Thermoelectric efficiency of topological insulators in a magnetic field

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We study the thermoelectric properties of three-dimensional topological insulators in magnetic fields with many holes (or pores) in the bulk. We find that at high density of these holes in the transport direction the thermoelectric figure of merit, $ZT$, can be large due to the contribution of the topologically protected conducting surfaces and the suppressed phonon thermal conductivity. By applying an external magnetic field a subgap can be induced in the surface states spectrum. We show that the thermoelectric efficiency can be controlled by this tunable subgap leading to the values of $ZT$ much greater than 1. Such high values of $ZT$ for reasonable system parameters and its tunability by magnetic field make this system a strong candidate for applications in heat management of nanodevices, especially at low temperatures.
Introduction. Topological insulators (TIs) recently attracted a lot of attention as potential candidates for spintronics applications. This interest is based on the remarkable properties of TIs, namely, the fact that their surfaces (for three-dimensional TIs) or edges (for two-dimensional TIs) possess topologically protected conducting states. In this paper we argue that these unique properties of TIs can also be employed to make very efficient thermoelectrics.

Good thermoelectric materials are characterized by a low thermal conductivity and high thermopower and electric conductivity. The large thermopower requires steep dependence of the electronic density of states on energy, which can be achieved by having the chemical potential close to the bottom of a band. The relatively high conductivity demands the gap to be low. These combined requirements point to semiconductors with heavy elements as the best candidates for the thermoelectric materials. Some of these semiconductors were recently rediscovered as TIs. We show that by making holes in these TI materials (see Fig. 1) and inducing subgap in their surface states by means of applied magnetic fields or proximity of ferromagnets one can significantly enhance their thermoelectric efficiency. The high density of holes in the direction of transport has two positive effects: 1) to trap phonons and thus reduce the thermal conductivity; 2) to increase the surface to bulk ratio and therefore effectively enhance the electric conductivity of the sample. The effect of the applied magnetic field is to increase the thermopower.

Thermoelectric figure of merit. The thermoelectric efficiency is defined as a ratio of an electric power generated to the total heat flux through the sample. Therefore, it is characterized by the dimensionless number

\[ ZT = \frac{\sigma S^2}{\kappa_e + \kappa_{ph}} T, \]

where \( \sigma \) is electric conductivity, \( S \) is Seebeck coefficient (or thermopower), \( T \) is temperature, and \( \kappa \) is thermal conductivity. The latter, in general, has contributions both from electrons (\( \kappa_e \)) and from phonons (\( \kappa_{ph} \)).

In the absence of magnetic field or magnetic impurities, the TIs have ungaped surface states. These propagating states are confined to the close proximity of the surfaces. Their existence is protected by the topology of the bulk band structure. These states have cone-like 2D Dirac spectrum, \( E = \pm v \hbar |k| \), where \( v \) is the constant Dirac electron velocity. Application of a magnetic field, doping with magnetic impurities, or hybridization of these states due
FIG. 1. (Color online) A sample of the topological insulator with many holes in the direction of transport.

to close proximity of two surfaces can induced a Dirac subgap $\Delta$ [22,24] which in the case of magnetic field $B$ is $\Delta \propto B$. Then the surface spectrum takes the form $E = \pm \sqrt{v^2\hbar^2k^2 + \Delta^2}$, see Fig. 2. Generally this subgap is much smaller than the bulk gap, $\Delta \ll \Delta_0$. For three-dimensional TIs $\Delta_0$ ranges from 0.15 eV to 0.3 eV for such as Bi$_2$Te$_3$ and Bi$_2$Se$_3$.

To study the thermal and electric transport in these materials we employ the linear response theory. The electric ($j^e$) and thermal ($j^q$) currents are given by linear combinations of the temperature and chemical potential gradients:

$$j^e/e = L_0 \nabla \mu + L_1 (\nabla T)/T,$$

$$j^q = -L_1 \nabla \mu - L_2 (\nabla T)/T,$$

where $e$ is the electron charge. Using Onsager relations, one can find from these equations the electrical conductivity $\sigma = e^2L_0$, Seebeck coefficient $S = -L_1/(eTL_0)$, and electron thermal conductivity $\kappa_e = (L_0L_2 - L_1^2)/(TL_0)$. The figure of merit, $ZT$, can then be represented in
terms of these linear coefficients as

$$ZT = \frac{L^2_{2,1}}{L_0(L_2 + \kappa_{ph}T) - L^2_1}.$$  \hspace{1cm} (4)

In Eq. (4) it is assumed that the transport coefficients have bulk and surface contributions $L_n = L_{b,n} + L_{s,n}/D$, where $D = (A - \sum_n \pi R^2_n)/\sum_n 2\pi R_n$ is the factor related to surface/bulk ratio (porosity) and has dimension of length. The holes in the sample does not have to form a periodic structure and can be placed randomly. The same idea applies to porous TI samples, see Fig. 3 (a). The parameter $D$ characterizes the average distance between the pores (holes) of the average radius $R$, see Fig. 3 (b). Here $\kappa_{ph}$ is the phonon contribution to the thermal conductivity in the bulk (phonon contribution to the thermal conductivity for the surface TI states is much smaller than that in the bulk).

To estimate the surface contribution of TI to the transport coefficients $L_n$ we assume the bands to be Dirac-like with a subgap $\Delta$ and use Boltzmann equation in the relaxation time approximation,

$$L_{s,n} = -2 \sum_i \int_{-\infty}^{\infty} \tau \left( \frac{\partial E_i}{\partial \hbar k} \right)^2 f'(E_i)(E_i - \mu)^n \frac{d^2 k}{4\pi^2}. \hspace{1cm} (5)$$

Here the sum is over the upper and lower bands, $i = \pm 1$, and $f'(E) = \partial f/\partial E$ with $f = 1/(e^{(E-\mu)/(k_B T)} + 1)$ being the Fermi distribution function. Then taking relaxation time $\tau$ to be independent of energy, we find

$$L_{s,n} = \frac{\tau(k_B T)^{1+n}}{2\hbar^2} \int_{\Delta} \frac{x^2 - \bar{\Delta}^2}{x} \left[ \frac{(x - \bar{\mu})^n}{\cosh^2 \frac{x - \bar{\mu}}{2}} + \frac{(-x - \bar{\mu})^n}{\cosh^2 \frac{x + \bar{\mu}}{2}} \right], \hspace{1cm} (6)$$

where $h$ is Planck constant, $\bar{\Delta} = \Delta/(k_B T)$, and $\bar{\mu} = \mu/(k_B T)$.

When the chemical potential $\mu$ is far below the bottom of the conduction band, $(\Delta_0 - \mu)/(k_B T) \gg 1$, the contribution from the bulk to the transport coefficients is exponentially suppressed, $L_{b,n} \propto e^{-(\Delta_0 - \mu)/(k_B T)}$, and can be neglected. The same argument works also for the valence band contribution when $\mu$ is far from the valence band edge. Thus, the thermoelectric transport is dominated by the surface states and the only sensible bulk contribution is to the phonon thermal conductivity $\kappa_{ph}$. Then the figure of merit becomes

$$ZT = \frac{L^2_{s,1}}{L_{s,0}(L_{s,2} + D\kappa_{ph}T) - L^2_{s,1}}. \hspace{1cm} (7)$$

At small $D$, the contribution to $ZT$ mostly comes from 2D surface states and in this limit $ZT$ is given by $ZT_{2D} = \frac{L^2_{s,1}}{(L_{s,0}L_{s,2} - L^2_{s,1})}$, which is shown as a function of the chemical
FIG. 2. (Color online) A sketch of TI's band structure with the subgap $\Delta$ in the surface band. The bulk gap $\Delta_0$ is considered to be much larger than $\Delta$.

potential in the inset of Fig. 4 (a) for $\Delta/(k_B T) = 3$. The color plot of $ZT_{2D}$ as a function of the induced subgap $\Delta/(k_B T)$ and $\mu/(k_B T)$ is shown in Fig. 4 (a). The maximum $ZT$ achievable by tuning the chemical potential for a fixed induced gap $\Delta/(k_B T)$ is shown by a golden line in Fig. 4. The very high values of $ZT$ in reality are not reachable since any small contribution from the phonon thermal conductivity reduces $ZT$.

For the holey sample, the phononic contribution to the thermal conductivity can be characterized by the dimensionless parameter $K_{ph} = 2\kappa_{ph}Dh^2/(\tau k_B^3 T^2)$. Here the phonon thermal conductivity can be estimated to be $\kappa_{ph} \approx 1 W m^{-1} K^{-1}$ (as for Bi$_2$Te$_3$) and the average distance between the holes reaching $D \sim 10$ nm. Taking the relaxation time $\tau \approx 10^{-11}$ s, at room temperatures we estimate $K_{ph} \sim 1$ for these rather conservative values of parameters. In Fig. 4 (b), estimated $ZT$ is shown as a function of $\Delta$ and $\mu$ for the phononic
FIG. 3. (Color online) (a) A schematic view of a TI sample’s part with pores propagating in the direction of transport. (b) Top view of the TI sample with the average distance between the holes/pores given by $D$.

bulk contribution characterized by the dimensionless parameter $K_{ph} = 3$. Although reduced considerably from its pure 2D value, $ZT$ remains substantially larger than any value thus far achieved in these materials and can be tuned significantly by applied magnetic fields.

Summary. We have studied the thermoelectric properties of three-dimensional TIs in magnetic fields with high density of holes in the sample. By applying an external magnetic field a subgap can be induced in the surface states spectrum. We show that the thermoelectric efficiency can be controlled by this tunable subgap. We have find that the thermoelectric figure of merit $ZT$ in these materials can be much greater than 1. This is due to the high contribution of the topologically protected conducting surfaces and the suppressed phonon thermal conductivity. High $ZT$ values for reasonable system parameters and its tunability by magnetic field or magnetic impurities make this system a strong candidate for applications in heat management of nanodevices.

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FIG. 4. (Color online) Thermoelectric figure of merit, $ZT$, as a function of surface subgap $\Delta$ and chemical potential $\mu$. Light solid curve shows the maximum of $ZT$. (a) $ZT$ for the infinitely high density of holes. The inset shows $ZT(\mu)$ for the case of $\Delta/(k_B T) = 3$. (b) $ZT$ for a finite density of holes characterized by the dimensionless parameter $K_{ph} = 3$. Because of the phononic contribution to the thermal conductivity $ZT$ is reduced compared to the case (a).
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