Exciton condensation in thin-film topological insulator

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Abstract – We study the many-body physics in thin-film topological band insulator, where the inter-edge Coulomb interaction can lead to an exciton condensation transition. We investigate the universality class of the exciton condensation quantum critical point. With different chemical potentials and interactions, the exciton condensation can belong to \(z = 2\) mean field, or 3d XY, or Yukawa-Higgs universality classes. The interplay between exciton condensate and the time-reversal symmetry breaking is also discussed. Predictions of our work can be tested experimentally by tuning the chemical potentials on both surfaces of the thin film through gate voltage. We also show that all the analysis of the exciton condensate can be directly applied to a spin-triplet superconducting phase with attractive inter-edge interaction.

Quantum phases protected by topology have shown enormous interesting behaviors. Despite unusual quantized responses to external fields [1,2], topological phases usually manifest themselves with their stable edge states. For instance, the three-dimensional topological band insulator (TBI) is characterized by its single Dirac cone edge state, with the Dirac point located at the time-reversal (\(T\)) invariant point in the edge Brillouin zone. These edge states were predicted theoretically, and also observed very successfully experimentally in materials such as BiSb, Bi\(_2\)Se\(_3\) and Bi\(_2\)Te\(_3\) [3–8]. It was understood that \(T\) is crucial to the stability of the edge states [7,9–11], basically because one cannot open up a \(T\)-invariant Dirac mass gap for a single edge. Enormous interest was devoted to the \(T\) breaking at the edge states of TBI, including the cases with \(T\) broken by magnetic impurities and broken spontaneously due to interactions [12–17].

In a thin-film sample of TBI, since the two edges are close enough to interact with each other, \(T\) is no longer sufficient to protect the stability of the edge states, i.e., it is allowed to open up a \(T\)-invariant gap for both edge states. Recently, the gap at the edge states was indeed observed in experiments on thin-film TBI, when the thickness of the film is small [18–20]. It was proposed that even without direct inter-edge tunnelling, the local Coulomb interaction can also gap out the edge states through exciton condensation [21], i.e., a particle-hole pair bound state across the thin film condenses.

This effect is most prominent when a specific biased gate voltage is applied to two edges, where there is a “nesting” between two Fermi surfaces, and the “exciton” susceptibility diverges [21]. Lately it was proposed that large dielectric constants of these materials increases the layer separation range over which the inter-surface coherence survives [22]. In our current paper we hope to go beyond the mean-field consideration in ref. [21] and study the critical properties of the exciton condensate physics.

We illustrate our main results of this paper in the phase diagram (fig. 1) plotted against the chemical potentials of the two edges, which we assume can be separately tuned with gate voltages on both edges. The color in this phase diagram denotes the critical Coulomb interaction \(U_c\) required to drive the exciton condensate, and at the line \(\mu_1 + \mu_2 = 0\) except for the origin, \(U_c = 0\) due to the divergence of exciton susceptibility. In most of the area of this phase diagram, the quantum critical point (QCP) belongs to the \(z = 2\) mean-field universality class. At the origin \(\mu_1 = \mu_2 = 0\), the transition is described by the Yukawa-Higgs theory; and at the special line \(\mu_1 = \mu_2 \neq 0\), the transition belongs to the 3d XY universality class. The same phase diagram and universality classes apply to the superconducting transition with attractive inter-edge “Coulomb” interaction.

The effective Hamiltonian of the surface states reads

\[
\mathcal{H} = \sum_{l=1,2} \psi_l^\dagger (v_l \vec{\sigma} \cdot \vec{p} - \mu_l) \psi_l + U n_1 n_2, \tag{1}
\]
where \(v_l = (-1)^{l+1} v_f\) because the two edges of the TBI have opposite helicities. This Hamiltonian clearly has time-reversal symmetry \(T\): \(\psi_l \rightarrow i\sigma^y \psi_l, \vec{k} \rightarrow -\vec{k}\). There is also an inversion symmetry \(I\): \(\psi_1 \leftrightarrow \psi_2, \vec{k} \rightarrow -\vec{k}\) when \(\mu_1 = \mu_2\), and the inversion is also a generic symmetry of materials such as Bi2Te3 and Bi2Se3. Gate voltages determine the relative chemical potentials, \(\mu_l\). The second term of eq. (1) describes the short-ranged inter-edge Coulomb interaction. We assume the screening length of Coulomb interaction is always larger than the thickness of the think film, therefore the inter-edge Coulomb interaction is still important even when the direct inter-edge electron tunnelling is ignorable. The intra-edge Coulomb interaction is also tentatively ignored in this Hamiltonian, its effects will be discussed later.

Without inter-edge tunnelling, electron number in each layer is independently conserved. This enlarged \(U(1) \times U(1)\) symmetry is spontaneously broken down to the diagonal \(U(1)\) symmetry by exciton condensation with order parameter \(\phi \sim U(\psi_1^\dagger \psi_2)\), which also lowers the energy of the system. Then a mean-field Hamiltonian can be obtained from the Hubbard-Stratonovich transformation of the original Hamiltonian equation (1) [21]:

\[
H_{MF} = \sum_{l=1,2} \psi_l^\dagger \left( v_l \vec{\sigma} \cdot \vec{p} - \mu_l \right) \psi_l + \left( \phi^* \psi_1^\dagger \psi_2 + \mathrm{H.c.} \right) + \frac{|\phi|^2}{U}.
\]

The complex order parameter \(\phi\) is invariant under \(T\), but becomes its complex conjugate under inversion \(I\). Clearly there are also other mean-field channels of the Coulomb interaction such as \(\langle \psi_1^\dagger \sigma^z \psi_2 \rangle\), but the exciton order \(U(\psi_1^\dagger \psi_2)\) has the lowest mean-field energy because it opens up a Dirac mass gap, therefore we will focus on this order parameter in our current work.

After integrating out the fermions, the static and uniform renormalization to the mean-field Hamiltonian of \(\phi\) is \(\mathcal{L}_{eff} = (1 - \chi_0)|\phi|^2\), \(\chi_0\) is the susceptibility of order parameter \(\phi\) which can be evaluated from the Boson self-energy loop diagram in fig. 2:

\[
\chi_0 = \Sigma_{\phi}(0,0) = -\int_{i\omega,\vec{k}} \text{Tr}(\hat{G}_1(k,i\omega)\hat{G}_2(k,i\omega)), \quad (2)
\]

where \(\hat{G}_1\) is Green’s function of fermion. This integral increases linearly with the ultraviolet cut-off \(\Lambda\), \(i.e.,\) it is not just a Fermi surface effect. For instance, when \(\mu_1 = \mu_2 = \mu, \chi_0 \sim \Lambda - |\mu|\). Had we included the other mean-field order parameter \(\psi_1^\dagger \sigma^z \psi_2\), since the susceptibility of this order parameter only comes from the Fermi surface, it would never have beaten the order parameter \(\phi \sim U(\psi_1^\dagger \psi_2)\) under consideration, as long as the size of the Fermi surface is small compared with the UV cut-off.

If we fix \(\mu_2\), the critical Coulomb interaction \(U_c\) is plotted in fig. 3. As we mentioned, \(U_c\) itself is cut-off dependent. However, the relative difference between \(U_c\) is UV cut-off independent, hence we can still compare \(U_c\) with no ambiguity. As we can see, at \(\mu_1 = -\mu_2 \neq 0\), the critical Coulomb interaction is zero, due to the fact...
that the exciton susceptibility diverges logarithmically at this point. The logarithmic divergence is a consequence of the Fermi surface nesting between the two edges [21]. At \( \mu_1 = \mu_2 \neq 0 \), although the two Fermi surfaces still have the same size, the wave function overlap \((\psi_{1,\mathbf{k}}\psi_{2,\mathbf{k}}) = 0 \) for any momentum \( \mathbf{k} \) at the Fermi surface, therefore, the susceptibility is not divergent. This matrix element suppression is due to the opposite helicity of the two edges, and as we will see, this suppression will also affect the dynamics and universality class of QCP.

Now let us go beyond the mean-field formalism and move on to the universality class of the QCPs. Without fermions, the exciton condensation would certainly belong to the 3d XY universality class, while coupling to fermions will likely modify the universality class. Let us first discuss the case with \( \mu_1 = \mu_2 = 0 \). At this point, after redefining \( \psi_2 = \sigma_z \psi_2 \), the phase transition is described by the following Lagrangian:

\[
\mathcal{L}_{\text{Higgs}} = \bar{\psi} \gamma^\mu \partial_\mu \psi + \lambda \bar{\psi} \sigma^a \tilde{\psi} a^b \psi + |\partial \phi|^2 + v_\phi^2 |\phi|^2 + \frac{u}{4} |\phi|^4 + \cdots,
\]

Here \( \gamma_\mu = (\sigma^x, \sigma^y, \sigma^z) \), \( \eta^a \) and \( \eta^b \) are two Pauli matrices that mix the two edges. This model becomes precisely the Higgs-Yukawa model which describes the chiral symmetry breaking of the Dirac fermion, at least when \( v_\phi = v_\psi \).

The transition of \( \phi \) is not the 3d XY transition because the coupling \( \lambda \) is relevant at the 3d XY fixed point, based on the well-known scaling dimensions [\( \psi = 1 \), and \( \phi = (d-2)/2 + \eta/2 = 0.519 \) at the 3d XY fixed point [23]. The critical exponents of this transition with large N have been calculated by means of \( 1/N \) and \( \epsilon = 4-d \) expansions [24–27], and a second-order transition with non-Wilson-Fisher universality class was found. Therefore, we conclude that the transition is still second order, with different universality class from the 3d XY transition.

If \( \mu_1 \neq \mu_2 \), due to the mismatch of the size of the Fermi surface, the loop diagram in fig. 2 will not induce to a singular behavior for the boson self-energy at low frequency and small momentum. However, the Fermi surface mismatch breaks the inversion symmetry of the Hamiltonian equation (1); therefore, the following term is allowed in the Lagrangian:

\[
\mathcal{L}_1 = \hbar (i \psi^\dagger \partial_t \psi - i \psi \partial_t \psi^\dagger) \sim \hbar \sigma_x \partial_t \phi, \quad \hbar \sim \mu_2 - \mu_1.
\] (3)

\( \mathcal{L}_1 \) leads to a \( z = 2 \) dynamical exponent, which is analogous to the Mott insulator (MI)-superfluid transition in the Bose-Hubbard model away from the tip of the MI lobe [28], and also the XY magnetic transition in magnetic field. In two spatial dimensions, the \( z = 2 \) transition is a mean-field transition with marginally irrelevant perturbations.

If \( \mu_1 = \mu_2 \neq 0 \), then the exciton condensation is similar to a ferromagnetic transition in Fermi liquid, which usually has a \( z = 3 \) over-damped quantum critical mode [29, 30]. However, in our case there is the matrix element suppression effect mentioned before, namely:

\[
|\mathcal{M}_{k,k+q}|^2 = |\langle k + q, 1|\psi^\dagger_{1,k+q} \psi_{2,k}|k, 2\rangle|^2 = \sin^2(\theta_{k+q} - \theta_k) \sim q^2/k_\perp^2.
\] (4)

This matrix element suppression strongly affects the low-energy dynamics of the quantum critical fluctuations. For instance, the damping rate of the quantum critical modes due to particle-hole excitations can be calculated through the boson self-energy diagram in fig. 2(a):

\[
\text{Im}[\Sigma_\phi(\omega, q)] \sim g^2 \int \frac{d^2k}{(2\pi)^2} [f(\varepsilon_{k+q}) - f(\varepsilon_k)]
\times \delta(\omega - \varepsilon_{k+q} + \varepsilon_k) |\mathcal{M}_{k,k+q}|^2 \sim g^2 \frac{|\omega| q}{v_\phi k_\parallel^2}.
\] (5)

This term will not lead to over-damped \( z = 3 \) quantum critical modes. The same effect was noticed in ref. [15] in the context of \( T \) breaking at the edge state of TBI, and following the argument of ref. [15], we can conclude that this transition still belongs to the 3d XY universality class even though the order parameter \( \phi \) couples linearly to Fermi surface in eq. (2).

The quantum critical modes also modify the fermion’s self-energy. Using the Feynman diagram in fig. 2(b), the fermion self-energy reads

\[
\Sigma(i\omega) \sim \int d^2 k d G(i \epsilon + i \omega, \mathbf{k}) \langle \phi_{\mathbf{k}, \mathbf{k}'} | \phi_{\mathbf{k}' - \mathbf{k}, -\mathbf{k}} \rangle |\mathcal{M}_{\mathbf{k}, \mathbf{k}'}|^2.
\] (6)

Here we use the full correlation at the 3d XY fixed point: \( \langle \phi_{\mathbf{k}, \mathbf{k}'} \phi_{-\mathbf{k}' - \mathbf{k}, -\mathbf{k}} \rangle \sim (\epsilon^2 + \nu_\phi k^2)^{-\eta/2} \). \( \eta \) is the anomalous dimension of the order parameter \( \phi \) at the 3d XY fixed point. The leading-order contribution to the imaginary part of Fermion self-energy reads

\[
\Sigma(\omega)'' \sim (\lambda)^2 |\omega|^{2 + \eta} \text{sgn}[\omega] \ll |\omega|.
\] (7)

Therefore, the fermion self-energy correction is always dominated by the linear frequency term of the free-electron propagator, the linear coupling \( \lambda \) does not destroy the Landau quasiparticles.

In addition to the linear coupling, eq. (3), another quadratic interaction is also allowed by symmetry, but was omitted in the mean-field Hamiltonian equation (2):

\[
\mathcal{L}' = \lambda' \sum_i |\psi_i^\dagger \psi_i (\phi)|^2.
\] (8)

When \( \mu_1 = \mu_2 = 0 \), this term is clearly irrelevant based on straightforward power-counting. With finite Fermi surfaces, after integrating out the fermions, this quadratic interaction will induce the following four-body interaction:

\[
\mathcal{L}_2 = u(\phi^\dagger_{i\omega, \mathbf{q}} |\omega| \phi_{-i\omega, -\mathbf{q}} + \text{h.c.})
\] (9)
Note that the term with $|ω|$ comes from the Fermi surface effects. We want to estimate the scaling dimension of $u$ at the 3d $XY$ fixed point. Since the scaling dimension $[(\tilde{φ})^2] = 3 - 1/ν$, the scaling dimension of $u$ is $[u] = 2/ν - 3$, where $ν$ is the standard critical exponent defined as $ξ ≈ ν^{-1}$. Therefore, as long as $ν > 2/3$, $u$ is irrelevant. This criterion is indeed satisfied according to the well-known exponents of 3d $O(N)$ universality class [23]. $L_2$ also exists at the $z = 2$ QCP with $μ_1 ≠ μ_2$ discussed before; however, since there $|ω| = 2|q| = 2$, this term has a high scaling dimension and is clearly irrelevant. A similar analysis about the $|ω|/q$ term was first made in ref. [31].

Again we can evaluate effect of the coupling $L'$ on the fermion self-energy. The leading-order correction can again be calculated through the diagram in fig. 2(b), while now the dashed lines are correlation functions $⟨\tilde{φ}_{ic,k}^2 ϕ_{ic,−k}^2⟩ \sim (ε^2 + v_3^2 k^2)^{-1/2}$. With a finite Fermi surface, the leading-order contribution to the imaginary part of fermion self-energy reads

$$\Sigma(ω)'' \sim (λ)^2|ω|^{2/2} ν \text{sgn}|ω| \ll |ω|. \quad (10)$$

Hence this quadratic coupling $L'$ does not destroy the Landau quasiparticle at the QCP either.

Now let us turn on an extra intra-edge Coulomb interaction in eq. (1):

$$L_v = \sum_{\lambda} V_{n\lambda} n_{\lambda \downarrow}. \quad (11)$$

This term will favor to develop magnetization on each edge [17]. Since $V_{n\lambda} n_{\lambda \downarrow} \sim -V(ψ^\dagger \sigma^x ψ^\dagger)/2$, the Hubbard-Stratonovich transformation can give us the mean-field order parameters $Φ_1 \sim ψ^\dagger ψ$ and $Φ_2 \sim ψ^\dagger ψ^\dagger$ with Ising symmetry. Without exciton condensate in the background, these two Ising order parameters $Φ_1$ and $Φ_2$ are degenerate at the mean-field level. $Φ_1$ breaks only $\mathcal{T}$, while $Φ_2$ breaks both $\mathcal{T}$ and $\mathcal{I}$. In the background of exciton condensate, $Φ_2$ has lower fermion mean-field energy because the exciton order parameters anticommute with $Φ_2$, hence the exciton condensate favors to have an $\mathcal{I}$ breaking magnetization.

In ref. [21], it was shown that when $μ_1 + μ_2 = 0$, at the vortex core of the exciton condensate order parameter there is a Fermion zero mode, which carries charge $1/2$. This zero mode is protected by the symmetry of the Hamiltonian equation (1): $γ_2 H^* γ_2 = H$, and $γ_2 = iσ^y γ^y$. This symmetry guarantees that the spectrum is symmetric with $E = 0$, and it is valid even with the presence of an exciton vortex. With nonzero $Φ_2$, this symmetry is broken, and there is no longer a zero mode at the vortex core. By contrast, if the system develops the magnetization $Φ_1$, there is still a vortex core fermion mode at precisely zero energy.

Just like the exciton order parameter $Φ$, the order parameter $Φ_0$ also couples to the fermions both linearly and quadratically. Due to the same matrix element suppression effect as in eq. (5), the linear coupling does not lead to singular corrections to the QCP of $Φ_0$. However, using the similar argument as that below eq. (9), the quadratic coupling $L'' \sim λ \sum_{\lambda} ψ_{\lambda}^\dagger (Φ_0)^2$ will lead to a relevant perturbation at the 3d Ising fixed point as long as one of the edges has a finite Fermi surface, due to the fact $ν < 2/3$ at the 3d Ising universality class [23].

In addition to the Fermi surface, the Goldstone mode of the exciton condensate couples to the order parameter $Φ_0$ as well, if the QCP of $Φ_0$ occurs in the background of the exciton condensate. In the case without $I (μ_1 ≠ μ_2)$, the lowest-order coupling reads $L'''' \sim λ''''(\partial_\theta)(Φ_0)^2$. $θ$ is the phase angle of the exciton condensate: $φ \sim e^{iθ}$. With $L''''$, after integrating out the Goldstone mode $θ$, a singular term is induced for $Φ_0$:

$$L_3 = u_3(Φ_0)^2 \frac{ω^2}{ω^2 + v_0^2 q^2} (Φ_0)^2 \sim ω^2 Σ(ω)'''' \quad (12)$$

To determine the scaling dimension of this term, we again have to compare $ν$ of 3d Ising transition and 2/3: since $ν < 2/3$, this coupling $L_3$ is also relevant at the 3d Ising universality class. This relevant perturbation exists even when the fermions are fully gapped out by the exciton condensate. In the case with $I$, the coupling $L''''$ is forbidden, since $θ → -θ$ under $I$. In this case the coupling between $Φ_0$ and the exciton Goldstone mode will occur at higher order, hence no relevant perturbation is induced at the 3d Ising universality class.

Although the exciton is charge neutral, its transport effect has been verified in a bilayer quantum Hall system [22], by measuring the tunnelling conductance between the two layers [33]. A similar measurement can in principle be carried out in the thin-film topological insulator. The exciton condensate will lead to a sharp peak of the inter-surface tunnelling conductance. Inside the exciton condensate phase, the condensate will be destroyed by the thermal fluctuation through a Kosterlitz-Thouless transition at finite temperature. The scaling between the critical temperature $T_c$ of this KT transition and the tuning parameter $r$ depends on the universality class of the QCP, and $r$ can be taken as the interaction $U − U_c$. For example, for the $z = 2$ mean-field transition, $T_c \sim |r|$, while for the 3d $XY$ transition in the phase diagram (fig. 1), $T_c \sim |r|^{2ν} \sim |r|^{2/3}$. Thus, different quantum critical behaviors can be measured through $T_c$. The interaction $U$ between the two surfaces can be tuned by changing the thickness of the thin-film sample.

If $U$ in eq. (1) is attractive instead of repulsive, then the system favors to have superconductor pairing. After a particle-hole transformation for $ψ_2$: $ψ_2 \rightarrow σ^x ψ_1^\dagger$, both $U$ and $μ_2$ change sign, while all the other terms of the Hamiltonian remain unchanged. The most energetically favored pairing state is $ψ_1 σ^x ψ_2^\dagger$, because after particle-hole transformation this pairing becomes the exciton condensate $ϕ$. Therefore, all the analysis of the QCP and Goldstone mode about this superconducting state can be obtained by particle-hole transformation of the exciton case. For instance, at chemical potential $μ_1 = μ_2$, there is a logarithmic divergence of the pairing susceptibility,
while at $\mu_1 = -\mu_2$ there is a matrix element suppression at the interaction vertex between Cooper pair and fermions. The pairing $\psi_1^\dagger \sigma^x \psi_2$ is a spin triplet pairing with total $S^z = 0$, and the vortex core of this superconductor carries a fermion zero mode when $\mu_1 = \mu_2$.

In summary, we have studied the exciton condensation phase transition and its quantum critical properties in a phase diagram with edge-dependent chemical potentials and Coulomb interaction. Interplay between exciton condensate and other order parameters are also discussed. In addition to the TBI materials that are currently under intensive experimental studies, we expect our formalism to be applicable to TBI with strong correlation, for instance the materials with $5d$ electrons [34,35] which have been proposed recently.

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