

Topological Insulators and Nematic Phases from Spontaneous Symmetry Breaking in 2D Fermi Systems with a Quadratic Band Crossing

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We investigate the stability of a quadratic band-crossing point (QBCP) in 2D fermionic systems. At the non-interacting level, we show that a QBCP exists and is topologically stable for a Berry flux $\pm 2\pi$, if the point symmetry group has either fourfold or sixfold rotational symmetries. This putative topologically stable free-fermion QBCP is marginally unstable to *arbitrarily weak* short-range repulsive interactions. We consider both spinless and spin-1/2 fermions. Four possible ordered states result: a quantum anomalous Hall phase, a quantum spin Hall phase, a nematic phase, and a nematic-spin-nematic phase.

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Introduction— In multi-band fermionic systems, a band-crossing point (BCP) is a point in the Brillouin zone where two bands cross. As the chemical potential reaches a BCP, the Fermi surface shrinks to a point and new phenomena, not described by a Fermi liquid, result. The simplest and best studied is the case of a linear band crossing, whose low energy physics is described by a Dirac fermion. Dirac fermions are a good description of the low energy states of nodal superconductors, graphene and zero gap semiconductors.

In general, a Dirac point in a band structure is robust with respect to small changes in the effective potential which preserve the symmetries of the crystal, as has been extensively shown in various contexts [1, 2, 3, 4]. Moreover, short-range electron-electron interactions are perturbatively irrelevant for space dimension $d > 1$. Thus, there is a stable phase with free gapless Dirac fermions which becomes unstable above a critical interaction strength corresponding to a quantum critical point beyond which lie phases with spontaneously broken space or point group symmetries and/or broken time-reversal invariance [5, 6, 7].

In this letter we consider a system with a quadratic band crossing point (QBCP) somewhere in its 2D Brillouin zone. This problem has not been discussed in depth, and only a few aspects have been analyzed. The perturbative stability of a QBCP was studied for 2D noninteracting systems with C_{4v} symmetry in Ref. [8]. For interacting fermions, it was noted in Ref. [9] that a QBCP in 2D has instabilities, for arbitrarily weak interactions, leading to the spontaneous breaking of rotational symmetry (nematic phase) or time-reversal invariance, but its consequences were not explored in depth.

We begin by analyzing the general symmetry principles that protect a QBCP in lattice models of noninteracting fermions. We find that QBCPs are protected by time-reversal symmetry and C_4 or C_6 rotational symmetry. Explicit examples of lattice models with both symme-

tries are presented. We show that short-range repulsive interactions are marginally relevant in the renormalization group (RG) sense. The symmetry breaking phases and phase transitions, both quantum and thermal, are investigated by an RG analysis and mean-field approximations, both presumably reliable at weak-coupling.

We determined the structure of the phase diagrams for both spinless and spin-1/2 fermions. In the spinless case the leading weak-coupling instability is to a gapped phase with broken time-reversal invariance, a quantum anomalous Hall (QAH) effect, and topologically protected edge states. For stronger interactions, there is a subsequent transition to a nematic Dirac phase and an intermediate phase with QAH-nematic coexistence. For spin-1/2 fermions the phase diagram is more complex: in addition to spin singlet QAH and nematic phases, there are also a spin triplet quantum spin Hall (QSH) phase [10] and a nematic-spin-nematic (NSN) phase [11, 12, 13].

Quadratic band-crossing point— A BCP carries quantized Berry flux [14] as required by time-reversal symmetry: $-i \oint_{\Gamma} d\mathbf{k} \cdot \langle \psi(\mathbf{k}) | \nabla_{\mathbf{k}} | \psi(\mathbf{k}) \rangle = n\pi$, where Γ is a contour in the momentum space enclosing the BCP, $\psi(\mathbf{k})$ is the Bloch wave function in a band involved in the band crossing, and n is an integer. For a Dirac point, the Berry flux is $\pm\pi$. Instead, the Berry flux at a QBCP is either 0 or $\pm 2\pi$ [9]. The zero flux QBCP is an accidental band crossing, which can be removed by infinitesimal band mixing without breaking any symmetries, but a QBCP with $\pm 2\pi$ flux is robust and more interesting.

A natural question to ask is if a QBCP is protected by the symmetries of the non-interacting system. In general, there are two ways to remove a QBCP. One way is to split it into several Dirac points while preserving the total Berry flux. A QBCP with flux 2π , for example, can be split into two separate Dirac points each with flux π , or three Dirac points with flux π and one additional Dirac point with $-\pi$. The former case in general breaks the point group symmetry leaving, at most, a two-fold

rotational symmetry unbroken. The latter case can take place while preserving a three-fold rotational symmetry, such as the case of bilayer graphene [15, 16]. For a QBCP with a fourfold or sixfold symmetry axis, the split into Dirac points cannot occur without breaking that symmetry. The alternative is to open a gap by breaking time-reversal symmetry or a symmetry that is formally similar, such as the combined space and spin symmetry whose breaking leads to a spontaneous quantum spin Hall state, as discussed below. Thus, for a QBCP (with Berry flux $\pm 2\pi$) to be stable without fine tuning, two conditions are required: a) the system must be time-reversal invariant and b) the QBCP must have C_4 or C_6 symmetry.

An example of a QBCP in 2D with C_4 symmetry can be found in the checkerboard lattice [9] Fig. 1(a). This lattice can be regarded as the 2D projection of a 3D pyrochlore lattice. It is also the oxygen lattice in a CuO_2 plane of the cuprates. With one orbital per site, there are two bands crossing at a QBCP at (π, π) with a fourfold rotational symmetry. At half filling the QBCP is at the Fermi level. An example of a QBCP with C_6 symmetry is a tight-binding model on a Kagome lattice, which has three bands. The middle band touches the bottom band at $(0, 0)$, resulting in a QBCP with sixfold rotational symmetry. It lies at the Fermi level at $1/3$ filling.

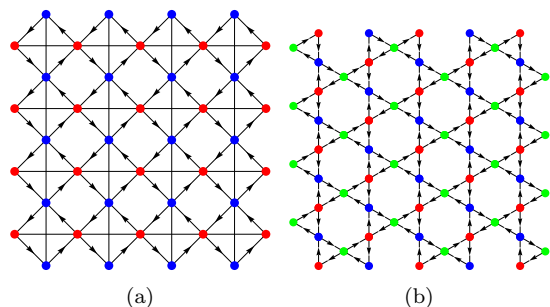


FIG. 1: (Color online) (a) A checkerboard lattice and (b) a Kagome lattice. The arrows represent currents in a spontaneously generated QAH state that breaks the time-reversal symmetry. See text for details.

In the presence of weak interactions, a BCP may become unstable if interactions are relevant in the RG sense. In 2D, a QBCP has a finite one-particle DOS, which implies that short-range interactions are marginal at tree level. We will show below, that at a 2D QBCP a short-range repulsive interaction is marginally relevant, and destabilizes this free fermion fixed point in weak coupling, leading to a state which spontaneously breaks one of the symmetries that otherwise would protect the QBCP.

General model— We first formulate the theory of possible symmetry breaking phases in a general way. We begin with the spinless-fermion case. Near a QBCP, in the low energy regime we have two species of interacting

charged Fermi fields, ψ_1 and ψ_2 , whose Hamiltonian is

$$H = \int d\mathbf{r} \left[\Psi^\dagger(\mathbf{r}) \mathcal{H}_0 \Psi(\mathbf{r}) + V \psi_1^\dagger(\mathbf{r}) \psi_1(\mathbf{r}) \psi_2^\dagger(\mathbf{r}) \psi_2(\mathbf{r}) \right], \quad (1)$$

where $\Psi^\dagger = (\psi_1^\dagger, \psi_2^\dagger)$, Ψ is its conjugate, and V is the coupling constant of the interaction.

The band structure near the QBCP is obtained by diagonalizing 2×2 Hermitian matrix $\mathcal{H}_0(\mathbf{k})$ for all Bloch-wave vectors in the neighborhood of the band crossing point, $|\mathbf{k}| \ll 1$. Quite generally we can choose the identity matrix I and the two real Pauli matrices σ^x and σ^z as a basis [17] and write $\mathcal{H}_0(\mathbf{k})$ as [18]

$$\mathcal{H}_0(\mathbf{k}) = d_I I + d_x \sigma^x + d_z \sigma^z, \quad (2)$$

where $d_I = t_I(k_x^2 + k_y^2)$, $d_x = 2t_x k_x k_y$, and $d_z = t_z(k_x^2 - k_y^2)$. The d -wave symmetry of d_x and d_z distinguishes a QBCP from a Dirac point in which their counterparts have a p -wave symmetry. It is this d -wave nature that gives rise to the $\pm 2\pi$ Berry phase of a QBCP. For a QBCP with a C_6 rotational symmetry, $|t_x| = |t_z|$. If the system has particle-hole symmetry, $t_I = 0$. The condition $|t_I| < |t_x|$ and $|t_I| < |t_z|$ is required to ensure that away from the QBCP, one of the bands lies above the degenerate point and the other band lies below.

At $V = 0$, in the model of Eq. (1), the fermions have a finite DOS but do not have a Fermi surface. They have a dynamic critical exponent $z = 2$, and an effective dimension $d_{\text{eff}} = d + z = 4$ [19]. Ψ has dimension one $[\Psi] = 1$, and the only local four-fermion operator allowed is marginal since $4[\Psi] = d_{\text{eff}}$. There is a single dimensionless coupling constant $g = V/|t_x|$.

This system is similar to $d = 1$ spinless fermions, a system with two Fermi points and dynamic critical exponent $z = 1$. In the 1D case the Fermi field has scaling dimension $1/2$, so there is only one interaction, four-Fermi backscattering, which is potentially important. However, due to a cancellation between the Cooper channel and the bubble term in 1D, the interaction is exactly marginal to all orders in perturbation theory [20], which is the origin of Luttinger liquid behavior in 1D. In contrast, no similar cancellation occurs for fermions in 2D with $z = 2$. Although the 4-Fermi interaction is superficially marginal it is actually marginally relevant. We find, that to one-loop order, the RG beta function for $g = V/|t_x|$ is

$$\beta(g) = \frac{dg}{dl} = \alpha g^2 + O(g^3), \quad (3)$$

where $\alpha = \frac{1}{2\pi^2} K \left(\sqrt{1 - (t_z/t_x)^2} \right)$, l is a momentum rescaling $k \rightarrow ke^{-l}$, and $K(x)$ is the complete elliptic integral. For $|t_x| = |t_z|$, *i.e.* a QBCP with C_6 symmetry, $\alpha = (4\pi)^{-1}$ [21]. Hence, Eq.(3) implies that for $g > 0$ the effective coupling constant flows to strong coupling.

To explore the consequences of this instability, we investigated, in a mean-field level, possible orderings of bi-

linear order parameters:

$$\begin{aligned}\Phi &= \langle \Psi^\dagger(\mathbf{r}) \sigma_y \Psi(\mathbf{r}) \rangle, \\ Q_1 &= \langle \Psi^\dagger(\mathbf{r}) \sigma_z \Psi(\mathbf{r}) \rangle, \quad Q_2 = \langle \Psi^\dagger(\mathbf{r}) \sigma_x \Psi(\mathbf{r}) \rangle.\end{aligned}\quad (4)$$

Φ is the order parameter of a time-reversal symmetry breaking gapped QAH phase [3, 7]. This phase has a zero-field quantized Hall conductivity $\sigma_{xy} = e^2/h$. Q_1 and Q_2 describe the nematic phases in which the C_4 or C_6 rotational symmetry is broken down to C_2 by splitting the QBCP into two Dirac points located along the direction of one of the main axes (Q_1), or along a diagonal (Q_2). The nematic phase is an anisotropic semimetal. Unlike in graphene, where the two Dirac points have Berry fluxes π and $-\pi$, in the nematic phase both Dirac points have the same Berry flux. There is also a phase in which nematic ($Q_1 \neq 0$ or $Q_2 \neq 0$) and QAH orders ($\Phi \neq 0$) coexist, an insulating analog of the metallic time-reversal breaking nematic β phases of Ref. [9].

Since there is only one coupling constant (V) in Eq.(1), the weak-coupling ordering tendencies are determined by the logarithmically divergent normal state susceptibilities χ_Φ (QAH order) and χ_{Q_1} and χ_{Q_2} (nematic order). For general t_x and t_z , they satisfy $\chi_\Phi = \chi_{Q_1} + \chi_{Q_2}$. Hence, $\chi_\Phi > \chi_{Q_i}$ ($i = 1, 2$), so the leading weak coupling instability is to the (gapped) QAH state.

The mean-field Hamiltonian is

$$\begin{aligned}H_{\text{MF}} &= \int d\mathbf{r} \Psi^\dagger(\mathbf{r}) \left[\mathcal{H}_0 - \frac{V}{2} (Q_1 \sigma_z + Q_2 \sigma_x + \Phi \sigma_y) \right] \Psi(\mathbf{r}) \\ &+ \frac{V}{4} \int d\mathbf{r} (Q_1^2 + Q_2^2 + \Phi^2)\end{aligned}\quad (5)$$

By minimizing the ground state energy of H_{MF} we find that at weak coupling the ground state is indeed the QAH phase, with a gap $\Delta \sim \Lambda \exp(-2/\alpha g)$ (Λ is a cutoff) and a mean-field critical temperature $T_c \sim \Delta$, consistent with the scaling predicted by the RG. A 3D example of the QAH at finite coupling is discussed in Ref. [22].

Mean-field theory also predicts nematic phases provided that irrelevant operators, such as $\int d\mathbf{r} d\mathbf{r}' \sum_{i=1,2} U(\mathbf{r} - \mathbf{r}') \psi_i^\dagger(\mathbf{r}) \psi_i(\mathbf{r}) \psi_i^\dagger(\mathbf{r}') \psi_i(\mathbf{r}')$, are also included. The nematic phase Q_1 is energetically favored at small $V > 0$ and $U < 0$ if $|U/V|$ is large enough. As $|U/V|$ is reduced, the nematic phase gives way to the QAH phase (and to a mixed phase).

Lattice models— We consider the following minimum model on a checkerboard lattice with a QBCP.

$$H = \sum_{ij} -t_{ij} c_i^\dagger c_j + V \sum_{\langle ij \rangle} c_i^\dagger c_i c_j^\dagger c_j, \quad (6)$$

where t_{ij} is the hopping amplitude between sites i and j and $V > 0$ is the nearest-neighbor repulsion. Here, $t_{ij} = t, t', t''$, respectively for nearest neighbors, and next-nearest neighbors connected (or not) by a diagonal bond, Fig. 1(a). There are two sublattices A (red) and B

(blue). The fermion spinor is $\Psi^\dagger = (c_A^\dagger, c_B^\dagger)$. The parameters of the free fermion Hamiltonian [Eq. (2)] are $d_I = -(t' + t'')(\cos k_x + \cos k_y)$, $d_x = -4t \cos \frac{k_x}{2} \cos \frac{k_y}{2}$, and $d_z = -(t' - t'')(\cos k_y - \cos k_x)$. The QBCP is $M = (\pi, \pi)$, at the corner of the Brillouin zone. The parameters of the continuum Hamiltonian (near the QBCP) of Eq. (1) are $t_I = (t' + t'')/2$, $t_x = t/2$, $t_z = (t' - t'')/2$. The order parameters are $Q_1 = \frac{1}{4} \sum_\delta \langle c_{A,i}^\dagger c_{A,i} - c_{B,i+\delta}^\dagger c_{B,i+\delta} \rangle$ (“site nematic”), $Q_2 = \frac{1}{2} \sum_\delta D_\delta \text{Re} \langle c_{A,i}^\dagger c_{B,i+\delta} \rangle$ (“bond nematic”), and $\Phi = \frac{1}{2} \sum_\delta D_\delta \text{Im} \langle c_{A,i}^\dagger c_{B,i+\delta} \rangle$ (QAH), where $\delta = \pm \hat{x}/2 \pm \hat{y}/2$ connects nearest neighbors. $D_\delta = \pm 1$, $D_{\pm(\hat{x}/2 + \hat{y}/2)} = 1$ and $D_{\pm(\hat{x}/2 - \hat{y}/2)} = -1$.

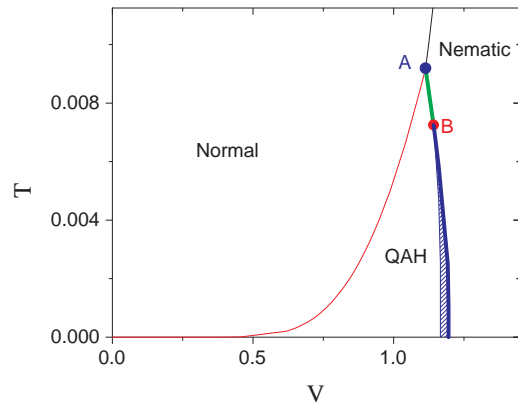


FIG. 2: (Color online) Mean-field $T - V$ phase diagram of a half-filled checkerboard lattice with $t'/t = 0.5$, $t''/t = -0.2$. Nematic and QAH orders coexist in the shaded area. Thick (thin) lines are first (second) order transitions. A is a bicritical point and B is a critical-end point.

A mean-field theory analysis [23] (similar to Eq.(5)) of the lattice model, Eq.(6), yields the $T - V$ phase diagram of Fig. 2. (The details depend on t'/t and t''/t .) A QAH phase is found for V small and below a critical temperature. This phase has a zero-field quantized Hall conductivity e^2/h , and that the quasiparticle spectrum has topologically protected chiral edge states, as predicted by general considerations [24]. A site-nematic phase is found for $V \sim |t' - t''|$, while the bond-nematic is not favored. For $|t'| \geq |t''|$ and $|t''|/|t'| \ll 1$, there is a direct nematic-QAH first order transition. If $|t''|/|t'| \sim 1$, there is also a coexisting QAH+nematic phase. For other values, there are a direct first-order transition and a coexisting phase.

Near a QBCP, a next-nearest-neighbor attraction $V_{nnn} < 0$ [25] generates the (irrelevant) interaction U . For $|V_{nnn}/V| \gtrsim 1$, a site-nematic phase (Q_1) becomes stable, even at weak coupling. A site-nematic phase is stabilized at large enough $V > 0$ ($V_{nnn} = 0$). In the strong coupling limit, at this filling, this system is known to be in an insulating site-nematic phase [26].

Spin-1/2 fermions— Let us consider briefly the case of a system of spin-1/2 fermions at a QBCP. Details will be given in Ref. [23]. We consider the four shortest-range

interactions on a lattice: a) an on-site repulsive Hubbard U , b) a nearest neighbor repulsion V , c) a nearest neighbor exchange interaction J , and d) a pair-hopping term W . In addition to spin-singlet order parameters (*c.f.* Eq (5)), there are also spin-triplet order parameters:

$$\begin{aligned} \vec{Q}_1^t &= \langle \Psi^\dagger(\mathbf{r})(\vec{\tau} \otimes \sigma_z)\Psi(\mathbf{r}) \rangle, \quad \vec{Q}_2^t = \langle \Psi^\dagger(\mathbf{r})(\vec{\tau} \otimes \sigma_x)\Psi(\mathbf{r}) \rangle, \\ \vec{S} &= \langle \Psi^\dagger(\mathbf{r})(\vec{\tau} \otimes I)\Psi(\mathbf{r}) \rangle, \quad \vec{\Phi}^t = \langle \Psi^\dagger(\mathbf{r})(\vec{\tau} \otimes \sigma_y)\Psi(\mathbf{r}) \rangle. \end{aligned} \quad (7)$$

where $\vec{\tau}$ are the three Pauli matrices. Here, \vec{S} is the spin density. For $\vec{Q}_1^t \neq 0$ the QBCP splits into four Dirac points displaced along the main axes. This state has reversed spin polarization along x and y axes. For a QBCP with C_4 symmetry, the charge sector is still C_4 invariant, but the spin sector changes sign under a rotation by $\pi/2$. Thus, $\vec{Q}_1^t \neq 0$ is a NSN state [11, 12, 13]. $\vec{Q}_2^t \neq 0$ describes NSN order along the diagonals.

A state with $\vec{\Phi}^t \neq 0$ is a QSH phase [7, 27, 28, 29] with helical edge states [30, 31]. In this phase, the two spin components have opposite Hall conductivity. The QSH topological insulator has a quantized spin Hall conductivity, and it is a spin triplet version of the QAH phase. It is an insulating analog of the β -phase of Refs. [13, 32].

A scaling analysis similar to the spinless case finds six marginally relevant operators, associated with the four nematic order parameters (singlet and triplet) and the QAH and QSH orders. We have obtained the phase diagram in mean-field theory for spin-1/2 fermions on a checkerboard lattice at a QBCP with $U > V > 0$ at $T = 0$ [33]. For simplicity we take t , t' and t'' such that $t_x \sim t_z$, and $W = 0$. Once again all the susceptibilities are logarithmically divergent with $\chi_{\vec{\Phi}} = \chi_{\Phi}$, and $\chi_{\vec{Q}_i} = \chi_{Q_i}$ ($i = 1, 2$), so the interactions are marginally relevant. For $U > 2V > 0$, the system is in the NSN phase at low temperatures. For $2V > U > 0$ we find the QAH phase for $J > 0$, and the QSH phase for $J < 0$. Both gapped phases are topological insulators. The gaps and critical temperatures obey a scaling law similar to the spinless case [23]. For $U \rightarrow \infty$ (and $J = 0$), there is a NSN state, while $V \rightarrow \infty$ stabilizes a nematic phase.

Using RG methods and mean-field theory we showed that a system of interacting fermions, with or without spin, at a QBCP have topological insulating QAH or QSH phases, at arbitrarily weak short-range repulsive interactions. These perturbatively accessible topological insulating phases are due to spontaneous symmetry breaking, described by order parameters, and are not due to spin orbit effects in the band structure. At intermediate coupling we also find nematic (and coexisting) phases. Using large N methods and a $2 + \epsilon$ expansion, we infer the existence of these phases in 3D (similar to those of Ref.[22]), but at a finite critical coupling[23].

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