Thermoelectric figure of merit in topological insulators

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Abstract. Transport behavior of two-dimensional topological insulators is theoretically studied in narrow ribbon geometry. The system has perfectly conducting edge channels, which are free from backscattering. At high temperature, the bulk states dominate in the transport phenomenon. However, at low temperature the conducting channels along the edges become dominant. It causes a bulk-to-edge crossover. Namely, by lowering temperature, the figure of merit first decreases by a competition between the bulk and the edge transport, and then increases again because the edge transport become larger.

1. introduction
Thermoelectric transport of materials is characterized by the thermoelectric figure of merit $ZT = \frac{\sigma S^2 T}{\kappa}$ [1], where $T$ is the temperature, $\sigma$ is the electrical conductivity, $S$ is the Seebeck coefficient, and $\kappa$ is the thermal conductivity from electrons and phonons. To achieve efficient energy conversion, high $ZT$ is favorable. One of the prevailing approaches is the phonon glass and electron crystal (PGEC) [2]. Phonon conduction reduces thermoelectric efficiency because the phonon transport increases $\kappa$. A relatively new approach is “low-dimensionality” [3]: a peaked structure in the density of states in low dimensions enhances $S$.

Recently we proposed that the two-dimensional topological insulators (2D TI) have a potential to enhance thermoelectric figure of merit at low temperature [4]. In this paper we explain the calculations made in [4], and discuss the results. The 2D TIs are qualitatively a new state of matter [5, 6, 7], realized experimentally. The 2D TI is an insulator in the bulk, and has gapless edge states which are stable against nonmagnetic impurities [8, 9]. Therefore we assume that in impure systems, electron conduction contributed from the edge states remains good, while phonon conduction is suppressed, satisfying the PGEC condition. At the same time, the edge currents are one-dimensional (1D), which fulfills the “low-dimensional” criterion. In addition, the 3D TI was observed in good thermoelectric materials such as Bi$_{1-x}$Sb$_x$ [10], Bi$_2$Se$_3$ [11], and Bi$_2$Te$_3$ [12]. Although these are 3D TIs, there is a close relationship between 2D and 3D TIs, and the candidate materials are largely in common between 2D and 3D TIs.
Therefore we study thermoelectric transport of 2D TI in this paper [4]. In 2D TIs in ribbon structure, both the bulk states and edge states contribute to the transport. To discuss transport phenomena where the edge states can have comparable or even larger contribution compared with the bulk, we set the ribbon width to be very narrow. We then show that the bulk and edge contributions to the thermoelectric phenomenon compete each other, and this competition gives rise to a bulk-to-edge crossover. The edge contribution to the transport is largely affected by inelastic scattering length $\ell$ of the edge states because the inelastic scattering breaks their coherence. As the system is cooled, $\ell$ becomes longer, and the edge states become dominant in thermoelectric transport. We note that at room temperature the bulk transport is completely dominant because $\ell$ might become very short.

2. Model calculation and results

The transport matrix is given by

$$
\begin{pmatrix}
\frac{j}{q} \\
\frac{w}{w}
\end{pmatrix} = \begin{pmatrix}
L_0 & L_1 \\
L_1 & L_2
\end{pmatrix} \begin{pmatrix}
\frac{d\mu}{dx} \\
\frac{1}{T}
\end{pmatrix},
$$

(1)

where $j$ is the electric current, $w$ is the thermal current, $q$ is the electron charge $-e$, and $\mu$ is the chemical potential. From the matrix, the transport properties are given by

$$
\sigma = e^2 L_0, \quad S = -\frac{1}{eT} L_1, \quad \kappa_e = \frac{1}{T} \frac{L_0 L_2 - L_1^2}{L_0}, \quad ZT = \frac{L_1^2}{L_0 L_2 - L_1^2 + \kappa_L T L_0},
$$

(2)

where $\kappa_e$ is the electron thermal conductivity, $\kappa_L$ is phonon thermal conductivity, and $\kappa = \kappa_e + \kappa_L$. The total transport matrix elements are given by $L_0^b = L_0^e + L_1^b$, where the suffix $e$ and $b$ mean the edge transport and bulk transport, respectively.

Fig. 1 schematically shows the density of states. The energy $E$ is measured from the bottom of the bulk conduction band, and the chemical potential $\mu$ is assumed to be close to zero. We neglect the hole band i.e. $-\Delta/2 \ll \mu$ where $\Delta$ is the energy gap. In the calculation we used the parameters estimated for Bi$_2$Te$_3$ at $T = 1.8$K [4]. We assume that the edge states are perfectly conducting over the whole sample and keep its coherence. In coherent systems, transport properties are calculated by the Landauer formula, with the transmission coefficient being unity when the electron energy is in the bulk gap ($-\Delta < E < 0$). $L_0^b$ is then given by

$$
L_0^b = -\frac{\ell}{sh} \int dET(E)(E - \mu) \frac{\partial f}{\partial E} = c_0 \int_{-\Delta}^{-\mu} x_{\nu} \frac{e^x}{(e^x + 1)^2} dx, \quad c_e = \frac{2\ell}{sh},
$$

(3)

where $f$ is the Fermi distribution function, $h$ is the Planck constant, $s$ is the cross section of the sample, the factor 2 comes from the two gapless channels of the 2D TI, $\mu = \mu/(k_B T)$ $\Delta = \Delta/(k_B T)$, and $k_B$ is the Boltzmann constant. We use the gap size of Bi$_2$Te$_3$: $\Delta = 0.15$ eV.

The bulk transport is calculated by the Boltzmann equation. We assume that the relaxation time $\tau$ is constant, and the bulk band is parabolic with an effective mass $m$. We use only the first subband because there is a large gap between the first subband and second subband due to the narrow–ribbon confinement. The transport coefficients are calculated as

$$
L_0^b = -\frac{1}{s} \int_{-\infty}^{\infty} \frac{dk}{2\pi} c_T v^2 (\epsilon - \mu) \frac{\partial f(\epsilon)}{\partial \epsilon} = c_b \int_{-\Delta}^{\infty} \frac{\sqrt{x + \mu} x \epsilon^x}{(e^x + 1)^2} dx, \quad c_b = \frac{4\sqrt{2\mu^* c}}{esh}
$$

(4)

where the coefficient $c$ is the number of the carrier pockets, and $\mu^*$ is the mobility.

The results are shown in Fig. 2. $\mu$ is assumed to be less than the bottom of the second subbands. The curves “Total” in Fig. 2 (a)(b) mean that both the bulk transport and the edge
transport are considered. While in the transport coefficients $L_i$, the bulk and edge contributions are summed, the Seebeck coefficient and $ZT$ from Eq. (2) are not simply the sums of the bulk and edge contributions. Fig. 2(b) shows that the maximum $ZT$ appears when the chemical potential $\mu$ is near the band edge. It comes from a competition between the bulk and the edge transport from the following argument. When the chemical potential $\mu$ is near the band edge ($\mu \sim 0$), the bulk charges are holes and edge carriers are electrons. Therefore the bulk and edge transport give positive and negative Seebeck coefficients, respectively. The Seebeck coefficient from the bulk states becomes larger when $\mu$ is in the bulk gap, while that from the edge states is larger when $\mu$ is in the bulk band. The behavior of the total Seebeck coefficients can be understood as such bulk-edge competition. This behavior of the Seebeck coefficients also governs the behavior of $ZT$, which roughly agrees with the Wiedemann-Franz law. This is why maximum of $ZT$ occurs when $\mu$ is around the band edge. The maximum $ZT$ in Fig. 2(b) is around 0.4 at 1.8K. For comparison, experimental value of $ZT$ of Bi$_2$Te$_3$ at room temperature is around unity [13]. Hence, in ribbon geometry at low temperature, by using the edge states, it might be possible to achieve $ZT$ comparable to the value at room temperature.

$$ZT_{\text{edge}} = \frac{\sigma_{\text{edge}}}{1 + \frac{\sigma_{\text{edge}}}{\kappa_{\text{therm}}}}$$

Fig. 3(a) shows that $ZT$ has two peaks, whose relative sizes vary as we change $\mu$. The crossover when the Seebeck coefficient vanishes as a function of the chemical potential. We see that for larger $\mu$, the Fermi energy is deep inside the bulk band, and crossover occurs at larger $\mu$.

From Fig. 3(a), when $g = 0$ or $r = 0$ (no edge transport), $ZT$ becomes very large; nevertheless, it cannot be realized because of relatively large phonon transport in real materials. Indeed, by increasing $g$ (phonon transport), $ZT$ is rapidly suppressed. Instead, in our theory we propose that increasing $r$ (edge transport) will be a promising route for enhancing $ZT$.

Fig. 3(a) shows that in usual material, i.e. for $r = 0$ (no edge transport), $ZT_{\text{max}}$ is sensitive to $g$ (phonon transport). Disorder suppresses the heat transport, but it also kill the electric transport, and $ZT$ is not enhanced so much. On the other hand, in the region where the $r$ is

3. Search for maximum $ZT$

To search for optimal thermoelectric figure of merit in 2D TIs by changing the physical parameters, we define the following dimensionless parameters: $r = c_e/c_b = \frac{\kappa_{\text{edge}}}{4\sqrt{2m_kT}k_B\mu^2}$, $g = \frac{\kappa_{\text{therm}}}{c_b} = \frac{\kappa_{\text{therm}}}{4\sqrt{2m_kT}k_B\mu^2}$, $r$ represents the ratio of the edge transport compared with the bulk transport, and $g$ represents the ratio between the phonon heat transport and the bulk transport. From these parameters, we calculate $ZT$ as a function of $\mu$, and then study the maximum $ZT_{\text{max}}$ when we vary $\mu$. Fig. 3(a) shows that $ZT_{\text{max}}$ becomes minimum at $r \sim 2.6$ because of a competition between the edge- and bulk-state transport. The value of $\mu$ is $\mu/(k_BT)$ where the $ZT$ becomes maximum as a function of $\mu$ is shown in Fig. 3(b). It prominently indicates this competing transport. A jump appears in Fig. 3(b) at around $r \sim 2.6$, because $ZT$ as a function of $\mu$ has two peaks, whose relative sizes vary as we change $r$. The crossover occurs when $\mu$ is fixed and $r$ is varied. Fig. 4 shows the value of $r = r_{\text{crossover}}$ when the Seebeck coefficient vanishes as a function of the chemical potential. We see that for larger $\mu$, the Fermi energy is deep inside the bulk band, and crossover occurs at larger $r$.

Figure 1. Schematic bands for the bulk and edge states.

Figure 2. Calculation result of (a) the Seebeck coefficient and (b) $ZT$ as a function of $\mu$. 
Figure 3. (a) ZT max and (b) μ max as a function of r and g.

much larger than the crossover “valley” around r ~ 2.6, the figure of merit becomes relatively insensitive to g. Disorder will lower the bulk mobility, and r becomes large. Then the ZT will be enhanced. In ordinary metals, both r and g generally become large as T decreases at low temperature. An estimation on Bi_2Te_3 at T = 1.8K gives r = 9.4 and g = 8.2, which is located in the edge-dominated regime. We estimate the crossover temperature to be 5K-10K for Bi_2Te_3 narrow ribbon by taking into account the temperature dependence μ*, κ_L, and ℓ. To keep the edge transport robust, the ribbon width w should be much larger than the penetration depth λ of the edge states; if w is less or equal to λ, a hybridization of the gapless edge states at the opposite edges occurs, and opens a sizable gap [14], killing the gapless edge channels.

4. Conclusion
In conclusion, we study thermoelectric properties of two-dimensional topological insulators. Around 5K-10K for narrow ribbons the edge states begin to dominate thermoelectric transport as the temperature is lowered. The bulk-to-edge crossover temperature becomes higher for longer inelastic scattering length of edge states.

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