Thermoelectric and optical probes for Fermi surface topology change in noncentrosymmetric metals

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Noncentrosymmetric metals such as Li2(Pd1−xPtx)3B have different Fermi surface topology below and above the band touching point where spin-degeneracy is not lifted by the spin orbit coupling. We investigate thermoelectric and optical response as probes for this Fermi surface topology change. We show that the chemical potential displays a dimensional crossover from a three-dimensional to one-dimensional characteristics as the descending Fermi energy crosses the band touching point. This dimensional crossover is due to the existence of different Fermi surface topology above and below the band touching point. We obtain an exact expression of relaxation time due to short-range scatterer by solving Boltzmann transport equations self-consistently. The thermoelectric power and figure of merit are significantly enhanced as the Fermi energy goes below the band touching point owing to the underlying one dimensional nature of noncentrosymmetric bulk metals. The value of thermoelectric figure of merit goes beyond two as the Fermi energy approaches to the van Hove singularity for lower spin-orbit coupling. Similarly, the studies of the zero-frequency and finite-frequency optical conductivities in the zero-momentum limit reflect the nature of topological change of the Fermi surface. The Hall coefficient and optical absorption width exhibit distinct signatures in response to the changes in Fermi surface topology.

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I. INTRODUCTION

Breaking of inversion symmetry has far reaching consequences in condensed matter physics. It gives rise to spin-orbit interaction (SOI) which itself serves as the backbone of the rich fast-growing field of spintronics1–3. At the interface of semiconductor heterostructures, the inversion symmetry is broken due to the band mismatch/external electric field, thus gives rise to a particular type of SOI known as Rashba spin-orbit interaction (RSOI)4,5. Besides the breaking of inversion symmetry in bulk semiconductors having zinc blende structures causes Dresselhaus spin-orbit interaction6. The RSOI has potential applications in developing spintronic devices as its strength is externally tunable7 and therefore it is mostly studied. It is revealed that the RSOI can host a plethora of exotic phenomena such as dissipationless spin current8,9, spin Hall effect10–15, spin-orbit torque15,16, and spin galvanic effect15,17.

Angle resolved photo emission spectroscopy has confirmed the existence of large spin splitting in several systems such as Bi/Ag(111) surface alloy18, topological insulators like Bi2Se3 etc.19,20. The spin-orbit coupling strength found in these systems are larger in magnitude at least by two orders than that found in conventional semiconductor heterostructures. The recent discovery of giant RSOI in three dimensional (3D) polar semiconductor BiTeX (X=Cl, Br, I) has triggered immense investigations in the field of spintronics both theoretically and experimentally. The surface states of BiTeX exhibit large Rashba splitting as a result of surface induced asymmetry. The origin of giant RSOI in the bulk of such materials has been unveiled by $\mathbf{k} \cdot \mathbf{p}$ perturbation analysis22 and is attributed to the distinct crystal structure of BiTeX and large SOI of Bi. Itinerant electrons also experience strong RSOI in $\text{B}_2\text{O}_3$ compounds20 and noncentrosymmetric metals such as Li2(Pd1−xPtx)3B27. The material Li2(Pd1−xPtx)3B exhibits superconductivity28,29 as result of inversion symmetry breaking whereas $\text{B}_2\text{O}_3$ compounds30–33 host nontrivial spin textures including spin helix and magnetic skyrmions. The spin-momentum locking in Li2(Pd1−xPtx)3B has distinct structure than that in the BiTeX family. Therefore, this noncentrosymmetric material has drawn immense interest from the perspective of superconductivity34. Kerr rotation27,35, spin susceptibility37,39 and Ruderman-Kittel-Kasuya-Yosida interaction37.

To probe electronic states in BiTeX materials various investigations have been performed recently in the context of transport38–44, thermoelectric45,46, and optical47–49 response. However, such studies are still missing in the case of spin-orbit coupled noncentrosymmetric metal like Li2(Pd1−xPtx)3B which has different Fermi surface topology below and above the band touching point. This lack of information motivates us to address the issue that whether the thermoelectric and optical probes can be used to extract the information about the topology of the Fermi surface in noncentrosymmetric metals like Li2(Pd1−xPtx)3B. In this work, we provide a systematic study of thermoelectric transport coefficients and optical responses in noncentrosymmetric metals. We find that the chemical potential exhibits a dimensional crossover from a 3D to 1D characteristics as the Fermi energy goes below the band touching point (BTP). This feature is attributed to the existence of different Fermi surface topology above and below the BTP. We obtain
exact expression of relaxation time assuming short-range electron-impurity scattering, by solving the Boltzmann transport equations including interband scattering self-consistently. We provide results of all thermolectric transport coefficients. The thermolectric power and figure of merit are significantly enhanced below BTP owing to the underlying 1D nature of this system as a consequence of change in Fermi surface topology. We obtain a remarkable value, more than 2 of thermolectric figure of merit for low density below BTP and \( \alpha = 0.2eV\mu m \). Similarly, the studies of the zero-frequency and finite-frequency optical conductivities shed some light on the nature of spin-split energy gap and would help to extracting the spin-orbit coupling strength. We find that Hall coefficient and optical absorption width respond differently to the change in the Fermi surface topology.

This paper is organized as follows. In section II, we provide a discussion on the ground state properties of the physical system considered. In Section III, we discuss various thermolectric properties. Section IV includes information of the Drude weight, Hall coefficient and finite-frequency optical conductivity. We summarize our main results in Section V.

II. GROUND STATE PROPERTIES

We consider conduction electrons in a 3D noncentrosymmetric metal. As mentioned in the introduction, the usual examples of noncentrosymmetric metals are LiI_{2}(Pd_{3-x}Pt_x)B and B_{2}O_{3} compounds. All these materials possess cubic crystal structure. In this particular lattice geometry, the low energy conduction electrons can be effectively described by the following Hamiltonian\(^{26,34}\)

\[
H = \frac{\hbar^2 k^2}{2m^*} + \alpha \sigma \cdot k,
\]

where \( m^* \) is the effective mass of electron, \( \sigma_0 \) is 2 \times 2 identity matrix, \( \sigma = \{\sigma_x, \sigma_y, \sigma_z\} \) is Pauli spin matrix, \( k = \{k_x, k_y, k_z\} \) with \( k = \sqrt{k_x^2 + k_y^2 + k_z^2} \) is the electron’s wavevector, and \( \alpha \) is the Rashba spin-orbit coupling. The RSOI term in Eq. (1) has the form \( \sigma \cdot k \) in which \( k_x, k_y \), and \( k_z \) are intertwined with \( \sigma_x, \sigma_y \), and \( \sigma_z \), respectively. This distinct spin-momentum locking is absent in 2D Rashba systems and 3D Rashba semiconductors such as BiTeI and therefore gives rise to particular Fermi surface topology, different than other Rashba systems, which will be discussed shortly. Note that the Hamiltonian commutes with the helicity operator \( k \cdot \sigma / k \) so that its eigenvalues \( \pm 1 \) are good quantum numbers. Thus, the eigenstates of the above Hamiltonian can be obtained as eigenstates of the helicity operator modulated by a plane wave like \( \psi_{k}^{\lambda}(r) = \phi_{k}^{\lambda} e^{i \mathbf{k} \cdot \mathbf{r}} / \sqrt{V} \), where \( V \) is volume of the system, \( \lambda = \pm \) represents two opposite helicity, and \( \phi_{k}^{\lambda} \) is helicity eigenstate which takes the following forms: \( \phi_{k}^{+} = [\cos(\theta/2), e^{i\phi} \sin(\theta/2)]^T \) for \( \lambda = + \) and \( \phi_{k}^{-} = [\sin(\theta/2), -e^{i\phi} \cos(\theta/2)]^T \) for \( \lambda = - \), with \( T \) being the transpose operation. Here, \( \theta \) and \( \phi \) are the polar and azimuthal angle, respectively, which represent the orientation of \( k \). The energy dispersion consists of two spin-split bands corresponding to \( \lambda = \pm \) having the structure \( E_{\lambda}(k) = 2\hbar^2 k^2 / (2m^*) + \lambda \alpha k \). This dispersion is depicted in Fig. 1(a). The band \( E_{-}(k) \) has a non-monotonic behavior for \( E < 0 \) and attains a minimum value \( E_{\min} = -E_{\alpha} = -\hbar^2 k^2 / (2m^*) \) at \( k = k_\alpha = m^* \alpha / \hbar^2 \). Although the energy spectrum in the present scenario looks similar to those for the 2D Rashba system found in III-V semiconductor heterostructures and 3D Rashba semiconductors, but it is different from the former ones in topological sense. In Fig. 1(b) and Fig. 1(c), constant energy surfaces are shown for \( E > 0 \) and \( E < 0 \), respectively. The wavevectors corresponding to \( E > 0 \) are given by \( k_\pm = \mp k_\alpha + \sqrt{k_\alpha^2 + 2m^* E / \hbar^2} \). Here, \( k_\pm \) represent the radii of the two concentric spherical constant surfaces as shown in Fig. 1(b). For \( E > 0 \), the topology of the Fermi surface has convex-convex shape on \( \lambda = + \) and \( \lambda = - \) bands respectively. The corresponding density of states for \( \lambda = \pm \) bands are given as

\[
D_{\pm}^\lambda(E) = \frac{1}{4\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \left[ \frac{E + 2E_\alpha}{\sqrt{E + E_\alpha}} \mp 2\sqrt{E_\alpha} \right].
\]

On contrary for \( E < 0 \), there exists only one energy band \( E_\alpha \) and the topology of energy surface changes completely as compared to \( E > 0 \). For \( E < 0 \), the topology of the Fermi surface has concave-convex shape on the inner and outer branches, respectively. The cross-section of the Fermi surface for \( E < 0 \) is shown in Fig. 1(c). This is characterized by the following wave vectors \( k_{1,2} = k_\alpha \mp \sqrt{k_\alpha^2 + 2m^* E / \hbar^2} \). It is worthy to mention that \( 0 \leq k_1 \leq k_\alpha \) and \( k_\alpha \leq k_2 \leq 2k_\alpha \). The region between two concentric spherical shells with the inner radius \( k_1 \) and outer radius \( k_2 \) contains the following available density of states

\[
D_{1,2}^{\lambda}(E) = \frac{1}{4\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \left[ \frac{E + 2E_\alpha}{\sqrt{E + E_\alpha}} \mp 2\sqrt{E_\alpha} \right].
\]

It is interesting to note that there is an inverse square-root divergence of \( D_{1,2}^{\lambda}(E) \) \((\eta = 1, 2)\) as \( E \to -E_\alpha \), similar to the van Hove singularity in conventional one-dimensional systems as well as in 2D Rashba systems. The large DOS in the very low-density \((E \to -E_\alpha)\) limit is due to the non-vanishing spherical energy surfaces with the radii \( k_{1,2} \) approach to \( k_\alpha \), and vanishing velocity as \( v(k) = (1/\hbar) \nabla_k E_\alpha(k) \propto \sqrt{E + E_\alpha} \).

For a given electron density \( n_e \), the chemical potential \( \mu \) at temperature \( T \) can be obtained from the normalization condition

\[
n_e = \sum_{\eta} \int_{-E_\alpha}^{0} f(E_\eta) D_{\eta}^{\lambda}(E) dE + \sum_{\lambda} \int_{0}^{\infty} f(E_\lambda) D_{\lambda}^{\lambda}(E) dE, \tag{4}
\]

where \( f(E) = [e^{(E-\mu)/(k_B T)} + 1]^{-1} \) is the Fermi-Dirac distribution function. In the \( T \to 0 \) limit, we obtain Eq.
known result of the Fermi energy for conventional 3DEG: \( \alpha \) changes at \( E \) changes at band touching point (BTP). (b) Cross-sections of the Fermi surface for \( E_F > 0 \) and \( E_F < 0 \). The Fermi surface topology has convex-convex shape and concave-convex shape for \( E_F > 0 \) and \( E_F < 0 \) respectively. The Fermi surface topology changes at band touching point (at \( E_F = 0 \)).

![FIG. 1: (a) Spin-split energy bands of the noncentrosymmetric metals: The two bands touch at \( k = 0 \) which is known as band touching point (BTP). (b) Cross-sections of the Fermi surface for \( E_F > 0 \) and \( E_F < 0 \). The Fermi surface topology changes at band touching point (BTP).](image1)

\[
3\pi^2 n_e = \sqrt{k_\alpha^2 + \frac{2m^* E_F}{\hbar^2}} \left[ 4k_\alpha^2 + \frac{2m^* E_F}{\hbar^2} \right].
\]

Note that with \( \alpha = 0 \) Eq. (5) correctly reproduces the known result of the Fermi energy for conventional 3DEG: \( E_F^0 = \frac{k_\alpha^2}{2m^*} (3\pi^2 n_e)^{2/3} \). The topology of the Fermi surface changes at \( n_e = n_t \) with \( n_t = 4k_\alpha^3/3\pi^2 \). For a given \( \alpha \), \( E_F < 0 \) when \( n_e < n_t \) and \( E_F > 0 \) when \( n_e > n_t \). At finite temperature, we obtain the chemical potential \( \mu \) by solving Eq. (4) numerically for \( \alpha = 0.1 \) eVnm. For three different temperatures, namely, \( T = 5, 10, \) and \( 20 \) K, the difference between the chemical potential and Fermi energy is shown in Fig. 2. We find that \( \mu - E_F \) exhibits a dimensional crossover as the Fermi energy changes its sign. For instance, \( \mu - E_F \) is negative when \( E_F > 0 \). This feature corresponds to the nature of chemical potential in 3D case. On contrary, for \( E_F < 0 \), \( \mu - E_F \) is positive. This behavior is clearly a hallmark of \( \mu \) in 1D case. However, this indirect signature of dimensional crossover is not clearly seen from the structures of the density of states corresponding to \( E_F > 0 \) and \( E_F < 0 \).

III. THERMOELECTRIC TRANSPORT

A. General Formalism

We consider the physical system is subjected to a spatially uniform electric field \( \mathbf{E} \) and a temperature gradient \( \nabla T \). The magnitude of the external electric field and temperature gradient are chosen in such a way that the linear response theory holds.

![FIG. 2: Difference between \( \mu \) and \( E_F \) as a function of \( E_F \) at a fixed \( \alpha = 10^{-10} \) eVnm for \( T = 5, 10, \) and \( 20 \) K. The change in sign of \( \mu - E_F \) at \( E_F = 0 \) implies the dimensional crossover.](image2)
present scenario. Let us now restrict ourselves to consider that the scattering mechanisms, responsible for thermoelectric transport, are due to the presence of weak spin-independent disorders distributed throughout the sample with an average density $n_{\text{imp}}$. The short-range disorder potential is given by $U(\mathbf{r}) = U_0 \sum_i \delta(\mathbf{r} - \mathbf{r}_i)$, where $U_0$ is the strength of the potential having dimension of energy times volume and $\mathbf{r}_i$ is the position of the $i$-th scatterer.

Note that the present situation is an example of isotropic case since the energy spectrum depends only on the magnitude of $\mathbf{k}$. In this case $L^{(r)}_{\nu'\nu} = L^{(r)}_{\nu} \delta_{\nu'\nu} \equiv L^{(r)}$. Also the expectation value of $\hat{n}_\nu(\mathbf{k})$ with respect to the state $\lambda$ is $\langle \hat{n}_\nu(\mathbf{k}) \rangle_\lambda = \frac{\hbar k_F}{m^*} + \lambda \frac{\hbar k_F}{e}$. Eq. (8) can be rewritten further as

$$L^{(r)} = \frac{e^2}{(2\pi)^3} \sum_{\lambda=\pm} \int \frac{d^3 k}{(2\pi)^3} (E_{k\lambda})^2 (\hat{n}_\nu(\mathbf{k}))^2 \left( \frac{\partial f_0^0}{\partial E_{k\lambda}} - \frac{\partial f_0^0}{\partial E_{k\lambda}} \right).$$

B. Results

Here we discuss the behavior of different thermoelectric coefficients obtained via the numerical solution of Eq. (12). For numerical calculation we consider following material parameters: effective mass of electron $m^* = 0.5m_e$, $m_e$ is the free electron mass and $\alpha_0 = 10^{-10}$eV.m.

Let us begin with the behavior of the electrical conductivity $\sigma = L_{11} = L^{(0)}$. From Eq. (12), we explicitly have $\sigma = 4e^2x_0/(3\hbar l_0)$. Figure 3(a) depicts the variation of $\sigma$ with chemical potential for $\alpha = 0.2\alpha_0$, $0.5\alpha_0$, and $\alpha_0$ at $T = 5$ K. The conductivity increases monotonically with $\mu$. For higher values of $\alpha$, the enhancement of $\sigma$ is significant. In the $T \to 0$ limit, we obtain the following analytical expression of $\sigma$ as (see Appendix for detail derivation)

$$\sigma = \frac{e^2}{\hbar m^* n_{\text{imp}} l_0^2} \left[ \frac{1}{2} - \frac{E_F^2}{6(E_F + E_f)^2} \right],$$

which shows that the zero temperature conductivity increases linearly with the Fermi energy. Note that the characteristics of $\sigma$ with $E_F$ in the $E_F > 0$ and $E_F < 0$ are the same. This is different from the behavior of $\sigma$ with $E_F$ in 2D Rashba systems$^{23}$ in which it was found that the zero temperature conductivity depends on the Fermi energy in linear (quadratic) fashion for $E_F > 0$ ($E_F < 0$). This feature was attributed to the fact that $\sigma(\mathbf{k})$ cannot be continuously differentiated at $E_F = 0$. In this 2D Rashba system density of states of individual bands/branches depends linearly on wave vector, which immediately implies that total density of states below and above BTP have different energy dependence. So relaxation time having same structures below and above the BTP will have different energy dependence. As a result of this the electrical conductivity being proportional to the relaxation time shows different energy dependence below and above BTP. However, in the present context,
Eq. (14) clearly demonstrates that $\sigma(E)$ is a continuously differentiable function at $E_F = 0$. This fact helped us to find same analytical structures of $\sigma(E_F)$ in both $E_F > 0$ and $E_F < 0$ regions. From Eq. (14) it is evident that $\sigma \propto E_\alpha$ at $E_F = 0$. The signature of this feature is also reflected in Fig. 3(a). The reason of not seeing the direct indication of change in Fermi surface topology in electrical conductivity in our case is that the density of states depends on square of the wave vector as a consequence of the 3D system. It implies that form of total density of states, and hence relaxation time will have the same below and above the BTP (see Appendix for more details).

![FIG. 3: Plots of (a) electrical conductivity $\sigma$ and (b) thermal conductivity $κ$ as a function of chemical potential $μ$ at temperature $T = 5$ K for three different values of $α$.](image)

The thermal conductivity $κ$ is obtained as $κ = (4/π^2)\kappa_0κ_I$, where $κ_0 = e^2E_0T/(\hbar\lambda_0)$ with $λ_0 = (π^2/3)(k_B/e)^2$ is the Lorentz number for 3D electron gas and $κ_I = X_2 - X_e^2/X_0$. The variation of the thermal conductivity with the chemical potential is depicted in Fig. 3(b). The thermal conductivity behaves with the chemical potential in a similar fashion as the electrical conductivity.

We obtain the thermopower through explicit calculation as $S = -(k_B/e)S_T$ where $S_T = X_1/X_0$. In Fig. 4, we show the dependence of $S$ on $μ$ for $α = 0.2α_0$, $0.5α_0$ and $α_0$. The thermopower is large at lower values of $α$ as compared to higher $α$. In the region below, $E_F = 0$, thermopower increases rapidly with $μ$. For $E_F > 0$, the rate of increase of $S$ with $μ$ is slow compared to the previous case. Moreover, for higher $α$, the thermopower attains a saturation value when $μ > 0.5E_α$. In the $|E_F| \gg k_BT$ limit, using the Mott relation one may obtain the following expression of thermoelectric power

$$S_{\text{Mott}} = -\frac{π^2k_BT}{3e} \frac{d\ln σ(E)}{dE} \bigg|_{E=E_F},$$ \hspace{1cm} (15)

one may obtain the following expression of thermoelectric power

$$S_{\text{Mott}} = -\frac{π^2k_BT}{3e(E_F + E_α)} \left[ 1 - \frac{2E_FE_α(E_F + E_α)}{(E_F + 2E_α)ξ_F} \right],$$ \hspace{1cm} (16)

where $ξ_F = E_0^2 + 6E_αE_F + 6E_0^2$. The inset of Fig. 4 shows the variation of $S/S_{\text{Mott}}$ as a function of chemical potential for different values of $α$ at $T = 5$ K. For lower values of $α$, namely, $α = 0.2α_0$, the Mott relation is valid only when $μ > 0.5E_α$. The degree of validity of the Mott relation increases with $α$. For $α = α_0$, the Mott formula is satisfied almost in the entire range of the chemical potential considered. It is known that the validity of Mott relation or the Sommerfeld expansion depends on the following simultaneous conditions: (1) $T \ll T_F$ where $T_F = E_F/k_B$ is the Fermi temperature and (2) whether the Taylor expansion of $σ(E)$ about $E = μ$ is possible or not. In our case Condition (2) is satisfied always because $σ(E)$ is a continuously differentiable function. Therefore we attribute the breakdown of Mott relation (as shown in Fig. 4) to the breakdown of the validity of Condition (1).

![FIG. 4: Plots of the thermopower $S$ as a function of chemical potential $μ$ at temperature $T = 5$ K for three different values of $α$.](image)

![FIG. 5: Plots of the thermoelectric figure of merit $ZT$ as a function of chemical potential $μ$ at temperature $T = 5$ K for three different values of $α$.](image)

The thermoelectric figure of merit is a dimensionless number which measures the efficiency of the thermoelectric performance of a material. It is defined as $ZT = S^2σT/κ$. In general, the symbol $κ$ used in the definition of $ZT$ should stand for the total thermal conductivity which is a sum of electronic and phononic contribution. But, in the temperature regime we are focusing...
on now, the electronic thermal conductivity dominates over the thermal counterparts. Therefore, we neglect lattice contribution to the thermal conductivity and proceed with the electronic counterpart for the subsequent calculation of ZT. Materials with higher figure of merit can be used for good thermoelectric devices. So a good thermoelectric material needs to possess following properties: large electrical conductivity, high thermopower, and low thermal conductivity. For the current scenario, we obtain ZT explicitly as \( ZT = S^2 T / \kappa L \). In Fig. 5 we show the dependence of ZT on the chemical potential at \( T = 5 \) K for three different values of \( \alpha \), namely, \( \alpha = 0.2 \alpha_0 \), \( 0.5 \alpha_0 \), and \( \alpha_0 \). It is clear that ZT behaves as a monotonically decreasing function of \( \mu \) for each \( \alpha \). The value of ZT is higher at lower \( \alpha \). This is obvious because the order of magnitude of \( \sigma \) and \( \kappa \) are almost same for each \( \alpha \) whereas the thermopower is large at lower \( \alpha \). In other words, the thermopower alone determines the behavior of ZT. Note that For \( \alpha = 0.2 \alpha_0 \), ZT attains a remarkable value greater than 2 when the chemical potential lies far below the BTP. To explain this feature explicitly, in Fig. 6 we plot \( D(E) \), \( D(E)\langle - \partial f^0 / \partial E \rangle \), and the integrand of \( L \) which is proportional to \( S^2 \) as a function of energy for a particular \( \alpha \), namely \( \alpha = \alpha_0 \). We consider two different densities, namely, \( n^{(1)}_e \) and \( n^{(2)}_e \) which in turn correspond to chemical potential \( \mu_1 \) and \( \mu_2 \), respectively, at some constant temperature \( T \). The chemical potential \( \mu_1 \) lies above the band touching point whereas \( \mu_2 \) falls well below of it. As expected the function \( D(E)\langle - \partial f^0 / \partial E \rangle \) exhibit a peak whenever the energy matches with the chemical potential. For \( n_e = n^{(1)}_e \), as expected the integrand of \( L \) changes sign when the energy crosses \( \mu_1 \) and exhibits a structure as shown by the shaded portion. It is hard to differentiate between the areas under the curves (shaded region in Fig. 6) below and above \( \mu_1 \). Therefore, when summed up it gives rise to negligible contribution to the thermoelectric power which is reflected in Fig. 4. When \( n_e = n^{(2)}_e \), the asymmetry between the magnitudes of \( L \) below and above \( \mu_2 \) can be visible. This increment in the asymmetry is responsible for the enhancement of thermopower below BTP. The amount of asymmetry increases as the chemical potential approaches \(-E_\alpha\). As we tune the chemical potential from positive to negative value the amount of asymmetry increases due to the dimensional crossover from 3D to 1D, which leads to an increase of thermopower as well as thermoelectric figure of merit. There have been several studies before, where it has been shown that the low dimensional systems lead to larger asymmetry in the density of states about the chemical potential, which give rise to larger thermopower and thermoelectric figure of merit and hence can be used for good thermoelectric device applications. Our result is consistent with these observations as we obtain larger value of figure of merit below the BTP due to the underlying 1D characteristics of our bulk 3D system. It can be verified that the amount of asymmetry will become more prominent for the cases of lower \( \alpha \). This asymmetry explains the higher values of ZT obtained for low \( \alpha \). Therefore, one has to struggle to fix both \( \alpha \) and \( n_e \) at reasonable values in order to use 3D noncentrosymmetric metal for good thermoelectric devices. Also the thermopower \( S \) and figure of merit \( ZT \) tend to diverge as \( \mu \) approaches \(-E_\alpha\). This fact is attributed to the presence of the van Hove singularity in the band structure, similar to quasi-1D systems.\(^{53}\)

\[
IV. \text{ZERO-MOMENTUM OPTICAL CONDUCTIVITY}
\]

In this section, we present optical signature of a change in the Fermi surface topology in noncentrosymmetric metals at \( T = 0 \). The zero-frequency and finite-frequency optical conductivities are manifestation of the intra-band and interband optical transitions, respectively. Consider the noncentrosymmetric metal is irradiated by a weak and spatially homogeneous electric field \( \mathbf{E} = E_0 \mathbf{e}^{\omega t} \) oscillating with the frequency \( \omega \) and amplitude \( E_0 \). The absorptive part of the charge optical conductivity tensor is given by \( \Re \Sigma_{\nu \nu'}(\omega) = \delta(\omega)D_{\nu \nu'}^{\omega} + \Re \sigma_{\nu \nu'}(\omega) \), where \( \nu, \nu' = x, y, z \) and \( D_{\nu \nu'}^{\omega} \) is the Drude weight (charge stiffness). The semiclassical expression of the Drude weight \(^{30}\) is given by

\[
D_{\nu \nu'}^{\omega} = \pi e^2 \sum_{\lambda} \int \frac{d^3k}{(2\pi)^3} \langle \hat{\mathbf{v}}_\nu \rangle_\lambda \langle \hat{\mathbf{v}}_{\nu'} \rangle_\lambda \delta(E_\lambda(k) - \nu E_F) \tag{17}
\]

This semiclassical expression has been successfully used in 2DEG with linear spin-orbit interaction as well as in 2D hole gas with \( k \)-cubic spin-orbit interaction.\(^{54}\) The exact analytical expression of the Drude weight is obtained as

\[
D_{\nu \nu'}^{\omega} = \pi e^2 n_e \frac{E_F + 2E_\alpha}{E_F + 4E_\alpha} \delta_{\nu \nu'} \theta(E_F + E_\alpha). \tag{18}
\]

The longitudinal Drude weight is isotropic i.e. \( D_{xx}^{\omega} = D_{yy}^{\omega} = D_{zz}^{\omega} = D_{\omega} \) and the off-diagonal Drude weight...
vanishes exactly. Setting $\alpha = 0$ in the above equation, we get the standard result of the Drude weight for 3DEG i.e. $D^0_w = \pi n_v e^2/m^*$. It shows that the spin-orbit coupling reduces the Drude weight as compared to the conventional 3DEG without spin-orbit coupling and further an increase in $\alpha$ decreases it more as shown in Fig. 7(a). We also see in Fig. 7(a) that similar to Drude conductivity, Drude weight also shows no signature of change in Fermi surface topology.

FIG. 7: Plots of the Drude weight $D_{\alpha}(a)$ and the Hall coefficient $R_H$ (b) as a function of carrier density $n_e$ for two different values of $\alpha$. Here $n_i^{\alpha}(i=1,2) = 4k_{i\alpha}/(3\pi^2)$ (with $i = 1, 2$) is the density at which $E_F$ changes its sign i.e. the topology of the Fermi surface changes at $n_t$.

It has been shown$^{55,56}$ that the Hall coefficient $R_H$ can be obtained from the Drude weight using the general expression

$$R_H = -\frac{1}{eD_w} \frac{\partial D_w}{\partial n_e}.$$  

This expression has been successfully used to calculate the Hall coefficient in various systems$^{55-57}$. For the present system, the exact Hall coefficient is given by

$$R_H = R_0^\alpha \left[ 1 + \frac{2E_\alpha(E_\alpha + E_F)}{3(2E_\alpha + E_F)^2} \theta(E_F + E_\alpha) \right],$$  

(19)

where $R_0^\alpha = -1/(eD_w)$ is the Hall coefficient for $\alpha = 0$ case. Equation (19) clearly shows the Hall coefficient is enhanced due to the presence of the spin-orbit coupling. In the low-density limit, $E_F$ is comparable to $E_\alpha$ and therefore pronounced effect of the spin-orbit coupling can be realized when $E_F < 0$ as seen in Fig. 7(b). It is interesting to notice here that Hall coefficient responds to the change in the Fermi surface topology. As shown in Fig. 7(b), it first rises sharply until $n_t$ where transition occurs and then starts decreasing with further increase in density. The peak in $R_H/R_0^\alpha$ at the BTP is the signature of the change in the Fermi surface topology. Generally we estimate carrier concentration from the Hall coefficient measurement. It is interesting to note that for noncentrosymmetric metals we can also estimate the strength of RSOI from this measurement by noting the transition density $n_t$ which depends on $\alpha$.

The finite-frequency optical conductivity $\sigma_{\nu\nu'}(\omega)$ is arising due to the transitions between the spin-split states. Within the linear response Kubo formalism, the frequency-dependent optical conductivity is given by

$$\sigma_{\nu\nu'}(\omega) = \frac{1}{\hbar(\omega+i0^+)} \int_0^\infty dt e^{i(\omega+i0^+)t} \langle [\hat{j}_\nu(t), \hat{j}_{\nu'}(0)] \rangle.$$  

Here $\hat{j}_\nu$ are the components of the charge current operator, $\nu = e\hat{v}_\nu \cdot \mathbf{r}$ and $f(E_\lambda(k))$ is the Fermi-Dirac distribution function.

FIG. 8: (a) Plots of the Re $\sigma_{\nu\nu'}$ as a function of $\hbar\omega$ for $E_F < 0$. Solid and dashed curves corresponds to same $\alpha$ but different densities and have optical absorption widths $\Delta_{\nu\nu}$ respectively. Here $\Delta_{\nu\nu}^1 < \Delta_{\nu\nu}^2$ as $n_{\nu\nu}^1 < n_{\nu\nu}^2$, so $\Delta$ depends on density as mentioned in the text. (b) Plots of the Re $\sigma_{\nu\nu'}$ as a function of $\hbar\omega$ for $E_F > 0$. Solid and dashed curves corresponds to same $\alpha$ but different densities and have optical absorption widths $\Delta_{\nu\nu}$ respectively. Here $\Delta_{\nu\nu}^1 = \Delta_{\nu\nu}^2$ but $n_{\nu\nu}^1 < n_{\nu\nu}^2$, so $\Delta$ is independent of carrier density as mentioned in the text. Dotted-dashed curve corresponds to different values of $\alpha$ and $n_e$, here $\Delta$ becomes more narrow because of the smaller value of $\alpha$. (b) Plots of the Re $\sigma_{\nu\nu'}$ as a function of $\hbar\omega$ for $E_F > 0$. Solid and dashed curves corresponds to same $\alpha$ but different densities and have optical absorption widths $\Delta_{\nu\nu}$ respectively. Here $\Delta_{\nu\nu}^1 = \Delta_{\nu\nu}^2$ but $n_{\nu\nu}^1 < n_{\nu\nu}^2$, so $\Delta$ is independent of carrier density as mentioned in the text. Dotted-dashed curve corresponds to different values of $\alpha$ and $n_e$, here $\Delta$ becomes more narrow because of the smaller value of $\alpha$. The dotted thin line in both the parts shows the finite temperature behavior of the optical conductivity for $\alpha_1$ and $n_{e1}$.

After some straightforward calculation, the real part of charge optical conductivity is given by

$$\text{Re } \sigma_{\nu\nu'}(\omega) = \frac{e^2}{8\pi^2\omega} \int d^3k [f(E_-(k)) - f(E_+(k))] v^+_{\nu\nu'}(k) \times v^+_{\nu\nu'}(k) \delta(E_+(k) - E_-(k) - \hbar\omega),$$  

(20)

where

$$(v^+_{\nu\nu}(k) = \frac{\alpha}{\hbar} [e^{-2i\phi \sin^2(\theta/2) - \cos^2(\theta/2)}],$$  

(21)

$$(v^+_{\nu\nu}(k) = \frac{\alpha}{\hbar} [e^{-2i\phi \sin^2(\theta/2) + \cos^2(\theta/2)}],$$  

(22)

$$(v^+_{\nu\nu}(k) = \frac{\alpha}{\hbar} e^{-i\phi} \sin \theta$$  

(23)

and $v^+_{\nu\nu}(k) = [v^+_{\nu\nu}(k)]^*$. The only root of the equation $E_+(k) - E_-(k) - \hbar\omega = 0$ is $k_\omega = \hbar\omega/2\alpha$. Using the result
of the following angular integrations,
\[ \int_0^\pi \int_0^{2\pi} u^{\nu,\nu'}_\nu(\mathbf{k}) \sin \theta d\theta d\phi = \frac{8\pi a^2}{3h^2} \delta_{\nu\nu'}, \quad (24) \]
the final expression of real part of the optical conductivity at \( T = 0 \) is given by,
\[
\Re \sigma_{\nu\nu'}(\omega) = \frac{e^2 k_F}{h} \left[ \theta(2\alpha k_F - \hbar \omega)\theta(\hbar \omega - 2\alpha k_F)\theta(E_F) \\
+ \theta(2\alpha k_F - \hbar \omega)\theta(\hbar \omega - 2\alpha k_F) \times \theta(-E_F)\theta(E_F + E_a) \right] \delta_{\nu\nu'}. \quad (25)
\]
Equation (25) shows the isotropic nature of the longitudinal optical conductivities: \( \Re \sigma_{xx}(\omega) = \Re \sigma_{yy}(\omega) = \Re \sigma_{zz}(\omega) \equiv \Re \sigma(\omega) \) and absence of the off-diagonal conductivities: \( \Re \sigma_{\nu\nu'}(\omega) = 0 \) for \( \nu \neq \nu' \).

For \( E_F \geq 0 \), the interband optical transitions would occur when the photon energy (\( \hbar \omega \)) obeys the inequality \( 2\alpha k_F^2 \leq \hbar \omega \leq 2\alpha k_F^2 \) at \( T = 0 \). On the other hand, for \( E_F \leq 0 \), the interband optical transitions take place when the photon energy satisfies the inequality \( 2\alpha k_F^2 \leq \hbar \omega \leq 2\alpha k_F^2 \) at \( T = 0 \). The optical absorption width, the region where \( \Re \sigma(\omega) \) remains non-zero, is \( \Delta_+ = 8E_a \) for \( E_F \geq 0 \) and \( \Delta_- = 8\sqrt{E_a^2 + E_a E_F} \) for \( E_F \leq 0 \). Interesting to note that \( \Delta_+ \) is independent of the carrier density, whereas \( \Delta_- \) depends on the both carrier density as well as Rashba energy \( E_a \) as shown in Fig. 8. The density dependence of \( \Delta_- \) is attributed to the topological change in the Fermi surface. So the optical conductivity shows a distinct response to the change in the Fermi surface topology. The absorption widths can be used to determine the value of \( \alpha \) experimentally. The magnitude of the optical conductivity at the left and right edges, respectively, are \( \sigma_{L/R}^+ = \frac{e^2 k_F^2}{3h} \) for \( E_F \geq 0 \) and \( \sigma_{L/R}^- = \frac{e^2 k_F^2}{3h} \) for \( E_F \leq 0 \). We observe that \( \sigma_L^+ < \sigma_R^+ \) and \( \sigma_L^- < \sigma_R^- \) which is also clear from Fig. 8. It is interesting to note that the spin-split energy gap is of the order of 0.1 eV for the carrier density \( n_c = 10^{25} \text{ m}^{-3} \) and \( \alpha = 1.0 \times 10^{-10} \text{ eV-m} \). This energy scale is comparable to the electromagnetic radiation with high frequency \( \omega \sim 10^3 \text{ Hz} \). The high-frequency radiation would flip the spin in a very short time. The non-centrosymmetric semiconductors can be used for high-speed electronic devices.

V. SUMMARY AND CONCLUSIONS

In summary, we have theoretically studied signatures of the Fermi surface topology change in thermoelectric and optical properties of noncentrosymmetric metals. The noncentrosymmetric metals possess distinct Fermi surface topology which depends on the sign of the Fermi energy. As a result of this, the chemical potential is found to exhibit a dimensional crossover from 3D to 1D behavior as the Fermi energy switches its sign from positive to negative one. It is shown that the electrical conductivity is continuously differentiable at the band touching point, as opposed to 2D Rashba systems. There is a significant enhancement of thermopower in the low density regime which is responsible to obtain a remarkable thermoelectric figure of merit with value more than 2. However the figure of merit is found to decrease with the increase of the strength of the Rashba spin-orbit interaction. This feature is explained qualitatively. It is shown that the Hall coefficient first rises sharply until BTP and then starts decreasing with further increase in density. The absorption width above the BTP depends solely on the spin-orbit coupling strength. Hence Hall coefficient and optical conductivity measurements can be used to extract \( \alpha \) experimentally. On the other hand, the absorption width below the BTP depends on both the density and \( \alpha \). The spin-split energy gap is comparable to the electromagnetic radiation with high frequency \( \omega \sim 10^3 \text{ Hz} \). The corresponding spin-flip time scale will be very small. Therefore, noncentrosymmetric bulk materials can be used for good thermoelectric as well as spintronics devices.

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Appendix A

1. Calculation of the relaxation time

Relaxation time approximation for multiband systems: In this Appendix, we present calculation of the relaxation time by solving the Boltzmann transport equation including the interband scattering for \( E > 0 \) and interbranch scattering for \( E < 0 \) self-consistently. We consider electrons in noncentrosymmetric semiconductors with spin-independent short-range scatterer. This system is subjected to a spatially uniform electric field \( \Xi \) and temperature gradient \( \nabla T \). The effective electric field due to charge redistribution results from \( \Xi \) is given by \( \Xi_{\text{eff}} = \Xi - (\nabla \mu)/e \). We now linearize the Fermi-Dirac distribution function \( f_\xi(E_\xi) = f^0_\xi(E_\xi) + \delta f_\xi \) around the equilibrium
solution $f_0^0(E_\xi)$. Here $\xi \equiv (\lambda, \mathbf{k})$ for $E \geq 0$ and $\xi \equiv (\eta, \mathbf{k})$ for $-E_\alpha \leq E \leq 0$ is the eigenstate index; and $\delta f_\xi$ is the out-of-equilibrium deviation which is linear in the external electric field. In nonequilibrium steady states, the linearized Boltzmann transport equation\textsuperscript{58} for the charge carriers is

$$F_\xi \cdot \mathbf{v}_\xi \frac{\partial f_0^0}{\partial E_\xi} = -\sum_{\xi'} W_{\xi', \xi}(\delta f_\xi - \delta f_{\xi'}).$$

(A1)

Here the generalized force acting on the state $\xi$ is

$$F_\xi = -\frac{(E_\xi - \mu)}{T} \nabla T + e \mathbf{z}_{\text{eff}}$$

(A2)

and $\mathbf{v}_\xi$ is the group velocity of the state $\xi$. Also, $W_{\xi', \xi}$ is the transition rate from the state $\xi$ to the state $\xi'$. We have used the fact that $W_{\xi', \xi} = W_{\xi, \xi'}$ in the Boltzmann transport equation. Within the lowest-order Born approximation, the intra-band transition rate between the states $\xi$ and $\xi'$ is

$$W_{\xi', \xi} = \frac{2 \pi N_{\text{imp}}}{\hbar} |\langle \phi_{\xi'}(\mathbf{k}') | U(\mathbf{r}) | \phi_\xi(\mathbf{k}) \rangle|^2 \delta(E_\xi - E_{\xi'}).$$

Here, $N_{\text{imp}}$ is the number of $\delta$-scatterer randomly distributed in the system at various locations $\mathbf{r}_i$. The corresponding spin-independent impurity potential produced by the $\delta$-scatterer is given by $U(\mathbf{r}) = U_0 \sum_{i=1}^{N_{\text{imp}}} \delta(\mathbf{r} - \mathbf{r}_i)$. Here $U_0$ being the strength of the impurity potential, whose dimension is energy times volume. The Fourier transform of the potential $U(\mathbf{r})$ is $U(\mathbf{q}) = U_0$. Upon simplification, the transition rates are obtained as

$$W_{\lambda', \lambda} = \frac{1}{u_0 V} (1 + \lambda \lambda' \cos \theta) \delta(E_\lambda - E_{\lambda'}); \quad E \geq 0$$

(A3)

$$W_{\eta', \eta} = \frac{1}{u_0 V} (1 + \cos \theta) \delta(E_\eta - E_{\eta'}); \quad -E_\alpha \leq E \leq 0,$$

(A4)

where $1/u_0 = \pi n_{\text{imp}} U_0^2 / \hbar$ with $n_{\text{imp}}$ being the impurity density.

We need to solve the Boltzmann transport equation separately for $E \geq 0$ and $-E_\alpha \leq E \leq 0$. This is because the intraband and interband transitions take place when $E \geq 0$. Whereas intraband and interbranch transition occurs within the band $\lambda = -$. We are able to obtain exact analytical expression of the scattering time even if we keep the interband/interbranch contribution in the Boltzmann transport equation. Assuming the out-of-equilibrium distribution function is of the following form:

$$\delta f_\xi(E, \mathbf{v}(E_\xi, \theta, \phi)) = -\frac{\partial f_0^0(E)}{\partial E} F_\xi \cdot \mathbf{v}_\xi(E, \theta, \phi) \tau_\xi(E).$$

(A5)

Substituting Eq. (A5) into Eq. (A1), the self-consistent equation for the relaxation time $\tau_\xi(E)$ is

$$\frac{1}{\tau_\xi(E)} = \frac{V}{4 \pi} \sum_{\xi'} \int dE_{\xi'} D_{\xi'}(E_{\xi'}) \sin \theta' d\theta' d\phi' W_{\xi', \xi}(E_{\xi'}, E_{\xi}) \left[ 1 - \frac{F_{E_{\xi'}} \cdot \mathbf{v}(E_{\xi'}, \theta', \phi')}{F_{E_\xi} \cdot \mathbf{v}(E_\xi, \theta, \phi)} \frac{\tau_{\xi'}(E_{\xi'})}{\tau_\xi(E)} \right].$$

(A6)

First we consider $E \geq 0$ case. After some straight forward manipulation, we get the following self-consistent equation for the relaxation time $\tau_\lambda(E)$

$$\frac{1}{\tau_\lambda(E)} = \sum_{\lambda'} \frac{D_{\lambda'}(E)}{2u_0} \int d\theta' \sin \theta' (1 + \lambda \lambda' \cos \theta') \left[ 1 - \cos \theta' \frac{\tau_{\lambda'}(E)}{\tau_\lambda(E)} \right].$$

(A7)

Performing the integrals and summation, the above equation reduces to

$$\frac{1}{\tau_{\pm}(E)} = \frac{2 D_\pm(E)}{3 u_0} \frac{D_{\pm}(E)}{u_0} \left[ 1 + \frac{\tau_{\pm}(E)}{3 \tau_{\pm}(E)} \right].$$

(A8)

On solving the above coupled algebraic equations, the relaxation times of the two bands for $E \geq 0$ are obtained as

$$\tau_\lambda(E) = u_0 \left[ \frac{D_\lambda(E)}{(D_\pm(E))^2} + \frac{1}{2 D_\pm(E)} \right].$$

(A9)
For \(-E_\alpha < E < 0\), the self-consistent equations for the relaxation time \(\tau_\eta(E)\) are
\[
\frac{1}{\tau_\eta(E)} = \sum_{\eta} D_{\eta\eta} E \left[ \frac{D_{\eta\eta}(E)}{2u_0} \int d\theta^2 \sin \theta (1 + \cos \theta) \right] \left[ 1 - (-1)^{\eta - \eta} \cos \theta \frac{\tau_\eta(E)}{\tau_\eta(E)} \right].
\] (A10)
The solutions for the relaxation times are obtained as
\[
\tau_\eta(E) = u_0 \left[ \frac{D_{\eta\eta}(E)}{(D^2_{\eta\eta}(E))^{\frac{1}{2}}} \right] + \frac{1}{2D^2_{\eta\eta}(E)}.
\] (A11)
In our case total density of states for \(E \geq 0\) and \(E < 0\) have the same form
\[
D^+_\eta(E) \equiv D^-_\eta(E) = \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^\frac{3}{2} \left[ \frac{E + 2E_\alpha}{\sqrt{E + 2E_\alpha}} \right].
\] (A12)
As a consequence of the same energy dependence of the total density of states below and above the BTP, we also have the same form of the relaxation time for \(E \geq 0\),
\[
\tau_{\lambda\lambda}(E) = 2\pi^2 u_0 \left( \frac{\hbar^2}{2m^*} \right)^\frac{3}{2} \left( \frac{\sqrt{E + 2E_\alpha}}{E + 2E_\alpha} \right) \left[ 1 - 2\lambda \frac{\sqrt{E_\alpha(E + E_\alpha)}}{(E + 2E_\alpha)} \right],
\] (A13)
and for \(E < 0\),
\[
\tau_\eta(E) = 2\pi^2 u_0 \left( \frac{\hbar^2}{2m^*} \right)^\frac{3}{2} \left( \frac{\sqrt{E + E_\alpha}}{E + 2E_\alpha} \right) \left[ 1 - 2(-1)^{\eta\eta} \frac{\sqrt{E_\alpha(E + E_\alpha)}}{(E + 2E_\alpha)} \right].
\] (A14)

2. The electrical conductivity at \(T = 0\)

Within the semi-classical Boltzmann transport theory, the general expression of the electrical conductivity at \(T = 0\) for \(E \geq 0\) is given by
\[
\sigma_\nu^\nu = \frac{e^2}{2\pi} \sum_{\lambda = \pm 1} \int_0^\infty dE \left( -\partial_E f^\lambda(E) \right) \int_0^\pi \int_0^{2\pi} \sin \theta d\theta d\phi D_\lambda(E) \langle \hat{v}_\nu(E, \theta, \phi) \rangle_\lambda^2 \tau_\lambda(E),
\] (A15)
where \(\nu = x, y, z\) and \(\hat{v}_\nu(E, \theta, \phi)\) is the \(\nu\)-component of the velocity operator and \(\tau_\lambda(E)\) is the relaxation time. The expectation values of the velocity operator \(\hat{v}_\mu\) with respect to the \(\lambda = \pm 1\) states are \(\langle \hat{v}_\nu(E, \theta, \phi) \rangle_\lambda = \left( \frac{h k_\lambda(E)}{m^*} + \frac{\lambda \alpha}{\hbar} \right) \sin \theta \cos \phi\) and so on. As we have already seen that \(\tau_\lambda(E)\) is independent of angular variables so using
\[
\int_0^\pi \int_0^{2\pi} \langle \hat{v}_\nu(E, \theta, \phi) \rangle^2_\lambda \sin \theta d\theta d\phi = \frac{4\pi}{3} \left( \frac{h k_\lambda(E)}{m^*} + \frac{\lambda \alpha}{\hbar} \right)^2,
\] (A16)
which exhibits isotropic nature of the electrical conductivity: \(\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = \sigma\). Using the forms of density of states and Eq. (A13), we get
\[
\sigma^\nu = \frac{e^2}{\hbar} \frac{4\hbar^2}{3m^* n_{\text{imp}} U_0^2} \left[ \frac{3}{2} - \frac{E_F^2}{2(2E_\alpha + E_F)^2} \right] (E_\alpha + E_F).
\] (A17)
Similarly for \(E < 0\), the electrical conductivity becomes
\[
\sigma^- = \frac{e^2}{\hbar} \frac{4\hbar^2}{3m^* n_{\text{imp}} U_0^2} \left[ \frac{3}{2} - \frac{E_F^2}{2(2E_\alpha + E_F)^2} \right] (E_\alpha + E_F).
\] (A18)
It is clear from Eqs. (A17) and (A18) that electrical conductivity has same form below \((E_F < 0)\) and above \(E_F \geq 0\) the BTP. It is also clear from Fig. 3 that electrical conductivity has the same kind of energy dependence below and above the BTP. So in our case electrical conductivity will be continuously differentiable at the BTP.

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