u}{k} \right)\) is

\[
D \left( \frac{u}{k} \right) = \frac{1}{2} \epsilon^{\mu\nu\rho} \frac{\partial u^\mu}{\partial k^\rho} \frac{\partial u^\nu}{\partial k^\rho}.
\]

If we let

\[
|W_l| = |W(u, k^\mu_l)| = \beta_l,
\]  
(31)

one call \(\beta_l\) Hopf index of the map \(k \rightarrow u(k)\) on the manifold \(K\). It means that when the momentum \(k^\mu\) of the electron changes around the neighborhood of the topological vortex \(k^\mu_l(s)\) (shown in figure 1) once, the function \(u\) cover the corresponding region in \(u(k)\) space \(\beta_l\) times. Then the Dirac function \(\delta^2(u)\) is expanded as

\[
\delta^2(u) = \sum_{i=1}^{n} \frac{\beta_i}{|D \left( \frac{u}{k} \right)|} \delta^2(k^\mu - k^\mu(s).
\]  
(32)

Let us define

\[
\eta_l = \text{sign} \left[ D \left( \frac{u}{k} \right) \right] = \frac{D \left( \frac{u}{k} \right)}{|D \left( \frac{u}{k} \right)|} = \pm 1,
\]  
(33)

one call \(\eta_l\) the Brouwer degree of the map \(k \rightarrow u(k)\). For the vortex, \(\eta_l = 1\), for the anti-vortex, \(\eta_l = -1\). Finally, the Berry curvature is
\[ \Omega_{k'} = 2\pi\beta\eta\delta^2(k^\mu - k_0^\mu(s)) \frac{dk^\mu}{ds}, \]  

where

\[ \frac{dk^\mu}{ds} = \frac{D^\mu\left(\frac{\mu}{T}\right)}{D\left(\frac{\mu}{T}\right)} \]  

and

\[ D^\mu\left(\frac{\mu}{k}\right) = \frac{1}{2} \epsilon^{\alpha\beta}\epsilon_{\gamma\delta} \frac{\partial}{\partial k^\alpha} \frac{\partial}{\partial k^\beta} u^\gamma u^\delta. \]  

The vorticity of the vortex \( L_i \) is

\[ \Gamma_i = \int_{\Sigma_i} \Omega \cdot d\mathbf{K} = W_i, \]  

where \( d\mathbf{K} = dk^\mu dk^\nu = d^2k \). The vorticity is the topological invariant.

In section 2, one has defined the transverse electrical and thermal conductivity. Then, Put equation (34) into (9), the transverse electrical conductivity can be written as

\[ \sigma_{xy} = \frac{e^2}{\hbar} \sum_n \int d^2 k f(\varepsilon_{nk}) W_{nk} \delta^2(k_n^\mu - k_0^\mu(s)) \frac{dk_n^\mu}{ds}, \]  

where \( k_n^\mu \) and \( k_0^\mu(s) \) are the momentum in \( nth \) band. To calculate the integral with the Dirac function, we have the formula

\[ \sigma_{xy} = \frac{e^2}{\hbar} \sum_n W_{nk} \left( f(\varepsilon_{nk}) \frac{dk_n^\mu}{ds} \right)_{k_0^\mu(s)}. \]  

Put equation (34) into (11), the transverse thermal conductivity is

\[ \alpha_{xy} = \frac{2\pi\epsilon}{\beta\hbar} \sum_n \int \frac{d^2 k dk^\nu}{(2\pi)^2} \varepsilon_{nk} W_{nk} \delta^2(k_n^\mu - k_0^\mu(s)) \frac{dk_n^\mu}{ds}. \]  

Consider the integral, it is

\[ \alpha_{xy} = \frac{2\pi\epsilon}{\beta\hbar} \sum_n W_{nk} \left( \varepsilon_{nk} \frac{dk_n^\mu}{ds} \right)_{k_0^\mu(s)}. \]  

These formulas show the transverse electrical and thermal conductivity depend on the topological number: winding number. The winding number is bigger; the transverse electrical and thermal conductivity are bigger. Although when the electron’s momentum \( k^\mu = k_0^\mu(s) \) the Bloch wave function is zero, the momentum \( k_n^\mu(s) \) decides the transverse electrical and thermal conductivity. The reason is there are two quantities relate to the \( k_n^\mu(s) \): One is the distribute function \( f(\varepsilon_{nk}) \) and the other is \( \frac{dk_n^\mu}{ds} \). In order to see how the topological number function in the TE effect, we will plot the Seebeck coefficient \( S \) by considering the equations (5), (39) and (41). From figure 2, we find the Seebeck coefficient \( S \) increases as the increasing of the topological number. It
conforms to the fact the adding foreign atoms as doping to the TE materials, which are just the point defect, will enhance the TE effect.

In equations (39) and (41), the transverse electrical conductivity and thermal conductivity are decided by two correlative factors: the topological factor \(W_{nl}\) and nontopological factor. It should be noted that another important factor of the thermal conductivity is the lattice contribution [24]. The lattice contribution can affect the transverse electrical conductivity and thermal conductivity through the equilibrium distribution and entropy density. On the other hand, the reason that the topology play an important role in study of TE effect is the phonon resonance scattering can reduce the lattice thermal conductivity. However, the resonance scattering exists in the TE materials with topology insulator. In this case, the local resonance will strength the couple between the phonon and photon, then reduce the thermal conductivity. Moreover, the lattice contribution can affect the equilibrium distribution function and this lead to the change of the entropy density. This is another reason the topology is an important role in study of thermal conductivity.

4. Conclusion

In this paper, the thermoelectric effect has been investigated in the frame of the topological insulator. Because of the topology, the AHE and ANE is not overlooked. These effects lead to the transverse electrical and thermal conductivity, which can be expressed by the Berry curvature \(\Omega_\mathbf{k}\). By using the \(\varphi\)-mapping topological theory to the Block wave function in \(\mathbf{k}\)-momentum space, we find there is topological vortex when \(\Omega_\mathbf{k} \neq 0\). Furthermore, when the momentum \(k^\alpha = k^\alpha_{nl}\) the topological vortex exists in \(\mathbf{k}\)-momentum space. We also find the Block wave function is zero at \(k^\mu = k^\mu_{nl}\), which means the electron can not move in the band formed by \(k^\mu_{nl}\). The band is just the gap band. However, this momentum \(k^\mu_{nl}\) decides the transverse conductivities through the distribution function, entropy density and \(\frac{d\Omega_\mathbf{k}}{d\mu}\). Therefore, the topological vortex is in the The relationships between the topological vortex and the transverse electrical and thermal conductivity are found.

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ORCID iDs

Xuguang Shi https://orcid.org/0000-0002-0403-0659

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