Quantum Criticality between Topological and Band Insulators in 3+1 Dimensions

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Quantum criticality between topological and band insulators in $(3+1)$-dimensions

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Four-component massive and massless Dirac fermions in the presence of long range Coulomb interaction and chemical potential disorder exhibit striking fermionic quantum criticality. For an odd number of flavors of Dirac fermions, the sign of the Dirac mass distinguishes the topological and the trivial band insulator phases, and the gapless semi-metallic phase corresponds to the quantum critical point that separates the two. Up to a critical strength of disorder, the semi-metallic phase remains stable, and the universality class of the direct phase transition between two insulating phases is unchanged. Beyond the critical strength of disorder the semi-metallic phase undergoes a phase transition into a disorder controlled diffusive metallic phase, and there is no longer a direct phase transition between the two types of insulating phases. Our results are also applicable to even number of flavors of Dirac fermions, and the band inversion transition in various non-topological narrow gap semiconductors.

The low energy, long wavelength quasi-particle spectrum of various narrow gap semiconductors is well approximated by noninteracting $(3+1)$-dimensional massive Dirac fermions and by adjusting the chemical composition, or by applying pressure, the sign of the Dirac mass can be changed at a band-inversion transition (BIT). At BIT the system becomes semi-metallic (SM) and is described by massless Dirac fermions. The SM phase is an interesting example of $z=1$ fermionic quantum critical point (QCP). In the massless phase, the conduction and valence bands cross at a discrete number of diabolic points inside the Brillouin zone and depending on the number of inequivalent diabolic points we obtain multiple flavors of Dirac fermions. The narrow gap semiconductors such as $Pb_{1-x}Sn_xTe$ (four flavors), $Bi_{1-x}Sb_x$ and $Hg_{1-x}Cd_xTe$ (each with single flavor) are well known examples, which for special values of x, become massless [1]. For odd number of Dirac fermion flavors, the QCP describes the phase transition between a topological insulator (TI) and an ordinary band insulator (BI) [2–5]. The recent experimental observation of TI phase in different narrow gap semiconductors have spurred our interest in the $(3+1)$-dimensional Dirac materials [4, 5]. The low energy spectrum of materials like $Bi_{1-x}Sb_x$, Bi_2Te_3, Bi_2Se_3, where TI phase has been observed are all described in terms of a single flavor massive Dirac fermion [6, 7].

The stability of the disorder free SM phase in the presence of long range Coulomb interaction and the noninteracting SM phase in the presence of random chemical potential disorder were respectively addressed in Refs. [8] and [9]. Recently the noninteracting, disordered $(3+1)$-dimensional TI has been considered in Refs. [10, 11]. For the noninteracting disordered problem a symmetry based ten-fold classification of TI and superconductors has been described in Ref. [12], and the stability of the two dimensional surface states has been discussed on the basis of this symmetry classification. The noninteracting TI in the presence of generic time reversal symmetric disorder belongs to the symplectic AII class. In general such classification does not hold in the presence of interaction. The stability of the two dimensional disordered and interacting surface states of a TI has been addressed in Ref. [13]. However, the combined effects of interaction and disorder on the bulk fermions has not been considered before. Motivated by this and possible future experiments in which novel QCPs can be explored, we analyze the problem of both massive and massless Dirac fermions in the presence of Coulomb interaction and random chemical potential type disorder using a perturbative renormalization group (RG) analysis. Remarkably, the vanishing density of states at the Dirac points renders such a calculation reliable in comparison to the corresponding non-relativistic problem.

For orientation we first consider the disorder free noninteracting Dirac fermion action. For simplicity we consider only one species of Dirac fermion. Assuming inversion (parity) and time reversal symmetry and using a spinor basis $\psi^T = (c_{+,\uparrow}, c_{+,\downarrow}, c_{-,\uparrow}, c_{-,\downarrow})$, where $c_{\pm,s}$ respectively correspond to the annihilation operators for parity even and odd states, with spin projection s, we can write the following Euclidean action

$$S_0 = \int d^4x \bar{\psi}\Big[\gamma_0(\partial_0 - A\partial_j^2) + iv\gamma_j\partial_j + m - B\partial_j^2\Big]\psi. \quad (1)$$

The latin index j is a spatial index and $\Lambda \sim 1/a$ is the ultraviolet cutoff, where a is the lattice spacing. The parameter v is the Fermi velocity and m is the Dirac mass. The anti-commuting Euclidean γ matrices satisfy $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu,\nu}$, and $\bar{\psi} = \psi^\dagger\gamma_0$. The four-component spinor structure arises from the two-sublattice crystallographic structure and the two spin components. We have also incorporated two higher gradient terms involving A and B. The above action is invariant with respect to the parity ($\mathcal{P}$) and time reversal ($\mathcal{T}$) transformations: $\mathcal{P}\psi\mathcal{P}^{-1} = \gamma_0\psi$, $\mathcal{T}\psi\mathcal{T}^{-1} = -\gamma_1\gamma_3\psi$. For $A=0$, the action is also invariant under charge conjugation (particle-hole) transformation ($\mathcal{C}$): $\mathcal{C}\psi\mathcal{C}^{-1} = -\gamma_2\psi$. The particle-hole symmetry breaking term does not affect the topological properties, and can be off-set by adjusting of the chemical potential, and henceforth we will set $A=0$.

The fermion mass m and the higher gradient term Proportional to B break the $U(1)$ chiral symmetry of the massless Dirac fermions defined by $\psi \to e^{i(\theta/2)\gamma_5}\psi$, $\bar{\psi} \to \bar{\psi}e^{i(\theta/2)\gamma_5}$,

where $\gamma_5 = \gamma_0\gamma_1\gamma_2\gamma_3$. The TI and BI phases are respectively defined by the conditions $mB < 0$ and $mB > 0$ and are separated by a finite chiral angle $\delta\theta = \pi$. This is reflected in the quantized magneto-electric coefficients π and 0, respectively for TI and BI. At the critical point $m = 0$, the dynamic exponent $z = 1$, and in the RG sense the higher derivative terms can be ignored.

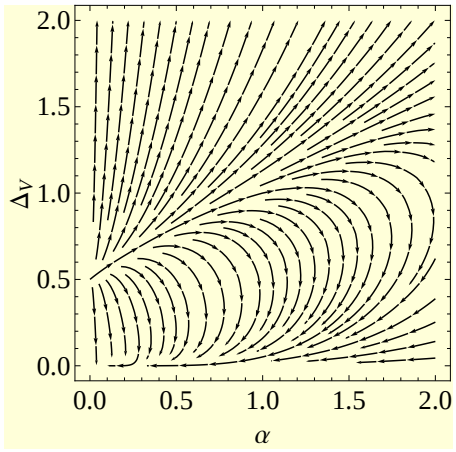
The Dirac structure of the Hamiltonian allows various types of disorder. The constraint of time reversal invariance allows the following six bilinears: $\bar{\psi}\gamma_0\psi$, $\bar{\psi}\psi$, $\bar{\psi}\gamma_0\gamma_5\psi$ and $\bar{\psi}\gamma_0\gamma_j\psi$ ($j = 1, 2, 3$). The bilinears $\bar{\psi}\gamma_0\psi$, $\bar{\psi}\psi$ respectively correspond to random chemical potential and random mass scattering. The physical description of other four bilinears depends on the crystallographic details. We shall concentrate on the random chemical potential as the dominant elastic scattering process, and add $S_D = \int d^4x V(\mathbf{x})\bar{\psi}\gamma_0\psi$ to the action S_0. The random potential $V(\mathbf{x})$ is a Gaussian white noise distribution specified by the disorder average $\langle\langle V(\mathbf{x})V(\mathbf{x}')\rangle\rangle = \Delta_V\delta^3(\mathbf{x}-\mathbf{x}')$. The detailed analysis for generic time reversal symmetric disorder is provided in the supplementary material [14].

Since typically $v/c \sim 10^{-2} - 10^{-3}$ (c is the velocity of light), the Coulomb interaction is instantaneous. Its strength is characterized by the the dimensionless parameter $\alpha = e^2/(4\pi\varepsilon v) \sim 2.2/\varepsilon - 22/\varepsilon$, where ε is the static dielectric constant of the material. We perform disorder average using the replica method, which we use merely as a book-keeping device for perturbative RG calculations. The replicated Euclidean action after disorder averaging of the partition function is

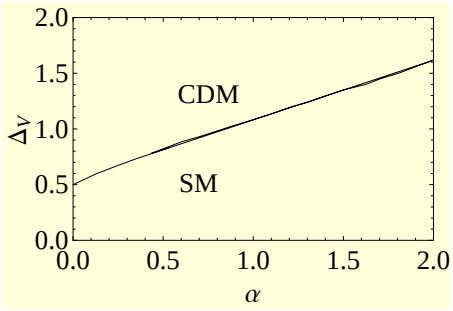
$$\overline{S} = \int d^4x \Big[\bar{\psi}_a\left\{\gamma_0(\partial_0 + ig\varphi_a) + v\gamma_j\partial_j + m - B\partial_j^2\right\}\psi_a + \frac{1}{2}(\partial_j\varphi_a)^2\Big] - \frac{\Delta_V}{2}\int d^3x dx_0 dx_0' \left(\bar{\psi}_a\gamma_0\psi_a\right)_{(x,x_0)} \times \left(\bar{\psi}_b\gamma_0\psi_b\right)_{(x,x_0')} \quad (2)$$

where $g = \sqrt{4\pi v\alpha}$, and a, b are replica indices. We have used the abbreviated notation $\left(\bar{\psi}_a\gamma_0\psi_a\right)_{(x,x_0)} \equiv \bar{\psi}_a(x, x_0)\gamma_0\psi_a(x, x_0)$. We have introduced an auxiliary scalar potential φ_a to decouple the four-fermion Coulomb interaction term. Unlike two dimensions, the Coulomb interaction manifests itself as $(\partial_j\varphi_a)^2$, which is analytic in momentum and g can certainly receive loop corrections. The action $\overline{S}$ preserves all three discrete symmetries $\mathcal{P}$, $\mathcal{T}$ and $\mathcal{C}$. For RG calculations we replace the couplings by the corresponding dimensionless couplings $m \to m/(v\Lambda)$, $B \to B\Lambda/v$ and $\Delta_V \to \Delta_V\Lambda/(2\pi^2v^2)$. The details of the RG calculation are provided in the supplementary material [14].

The density of states for massless and massive problems are, respectively, $\rho(E) \propto E^2$ and $\rho(E) \propto |E|\sqrt{E^2 - m^2}$. Since the the density of states vanishes at zero energy, the scattering rate $\tau^{-1}(E)$ calculated from lowest order Born approximation also vanishes at zero energy. At the tree level, B and Δ_V are irrelevant couplings, and α and m are respectively marginal and relevant couplings. Therefore we anticipate that the universality class of the QCP between TI and BI will be unchanged up to a critical strength of the disorder. This should be contrasted to the two dimensional problem, where the chemical potential disorder is a marginally relevant perturbation and invalidates the lowest order Born approximation result [15].



(a)



(b)

FIG. 1: (a)The RG flow and (b) the phase diagram in the $\alpha - \Delta_V$ plane for massless Dirac fermions with $m = B = 0$. The CDM phase represents a disorder induced massless, compressible diffusive metallic state with finite density of states and scattering rate at zero energy.

Consider first the massless Dirac fermions with $B = 0$. From a momentum shell renormalization group (RG) calculation to $\mathcal{O}(\alpha^2)$, $\mathcal{O}(\Delta_V^2)$, and $\mathcal{O}(\Delta_V\alpha)$, we find

$$\frac{dv}{dl} = v\left(z - 1 - \Delta_V + \frac{2\alpha}{3\pi}\right), \quad (3)$$

$$\frac{d\alpha}{dl} = \alpha\left(\Delta_V - \frac{4\alpha}{3\pi}\right), \quad (4)$$

$$\frac{d\Delta_V}{dl} = \Delta_V\left(-1 + 2\Delta_V - \frac{8\alpha}{3\pi}\right). \quad (5)$$

By keeping v fixed we obtain a scale dependent dynamic exponent $z(l) = 1 + \Delta_V(l) - 2\alpha(l)/3\pi$. There are two fixed points: (i) attractive, noninteracting, clean fixed point: $\Delta_V = \alpha = 0$, $z = 1$; and (ii)noninteracting finite disorder critical point: $\Delta_V = 1/2$, $\alpha = 0$, $z = 3/2$. For the noninteracting disordered problem, the fixed point (ii) controls the

transition between the two phases where disorder is respectively irrelevant (SM) and relevant. In the phase where disorder is relevant, both the zero energy density of states, and the zero energy scattering rates are finite. Therefore this disorder induced phase will be termed a compressible diffusive metal (CDM). The RG flow and the associated phase diagram are respectively shown in Fig. 1(a) and Fig. 1(b).

By linearizing the flow equations in the vicinity of the fixed point (ii), we find $\alpha(l) \approx \alpha_0 e^{l/2}$, and $\Delta_V - 1/2 - 8\alpha/(3\pi) \approx (\Delta_{V0} - 1/2 - 8\alpha_0/(3\pi))e^l$. Therefore at the disorder controlled critical point α is a relevant perturbation, and α shifts the SM-CDM phase boundary to a larger value of $\Delta_V = 1/2 + 8\alpha/(3\pi)$. Along this phase boundary the correlation length diverges with an exponent $\nu = 1$, but the dynamic exponent varies continuously as $z = 3/2 + 2\alpha/\pi$. Notice that CDM phase is a strongly interacting state of matter, and this was not addressed in Ref. 9–11. In the SM phase, the Coulomb interaction initially grows before curling back towards zero in a logarithmic manner, and the initial growth of α is controlled by the bare strength of Δ_V. This unusual flow will be reflected as a non-monotonic temperature dependence of the inelastic scattering rate. The critical behavior at the SM-CDM phase boundary should be contrasted with its $(2+1)$-dimensional counterpart. In $(2+1)$-dimensions, there is no perturbative loop correction to g, and the phase boundary is a line of critical points with $z = 1$[15].

Now we consider the role of m and B. Compared to the SM phase, we expect TI and BI to be stable up to a larger disorder, $\Delta_V(m) > (1/2 + 8\alpha/(3\pi))$. Due to the irrelevant nature of B, we expect it to cause non-universal shift of the phase boundaries, leaving the critical properties unchanged. For finite m and B, the RG equations are given by

$$\frac{dv}{dl} = v\left[z - 1 + \frac{2\alpha}{3\pi\sqrt{1+(m+B)^2}} - \frac{\Delta_V}{1+(m+B)^2}\right] \tag{6}$$

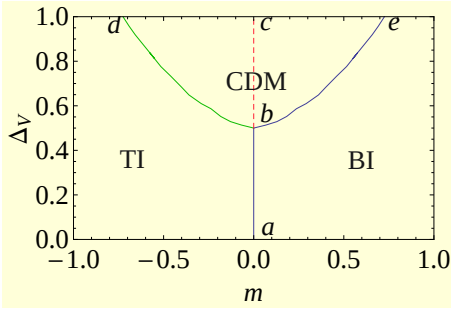
$$\frac{dm}{dl} = m\left[1 + \frac{\alpha}{3\pi\sqrt{1+(m+B)^2}} - \frac{\Delta_V}{1+(m+B)^2}\right] + B\left[\frac{\alpha}{\pi\sqrt{1+(m+B)^2}} - \frac{\Delta_V}{1+(m+B)^2}\right] \tag{7}$$

$$\frac{dB}{dl} = -B\left[1 + \frac{\alpha}{3\pi\sqrt{1+(m+B)^2}}\right] + m\frac{\alpha}{3\pi\sqrt{1+(m+B)^2}} \tag{8}$$

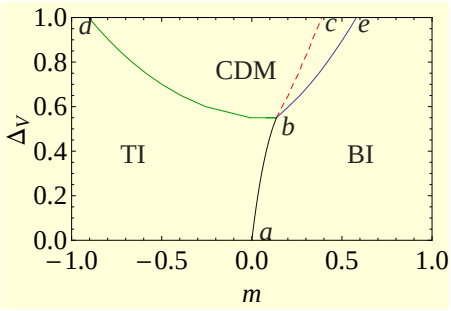
$$\frac{d\alpha}{dl} = \alpha\left[\frac{\Delta_V}{1+(m+B)^2} - \frac{2\alpha}{3\pi\sqrt{1+(m+B)^2}} - \frac{2\alpha}{3\pi}\frac{1+\frac{3}{2}(m^2+B^2)+mB}{[1+(m+B)^2]^{\frac{5}{2}}}\right] \tag{9}$$

$$\frac{d\Delta_V}{dl} = \Delta_V\left[-1 + \frac{2\Delta_V}{1+(m+B)^2} - \frac{4\alpha}{3\pi\sqrt{1+(m+B)^2}} - \frac{4\alpha}{3\pi}\frac{1+\frac{3}{2}(m^2+B^2)+mB}{[1+(m+B)^2]^{\frac{5}{2}}}\right] \tag{10}$$

In Fig. 2(a) we show the phase diagram for $B = \alpha = 0$ and in Fig. 2(b) we show the phase diagram for $\alpha = 0$ and a bare value $B_0 = 0.5$. When disorder is irrelevant, there is a direct phase transition between TI and BI phases along the line ab. In this region, $\Delta_V(l) \sim \Delta_V e^{-l}$, and $B(l) \sim B_0 e^{-l}$, and $\alpha(l) \sim \alpha_0(1 + 4\alpha_0 l/(3\pi))^{-1}$, and only relevant variable is fermion mass m. In this region for $\alpha_0 = 0$, we find $(m(l) - \Delta_V(l)B_(l)/3) \approx e^l(m_0 - \Delta_{V0}B_0/3)$. Therefore $(m - \Delta_V B/3)$ behaves as the effective mass, and for finite B, the TI-BI phase boundary shifts to $m = B\Delta_V/3$. This can be seen by comparing the segment ab in Fig. 2(a) and Fig. 2(b). The Coulomb interaction causes additional shift to $m = B\Delta_V/3 + B\alpha/(2\pi)$. Therefore in the weak disorder regime, it is possible to induce a transition between two insulating phases by tuning the strength of the disorder. As Δ_V and α are respectively irrelevant and marginally irrelevant couplings, z asymptotically approaches unity, and the universality class is described by the massless Dirac fermions. There are logarithmic corrections to the scaling properties due to marginally irrelevant nature of α and it is captured through the scale dependent z, and also by a factor $e^l(\alpha_0/\alpha)^{1/4}$ for the scaling dimension of m. The point b is a multi-critical point at which the massless SM phase undergoes a transition either into CDM or one of the two insulating phases. When disorder exceeds the critical strength corresponding to b, there is no longer a direct transition between two insulating phases. Along the TI-CDM and BI-CDM phase-boundaries respectively denoted by bd and be, z is non-universal, but the mean free path still has the exponent unity. The dashed line bc separates the disorder controlled CDM phase into two regions with negative and positive effective masses, which do not have any physical distinction. For a special case of chiral symmetric disorder and $B = 0$, the chiral symmetric diffusive metallic phase along bc becomes distinct from the rest of the CDM phase. In that case, due to the presence of additional diffusive modes, the weak anti-localization correction for a chiral symmetric CDM becomes two times larger than that of the chiral symmetry breaking CDM [10]. However for $B \neq 0$, or



(a)



(b)

FIG. 2: The phase diagrams in the $m-\Delta_V$ plane for (a)$B_0=\alpha_0=0$, (b)$B_0=0.5$, $\alpha=0$. The direct transition between TI and BI along ab is governed by massless Dirac fermions. When disorder exceeds a critical strength, the insulating phases are separated by CDM, and transitions along bd, and be have non-universal critical properties. The dashed line bc describes a cross-over between two regions of CDM with negative and positive effective masses.

generic disorder such distinction is lost and bc corresponds to a cross-over line. The Coulomb interaction shifts the point b to higher strength of disorder, and leads to additional non-universal shifts of the phase boundaries, and non-universal change of z.

In the weak disorder regime, the transition between TI and BI will be accompanied by interesting critical properties of massless Dirac fermions [14]. Since $(3+1)$-dimensions is marginal, some care is necessary to disentangle slow logarithmic corrections in many physical quantities. For example, the specific heat C_V and compressibility κ, instead of being proportional to T^3/v^3 will be proportional to $(T^3/v^3)\{1+4\alpha_0/(3\pi)\log(v\Lambda/T)\}^{-3/2}$. Similar logarithmic corrections in $(2+1)$-dimensions have been discussed in Ref. [16]. In the high temperature limit, the diamagnetic susceptibility instead of being a constant has logarithmic enhancement $\chi\approx -e^2v/(24\pi^2)\log(v\Lambda/T)$. A similar logarithmic correction proportional to $\log(B)$ appears in the strong field limit. However a finite particle-hole symmetry breaking term A and μ will lead to conventional diffusive Fermi liquid behavior in the low temperature limit specified by $\mu/T\gg 1$. Therefore the critical behavior will be limited to $T\gg\mu$. However by a careful adjustment of μ, the critical properties can be found even in the low T limit. The critical behavior will be found even for the massive fermions provided that $T>m$. In the critical regime the inelastic scattering rate $\sim\alpha^2T$ is larger than elastic scattering rate, and dominates the transport in the collision dominated regime $\omega\ll\alpha^2T$. A quantum Boltzmann equation leads to the conductivity

$$\sigma(\omega,T)=\frac{30.46T}{\alpha\log(1/\alpha)}\left[1-\left(\frac{i\omega}{T}\right)\frac{26.67}{\alpha^2\log(1/\alpha)}\right]^{-1} \quad (11)$$

The disorder induced initial growth of α will lead to non-monotonic temperature dependence of the inelastic scattering rate and the conductivity.

Our results are obtained for inversion symmetric systems, and do not apply for $Hg_{1-x}Cd_xTe$ due to broken inversion symmetry and the presence of additional gapless quadratic band at the Γ point. In the presence of inversion symmetry breaking Dirac mass such as $\gamma_0\gamma_5$ and $\gamma_0\gamma_j$, even for a clean system one can find a metallic phase, if the inversion symmetry breaking mass exceeds m. In the supplementary material we have considered the effects of inversion symmetry breaking disorder, and the generic phase diagrams shown in Fig.2 remain qualitatively unchanged [14]. In the strong disorder limit we have not accounted for the localization corrections for low energy diffusive modes, and such corrections can play important role in determining the more accurate scaling behavior in the strong disorder limit. The localization corrections are expected to drive a further phase transition from the CDM phase to disorder controlled insulating phase. The numerical work in Ref. 11 and Ref. 17 for noninteracting problem in the strong disorder limit have showed the existence of a disorder induced topological Anderson insulator phase. Our work suggests that, akin to the conventional metal-insulator transition problem [18], the interaction effects become strong in the diffusive metallic phase. The effects of strong interaction on metal-insulator transition and topological Anderson insulator will be addressed in a future publication.

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