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# Thermoelectric transport in the topological phase due to the coexistence of superconductivity and spin-density-wave

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**Abstract.** We study the thermoelectric transport in two dimensional topological system which has coexistence of superconductivity (SC) and spin-density wave (SDW). The SC is presumed to be of $d_{x^2-y^2}+(p_x+ip_y)$ type whereas the SDW order parameter is of $BCS$ symmetry. The Hamiltonian describing such a coexistence phase is shown to have topological phase in addition to the conventional one. The transport properties in such topological system have two distinct contributions: (i) the surface/edge and (ii) the bulk. The competition between the surface/edge versus the bulk transport is analyzed in different parameter regimes and the possibility of enhancing the figure of merit is discussed.

## 1 Introduction

In last few years, a new field in condensed matter systems has emerged which is called "Topological insulators and superconductors" [1,2]. It is based on the realization that the spin-orbit interaction in materials can lead to such electronic phases [3–6] which has been observed in real materials [7–9]. A topological insulator, similar to an ordinary insulator has a bulk energy gap separating the highest occupied electronic band from the lowest empty band [10–13]. It is closely related to the two-dimensional integer quantum Hall states [14] which have unique edge states. The surface of such insulators however, necessarily has gapless states (edge states) that are protected by time reversal symmetry. These states are conducting with properties unlike any other known one-dimensional or two-dimensional electronic systems. These states are predicted to have special properties which are thought to be useful for applications ranging from spintronics to quantum computation [15]. Due to such technological importance the field of topological systems has grown rapidly over the years. Since one of the compelling criteria of a material to be topological is that the system ought to have an energy gap, the topological concept extends over to any gapped systems such as superconductors and superfluids, etc. [16–18]. Recently, a possibility of a topological phase in the coexistence phase of superconductivity and spin-density wave has been discussed [19–22]. The nature of such topological phase depends on the symmetry as well as the amplitudes of both the order parameters.

Recently, the photoemission and the scanning tunnelling spectroscopy have become an important experimental tool in identifying the surface states in topological systems but the signature of such states in transport measurements is still under debate. The focus of experimental studies thus has shifted to the separation of bulk conduction from the surface conduction. Recently, there is an attempt to formulate the thermoelectric transport in topological insulators theoretically [23]. Thermoelectric transport is basically conversion of heat to energy. The efficiency of such energy conversion depends on the "figure of merit" of the material which is defined as, $ZT = \frac{\sigma S^2 T}{\kappa}$ [24], where $T$ is the temperature, $S$ is the Seebeck coefficient and $\sigma$ and $\kappa$ are respectively the electrical and thermal conductivities. In order to achieve a high $ZT$, the system should be a good electronic conductor whereas a bad lattice conductor. Further, the material low-dimensionality also have large $S$ and have high efficiency due to their peaked density of states [25]. Despite such proposals it was very hard to discover good thermoelectric materials in the past. This is due to the fact that $\sigma$, $S$ and $\kappa$ cannot be independently controlled, namely, a material with large electrical conductivity $\sigma$ has large thermal conductivity $\kappa$. The discovery of topological systems gives some hope on the above issues due to the fact that the edge state conduction remains good whereas the phonon conduction is suppressed. The edge states are one-dimensional which satisfies the low dimensionality [26] criteria mentioned above. The topological phenomena which has already been observed in materials such as $Bi_{1-x}Sb_x$ [27], $Bi_2Se_3$ [28] and $Bi_2Te_3$ [29] are known as good thermoelectric materials.

In this communication, we study the thermoelectric transport in two-dimensional topological system which has coexistence of superconductivity (SC) and spin-density wave (SDW). The symmetry of SC is considered to be of $d_{x^2-y^2}+(p_x+ip_y)$ type whereas the SDW order parameter is of $BCS$ symmetry. The Hamiltonian having

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such a structure is shown to have topological coexistence phases in addition to the conventional one. The thermoelectric transport in such topological system is discussed with respect to two distinct contributions: (i) the surface and (ii) the bulk. The competition among the surface versus the bulk transport is analyzed in different parameter regimes and the possibility of enhancement of figure of merit is discussed in these systems.

## 2 Model Hamiltonian

In the present work, we consider the coexistence of SDW and $d$-wave superconductivity which can generate a triplet and non-zero center of mass superconducting order parameter. We, thus start with a Hamiltonian on a 2D square lattice [21,22] as:

$$\mathcal{H} = \sum_{k,\sigma} \xi_k c^\dagger_{k,\sigma} c_{k,\sigma} + \frac{U}{N} \sum_{k,k'} c^\dagger_{k,\uparrow} c_{k+Q,\uparrow} c^\dagger_{k'-Q,\downarrow} c_{k',\downarrow} + \sum_{k,k'} V^1(k,k') c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} c_{-k',\downarrow} c_{k',\uparrow} + \sum_{k,k'} V^2(k,k') c^\dagger_{k,\uparrow} c^\dagger_{-k-Q,\downarrow} c_{-k'-Q,\downarrow} c_{k',\uparrow}. \quad (1)$$

Here, $\xi_k$ is the bare dispersion due to the tight binding approximation on a 2D square lattice, $U$ is the on-site Coulomb interaction, $V^{1,2}$ are the pairing strengths for $d$-wave and $p$-wave superconductivity and $N$ is the number of sites. Also, $\xi_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu$ and $c^\dagger_{k\sigma}$ ($c_{k\sigma}$) denotes creation (annihilation) operator of the electron with spin $\sigma = (\uparrow, \downarrow)$ at $\mathbf{k} = (k_x, k_y)$. Here, $\sum'_k$ is the sum of $k$ over the reduced Brillouin zone (RBZ). We express the wave-vector $k$ in units of $\frac{\pi}{a}$, with '$a$' the lattice parameter of the underlying square lattice. $\mathbf{Q} = (\pi, \pi)$ is the SDW nesting vector in 2D. We assume here a commensurate SDW so that $\mathbf{k} + \mathbf{Q} = \mathbf{k} - \mathbf{Q}$. The staggered spin magnetization is defined as $M_0 = -\frac{U}{N} \sum_{k,\sigma} \sigma \langle c^\dagger_{k+Q,\sigma} c_{k,\sigma} \rangle$. Since the discussion would be about three order parameters below, the crystal symmetry are such that the commutator of any two of them should give the third one. Thus, if $V^1$ is assumed to be of singlet $d$-wave symmetry, the SDW state guarantees that $V^2$ should be of triplet type. So we get the singlet interaction $V^1_{k,k'} = V^1_0 s_k s_{k'}$ and $V^2_{k,k'} = V^2_0 p_k p_{k'}$, where $s_k = \frac{1}{2}(\cos k_x - \cos k_y)$ and $p_k = \sin k_x + i \sin k_y$. We further assume that $V^{1,2}$ are attractive. The SC order parameters are defined as, for singlet state,

$$\triangle^1_{k'} = \triangle^1_0 s_{k'} = V^1_0 s_{k'} \sum_k s_k \left\langle c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} \right\rangle = V^1_0 s_{k'} \sum'_k s_k \left\langle c^\dagger_{k+Q,\uparrow} c^\dagger_{-k+Q,\downarrow} \right\rangle.$$

On the other hand, the triplet order is

$$\triangle^2_{k'} = \triangle^2_0 p_{k'} = V^2_0 p_{k'} \sum_k p_k \langle c_{-k,\downarrow} c_{k+Q,\uparrow} \rangle = \triangle^2_0 (\sin k_x + i \sin k_y) = \triangle^2_{1,k} + i \triangle^2_{2,k}$$

while

$$\triangle^{2*}_{k'} = V^2_0 p^*_{k'} \sum_k p^*_k \left\langle c^\dagger_{k,\uparrow} c^\dagger_{-k-Q,\downarrow} \right\rangle.$$

Defining $\xi^+_k = -4t' \cos k_x \cos k_y - \mu$ and $\xi^-_k = -2t(\cos k_x + \cos k_y)$ and employing the nesting property in the band dispersion i.e. $\xi^+_{k+Q} = \xi^+_k$, $\xi^-_{k+Q} = -\xi^-_k$ and also the order parameters

$$\triangle^1_{k+Q} = -\triangle^1_0 \left( \frac{\cos k_x a - \cos k_y a}{2} \right) = -\triangle^1_k$$

and

$$\triangle^2_{k+Q} = -\triangle^2_k,$$

the Hamiltonian in the momentum space can be expressed as, $\mathcal{H} = \sum_k \psi^\dagger_k \mathcal{H}(k) \psi_k$ where the four-component spinor $\psi_k$ is, $\psi^\dagger_k = (c^\dagger_{k\uparrow}, c_{-k-Q\downarrow}, c_{-k\downarrow}, c^\dagger_{k+Q\uparrow})$. Thus, the Hamiltonian matrix $\mathcal{H}(k)$ in this basis is written as:

$$\mathcal{H}(k) = \begin{pmatrix} \xi^+_k + \xi^-_k & \triangle^2_k & \triangle^1_k & M_0 \\ \triangle^{2*}_k & -\xi^+_k + \xi^-_k & M_0 & -\triangle^1_k \\ \triangle^1_k & M_0 & -(\xi^+_k + \xi^-_k) & -\triangle^{2*}_k \\ M_0 & -\triangle^1_k & -\triangle^2_k & \xi^+_k - \xi^-_k \end{pmatrix}. \quad (2)$$

In what follows, we study the energy spectrum of the above Hamiltonian. The Hamiltonian (Eq. (3)) is diagonalized and the quasiparticle spectrum is obtained as,

$$E_{\pm,\pm}(k) = \pm \sqrt{\xi^{+2}_k + \xi^{-2}_k + (\triangle^1_k)^2 + \mid \triangle^2_k \mid^2 + M^2_0 \pm 2G}, \quad (3)$$

where

$$G = \sqrt{\xi^{-2}_k \mid \triangle^2_k \mid^2 + (\triangle^2_{1,k} \triangle^1_k - M_0 \xi^+_k)^2 + \xi^{+2}_k \xi^{-2}_k}.$$

It is obvious that the energy spectrum is fully gapped as shown in Figure 1 and the gap closes only when the rhs of the above equation vanishes. A straight forward calculation provides a condition where the gap closes at points $\mathbf{k} = (0,0)$ and $(\pi, \pi)$ is:

$$16t^2 + M^2_0 = (4t' + \mu)^2. \quad (4)$$

Thus, one can find a topologically trivial and non-trivial regions with respect to these parameters. Since the critical phase line is determined by the condition $16t^2 + M^2_0 = (4t' + \mu)^2$ the phase becomes topological in the region where $16t^2 + M^2_0 > (4t' + \mu)^2$ whereas it is trivial for $16t^2 + M^2_0 < (4t' + \mu)^2$. The details of these work have been discussed in a recent paper [22].

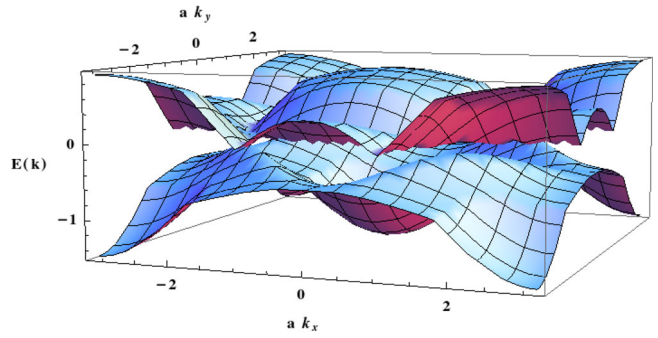


**Fig. 1.** Energy spectra $E_{\pm,+}(k)$, corresponding to coexistence of SC order parameters $d_{x^2-y^2}+(p_x+ip_y)$ and that of the SDW order parameter showing fully gapped spectrum. For illustration, here, we have chosen $t'=-0.3t$, $M_0=0.075t$, $\triangle_0^1=\triangle_0^2=0.005t$, $\mu=0.25t$ ($t=0.30$ eV).

## 3 Thermoelectric transport

In order to study thermoelectric transport in these system, we consider a 2D sample as a ribbon geometry where the ribbon width is taken to be very narrow. This is due to the fact that the edge states can have comparable contribution as compared with the bulk. Using a linear response theory [30], the electric current $j$ and thermal current $w$ which are coupled, are written as:

$$\begin{pmatrix} j/q \\ w \end{pmatrix} = \begin{pmatrix} L_0 & L_1 \\ L_1 & L_2 \end{pmatrix} \begin{pmatrix} -\frac{d\mu}{dx} \\ -\frac{1}{T}\frac{dT}{dx} \end{pmatrix}, \tag{5}$$

where $q$ is the electron charge $-e$, $\mu$ is the chemical potential. Here, the field used are the electric field and the thermal gradient. The electric and thermal transport coefficients are obtained as:

$$\sigma = e^2 L_0, \quad S = -\frac{1}{eT}\frac{L_1}{L_0}, \quad \kappa_e = \frac{1}{T}\frac{L_0L_2 - L_1^2}{L_0},$$
$$ZT = \frac{L_1^2}{L_0L_2 - L_1^2 + \kappa_L T L_0}, \tag{6}$$

where $\kappa_e$ is the electron thermal conductivitiy and $\kappa_L$ is phonon thermal conductivity. Here, $L_\nu$'s are the correlation functions determining the thermoelectric transport coefficients.

Since the topological systems have distinct edge and bulk states, we consider the transport due to both independently. We first consider the edge transport only. To describe the coherent transport of the edge states, we use the Landauer formula. The edge states are assumed to be perfectly conducting and the transmission coefficient $T(E)$ is taken as unity. This is true when the electron energy is within the bulk gap ($-\triangle < E < \triangle$), $\triangle$ being the effective gap. The energy here is measured from the bottom of the conduction band. While carrying out the calculation of the transport coefficients, we consider the bottom of the bulk conduction band and neglect the valence band such that we deal only with the edge states. We further, restrict the chemical potential $\mu$ to be within the gap. The edge state correlation function $L_\nu$ is given by:

$$L_\nu^{\rm e}(\mu) = \frac{2\ell}{sh}\int dE T(E)(E-\mu)^\nu \left(-\frac{\partial f}{\partial E}\right), \tag{7}$$

where the suffix '$e$' means the edge transport, $h$ is the Planck constant and $\ell$ and $s$ respectively are the length and the cross-section of the sample, the factor 2 comes from the two gapless channels of the 2D system. The integral in the above correlation function can be rewritten in a dimensionless form as:

$$L_\nu^e(\bar\mu) = \frac{2\ell}{sh}(k_BT)^\nu \int_{-\bar\triangle}^{\bar\triangle} dy(\bar y-\bar\mu)^\nu \frac{e^{(\bar y-\bar\mu)}}{(e^{(\bar y-\bar\mu)}+1)^2}, \tag{8}$$

where $\bar y = \frac{E}{k_BT}$, $\bar\triangle = \frac{\triangle}{k_BT}$, $\bar\mu = \frac{\mu}{k_BT}$ and $\beta = \frac{1}{k_BT}$, $T$ being the temperature. Using this edge-state correlation functions the thermoelectric coefficients are calculated. It is noticed that the edge contribution to the thermoelectric coefficients such as the figure of merit (ZT) is independent of the system size $\ell$ and $s$ eventhough the edge correlation functions are directly proportional to $\ell$ and inversely proportional to the cross-sectional area $s$. Further, ZT is unusually large and exceeds unity when the chemical potential is in the bulk band. This is due to the fact that when $\mu$ is in the bulk band, the correlation functions $L_0$ has only exponential dependence on $\mu$ but $L_1$ and $L_2$ have combined exponential and algebraic dependence. On the contrary, when the chemical potential is in the bulk gap, ZT becomes exponentially small ($\mu \to 0$) which is in agreement with the figures (see Figs. 2 and 3).

Next, we consider the bulk thermoelectric transport. The bulk transport are calculated using the Boltzmann transport theory. We assume that the relaxation time $\tau_e$ is constant. Since these transports are valid within the inelastic scattering length, we regard the inelastic scattering length as the effective system size. We use only the upper two subbands because there is a large gap between the upper and lower subbands due to the narrow-ribbon confinement. The bulk correlation function $L_\nu$ is written as:

$$L_\nu^{\rm b}(\mu) = \int dE(E-\mu)^\nu \left(-\frac{\partial f}{\partial E}\right) D(E)\tau_e v^2, \tag{9}$$

where the suffix '$b$' means the bulk transport and $\tau_e$ is the relaxation time which is assumed to be constant. Also $D(E)$ and $v$ respectively are the bulk DOS and the velocity. The above integral can be changed to integral over the momentum variables as:

$$L_\nu^b(\mu) = \frac{\tau_e}{c}\int \frac{d^2k}{(2\pi)^2}\left(\frac{\partial E_{+,+}(k)}{\hbar\partial k_x}\right)^2 (E_{+,+}(k)-\mu)^\nu \times \left(-\frac{\partial f(E_{+,+}(k)-\mu)}{\partial E_{+,+}}\right) + (E_{+,+}\to E_{+,-}). \tag{10}$$

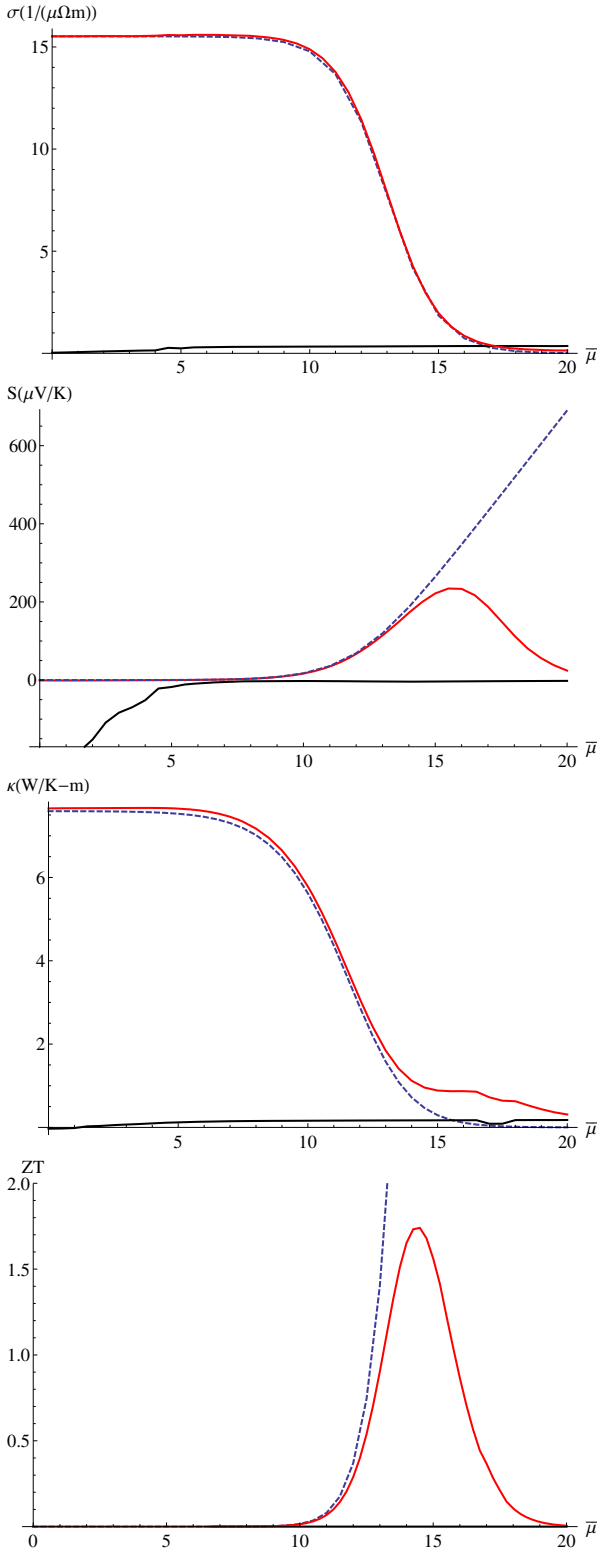


**Fig. 2.** Computation of longitudinal electrical conductivity, thermopower, electronic thermal conductivity and figure of merit as a function of the chemical potential ($\mu$) at $T = 20$ K for $\ell = 1$ $\mu$m. Black curve shows the bulk, dashed curve shows the edge and red curve shows the total contribution to the above quantities. For illustration, here, we have chosen $\triangle_0^1 = \triangle_0^2 = 0.005t$, $M_0 = 0.075t$, $t' = -0.3t$, $\kappa_L = 0.5$ W m$^{-1}$K$^{-1}$, $c = 0.1$ nm ($t = 0.30$ eV).

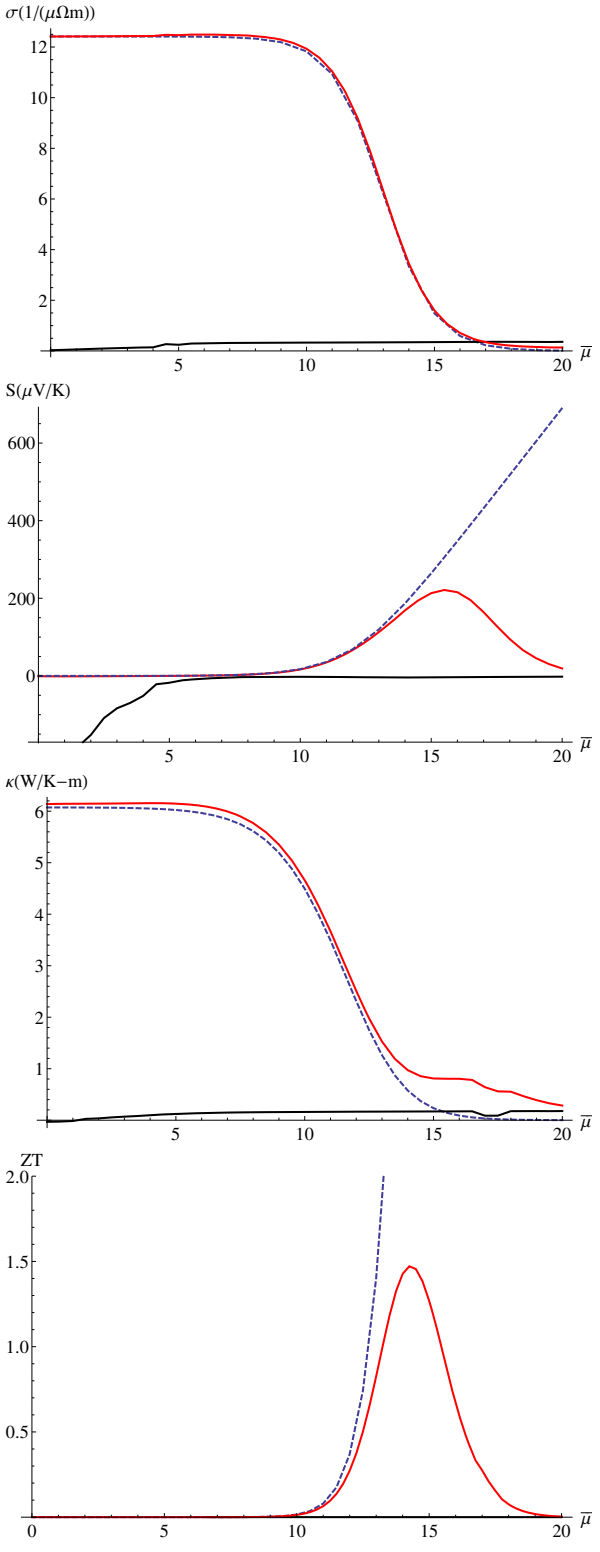


**Fig. 3.** Computation of longitudinal electrical conductivity, thermopower, electronic thermal conductivity and figure of merit as a function of the chemical potential ($\mu$) at $T = 20$ K for $\ell = 0.8$ $\mu$m. Black curve shows the bulk, dashed curve shows the edge and red curve shows the total contribution to the above quantities. For illustration, here, we have chosen $\triangle_0^1 = \triangle_0^2 = 0.005t$, $M_0 = 0.075t$, $t' = -0.3t$, $\kappa_L = 0.5$ W m$^{-1}$K$^{-1}$, $c = 0.1$ nm ($t = 0.30$ eV).

Using dimensionless variables namely $k_x a = y_1$ and $k_y a = y_2$, the above equation is written as:

$$L_\nu^b(\bar{\mu}) = \frac{\tau_e}{c\hbar^2}(k_B T)^{\nu+1} \int_{-\pi}^{\pi} dy_1 \int_{-\pi}^{\pi} dy_2 \left(\frac{\partial \bar{E}_{+,+}(y_1,y_2)}{\partial y_1}\right)^2 \times \left(\bar{E}_{+,+}(y_1,y_2) - \bar{\mu}\right)^\nu \frac{e^{\left(\bar{E}_{+,+}(y_1,y_2)-\bar{\mu}\right)}}{\left(e^{(\bar{E}_{+,+}(y_1,y_2)-\bar{\mu})}+1\right)^2} + \left(\bar{E}_{+,+} \to \bar{E}_{+,-}\right). \quad (11)$$

The variable $\bar{E}_{+,+(-)}$ in the above equations is written as, $\bar{E}_{+,+(-)} = \frac{E_{+,+(-)}}{k_B T}$ which is functions of $y_1 = k_x a$ and $y_2 = k_y a$. Using the parameters in the energy dispersion, the above correlation functions are calculated. It is noted that all the bulk correlations $L_\nu$ behave algebraically when the chemical potential is in the bulk band whereas they have combinations of algebraic and exponential dependence when $\mu$ is in the bulk gap. Meanwhile, the figure of merit is larger when the chemical potential is away from the band edge.

Since the actual thermoelectric transport coefficients involve both the edge and bulk correlation functions, we use $L_\nu = L_\nu^e + L_\nu^b$ and compute the transport properties. It has already been mentioned in the earlier section that the thermoelectric transports in the topological systems are due to the competition between the edge and the bulk contributions. As has already been discussed above, the relative magnitudes of both the edge and the bulk transports for different chemical potentials are different, the figure of merit ZT is also different. When the chemical potential is in the bulk band, ZT from the edge becomes larger eventhogh the number of edge carriers are exponentially small. This is due to the fact that the edge transport is overridden by the bulk contributions and a high ZT from the edge never appears. In a similar way, ZT from the bulk becomes larger when the chemical potential is in the bulk gap. In this case, there are very few bulk carriers whereas there are some edge carriers for which the edge carriers dominate and hence ZT is suppressed. This is a clear indication that in topological system the edge and the bulk transport compete with each other suppressing the total ZT.

In order to compute the transport properties, we consider the following parameters: the hopping integral $t$ is taken as 0.30 eV and the next nearest neighbour hopping integral as $t' = -0.3t$. The SC and SDW order parameters respectively are considered to be $\triangle_0^1 = \triangle_0^2 = 0.005t$, $M_0 = 0.075t$. The computation is performed at a temperature $T = 20$ K. The relaxation time is taken to be $\tau_e = 10^{-13}$ s. The phonon thermal conductivity is taken to be constant which is $\kappa_L = 0.5$ W m$^{-1}$ K$^{-1}$. The effective system size $\ell$ is assumed to be 1 $\mu$m and the cross-sectional area $s$ is taken as 10 nm $\times$ 0.1 nm (Fig. 2) (the same is repeated for $\ell = 0.8$ $\mu$m, see Fig. 3). All these parameters are taken in an adhoc basis and the thermoelectric coefficients are computed. The results are shown in Figures 2 and 3. It is obvious from Figures 2 and 3 that the edge contribution to $\sigma$, $\kappa_e$ and ZT is much higher as compared to the bulk. On the contrary, the Seebeck coefficient has comparable contribution from both, a positive contribution from edge whereas a negative contribution from bulk. Thus, there is a partial cancellation due to opposite charge carriers in the edge and the bulk. This results a peak structure in the Seebeck coefficient near the band edge which makes the figure of merit large.

Due to the edge-bulk competition, there is a possibility that ZT could be maximum when the chemical potential is near the band edge. In such a case, the bulk conduction is dominant at high temperature. On lowering temperature, the bulk-edge cross-over takes place and there is a possibility that ZT might be higher as shown in Figures 2 and 3. The edge current in these system provides ballistic transport but such transport crucially depends on the inelastic scattering length $\ell$ of the edge states (see Figs. 2 and 3 for $\ell = 1$ $\mu$m and 0.8 $\mu$m) because they loose their coherence due to inelastic scattering. At high temperature, $\ell$ is short and the bulk transport is dominant but at low temperature, $\ell$ is long and the edge transport is dominant. This might be the reason why an enhanced figure of merit results at low temperature.

## 4 Conclusion

In conclusion, we summarize the main findings of the present work. The thermoelectric transport in a two-dimensional topological system has been studied. The topological system being a coexistence phase of SC ($d_{x^2-y^2} + (p_x + ip_y)$) and SDW whose topological nature has been studied in an earlier work [22]. Due to the appearance of distinct edge and bulk states in such a topological system, the thermoelectric transport is computed considering both separately. Landauer formulation has been used for the edge transport whereas the bulk transport is computed using Boltzmann transport theory. Since the actual transport involves both the contributions, the competition between them is analyzed in different parameter regimes. It is argued that at low temperature, since the bulk-edge crossover takes place, there might be a possibility that the figure of merit can have high value in such system.

## Author contribution statement

A. Gupta and D. Sa contributed equally to the theoretical research described in this paper and the writing of the manuscript.

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