Excitonic instabilities and spontaneous time-reversal symmetry breaking on the honeycomb lattice

Wei Liu

Physics Department, City College of the City University of New York, New York, New York 10031, USA

Alexander Punnoose*

Instituto de Física Teórica - Universidade Estadual Paulista, R. Dr. Bento Teobaldo Ferraz 271, Barra Funda, São Paulo - SP, 01140-070, Brazil

(Received 3 September 2013; published 16 January 2014)

We elucidate the close relationship between spontaneous time-reversal symmetry breaking and the physics of excitonic instabilities in strongly correlated multiband systems. The underlying mechanism responsible for the spontaneous breaking of time-reversal symmetry in a many-body system is closely related to the Cooper-like pairing instability of *interband* particle-hole pairs involving higher-order symmetries. Studies of such pairing instabilities have, however, mainly focused on the mean-field aspects of the virtual exciton condensate, which ignores the presence of the underlying collective Fermi-liquid excitations. We show that this relationship can be exploited to systematically derive the coupling of the condensate order parameter to the *intraband* Fermi-liquid particle-hole excitations. Surprisingly, we find that the *static* susceptibility is negative in the ordered phase when the coupling to the Fermi-liquid collective excitations are included, suggesting that a uniform condensate of virtual excitons, with or without time-reversal breaking, is an unstable phase at T=0.

DOI: 10.1103/PhysRevB.89.045126 PACS number(s): 75.10.-b, 05.30.Fk, 11.30.Er, 71.27.+a

I. INTRODUCTION

In multiband systems, the normal Fermi-liquid (FL) state of a partially filled band becomes unstable when the exciton [1] (electron-hole pair) binding energy E_B is tuned to become larger than the direct excitation threshold energy $E_D < |E_B|$ (see Fig. 1). When this happens, *virtual* excitons form spontaneously in the ground state and destabilize the FL state. As a cure for this instability, it was proposed many decades ago [2,3] that a new Hartree–Fock ground state may be constructed by hybridizing the bands. Such a state is characterized by a nonzero expectation value $\langle a_{\bf k}^{\dagger} b_{\bf k} \rangle \neq 0$, where $a_{\bf k}^{\dagger}$ and $a_{\bf k}$ and $b_{\bf k}^{\dagger}$ and $b_{\bf k}$ are the electron creation and annihilation operators, respectively, in the relevant bands. As a result, the relative phase between the bands is locked to form a uniform (q=0) condensate of interband particle-hole pairs.

To distinguish condensates of *interband* particle-hole pairs from quantum liquids that arise from instabilities in the *intraband* particle-hole channel found in single-band systems, like the Pomeranchuk instability [4], we refer to the former here as an "excitonic liquid" (XL).

The XL is to be contrasted with the much-studied *excitonicinsulator* state formed when the number of free conduction electrons and valence holes are finite. The latter can occur either naturally when the bands cross at the Fermi level (semimetal with band gap $E_G < 0$) or can be created artificially by optically pumping a semiconductor ($E_G > 0$). The two carrier types have their own chemical potentials which are tied together by thermodynamic considerations. The excitonicinsulator problem has been shown to be mathematically equivalent to the Bardeen–Cooper–Schrieffer (BCS) model with electron-hole pairs instead of electron-electron pairs [5–9]. Unlike the gapped excitonic-insulator state, the XL state has only one species of free carriers, hence away from

half filling the chemical potential lies in the band leading to a metallic state with a sharp Fermi surface (at least in the Hartree–Fock approximation). This raises the interesting question of the stability of the XL in the presence of gapless fermions at the Fermi surface.

The issue of the coupling of bosonic modes in the ordered phase to gapless fermions has received considerable attention recently, particularly concerning the applicability of the Hertz theory [10] to continuous quantum phase transitions at T = 0. The issue is that integrating the fermions out completely has been shown to give rise to a nonlocal (in time or frequency) bosonic theory that is dominated by Landau damping, which in most cases leads to an infinite number of marginal terms in the effective action [11]. (For a review of this and other related issues, see Ref. [12].) In all of these studies involving a single band, it is usually implicitly assumed that, to ensure the stability of the condensate, the opposite limit, i.e., the static limit, of the fluctuation of the order parameter $\lim_{q\to 0} \langle |\delta\phi(q,\omega=0)|^2 \rangle > 0$ is positive. We find that this assumption is generally violated in a multiband system when the coupling of the order-parameter of the XL state to the collective intraband particle-hole excitations is considered. We note that the issues originating from the dynamics of the gapless fermions leading to the Landau damping of the bosonic mode is irrelevant for us in establishing the stability of the condensed phase.

There is considerable interest to understand if a *uniform* XL can in principle exist. In fact, excitonic singularities in multiband systems is recognized to be one of the very few known mechanisms capable of introducing singularities in the irreducible interactions leading to the breakdown of FL theory [13]. At the mean-field level, the Hamiltonian couples linearly to the bilinear operators $a_{\bf k}^{\dagger}b_{\bf k}$ via a vertex function $\mathcal{A}({\bf k})$. The symmetries of $\mathcal{A}({\bf k})$ are dictated by the lattice symmetries. As a result, a nonzero expectation value $\mathcal{A}({\bf k})\langle a_{\bf k}^{\dagger}b_{\bf k}\rangle \neq 0$ partially breaks the point group symmetry. Furthermore, depending on the transformation properties of $\mathcal{A}({\bf k})$ under the corresponding

^{*}punnoose@ift.unesp.br

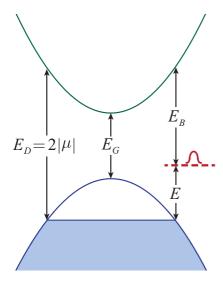


FIG. 1. (Color online) A simple direct band gap (E_G) model with quadratic bands of equal masses is shown. The location of the exciton level $E = E_D - E_B$ is marked by the dashed line. E_B is the exciton binding energy and E_D is the direct interband excitation threshold from the chemical potential μ (measured from the center of the gap). When $E_B = E_D$, the cost of creating virtual exciton pairs become negligible.

magnetic group, time-reversal (\mathcal{T}) symmetry may or may not be spontaneously broken in the ground state. Special interest in understanding the properties of electronic systems with broken \mathcal{T} symmetry stem from its proposed relevance to high-temperature superconductivity. An intriguing proposal, put forward originally by Varma as a candidate for a marginal Fermi liquid, posited a nonmagnetic, translationally invariant ground state with spontaneously broken \mathcal{T} invariance [14].

More generally, such ground states are novel in that they can exhibit anomalous Hall and Kerr effects without magnetic fields. Various nonmagnetic, translationally invariant states with broken \mathcal{T} symmetry that are ubiquitous in Hartree–Fock approximation schemes have been classified and analyzed in Ref. [15]. They were first demonstrated by Haldane in a simple two-dimensional model of noninteracting electrons on the honeycomb lattice with a periodic magnetic field arranged in such a way that the field averages to zero in each unit cell thus preserving the translational symmetry of the lattice [16]. It was later shown that interacting electrons on the honeycomb lattice with next-nearest-neighbor interactions can form exactly the same state as proposed by Haldane that spontaneously breaks \mathcal{T} invariance in the ground state [17].

Our main purpose in this paper is to analyze the stability of the mean-field solutions of particle-hole condensates both with and without \mathcal{T} symmetry breaking. We first show that the XLs are metallic *away* from half filling. Indeed, since the single-particle states in any mean-field approximation of a particle-number-conserving condensate remains in one-to-one correspondence with the FL states with well-defined quasiparticle excitations, at the Hartree–Fock level the condensates away from half filling are always metallic with a continuum of gapless fermionic excitations at the Fermi surface.

We show that the hybridization of the bands necessarily induces a coupling of the XL order parameter to the gapless

fermions at the Fermi surface. In the following, we analyze the static susceptibility originating from this coupling in two different two-band models, both of which stabilizes an XL phase at the mean-field level. The first model is a simplified continuum degenerate semiconductor model in which the $\mathcal T$ symmetry is left intact in the condensed phase, and the second model is a lattice model that supports a $\mathcal T$ -symmetry-broken phase.

II. THEORY OF XL STATE.

Our objective in this section is to analyze a simple model that undergoes a quantum phase transition to a uniform XL state. We consider the well-studied, continuum, two-band, spinless fermion model with a direct band gap $E_G > 0$ shown in Fig. 1. Keeping only the direct intraband scattering of the electrons and holes, the model is described by the Hamiltonian

$$K = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^{\dagger} (\epsilon_{\mathbf{k}} \tau_{3} - \mu) \psi_{\mathbf{k}} - \frac{1}{L^{d}} \sum_{\mathbf{k}', \mathbf{k}; \mathbf{q}} V_{\mathbf{k}\mathbf{k}'} a_{\mathbf{k}+\mathbf{q}}^{\dagger} b_{\mathbf{k}} b_{\mathbf{k}'}^{\dagger} a_{\mathbf{k}'+\mathbf{q}}.$$
(1)

The 2×2 Pauli-matrix τ_i 's act on the internal band space; τ_3 is the z component. The spinor $\psi_{\mathbf{k}}^{\dagger} = (b_{\mathbf{k}}^{\dagger}, a_{\mathbf{k}}^{\dagger})$ creates *electrons* in the conduction (b) and the valence (a) bands. The bands are assumed to be parabolic with equal masses $\epsilon_{\mathbf{k}} = E_G/2 + k^2/(2m)$. The chemical potential μ constraints the electron number $N = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^{\dagger} \psi_{\mathbf{k}}$. Hole doping is assumed throughout, i.e., partially filled valence band and empty conduction band; hence $\mu < 0$. All energies are measured from the center of the gap.

For the interaction, only the dominant scattering channel, the direct intraband scattering of the electrons and holes, are retained. The Hamiltonian K has been used extensively as a minimal model to analyze the excitonic properties of optically pumped degenerate semiconductors [9,18,19]. We note that because optical pumping fixes the number of electrons and holes $N_{ph} = \sum_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + a_{\mathbf{k}} a_{\mathbf{k}}^{\dagger}$, the chemical potential μ_{ph} in these systems appears as [9,20] $K_{ph} =$ $H - \mu_{ph} N_{ph} = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^{\mathsf{T}} [(\epsilon_{\mathbf{k}} - \mu_{ph}) \tau_3] \psi_{\mathbf{k}} + H_{\text{int}}$. A particlehole transformation, $a_{\mathbf{k}} \to c_{-\mathbf{k}\downarrow}^{\dagger}$ and $b_{\mathbf{k}} \to c_{\mathbf{k}\uparrow}$, maps K_{ph} to the continuum fermion model with attractive interactions [21,22] whose mean-field solution corresponds exactly to the BCS Hamiltonian. In contrast, the same transformation maps K in Eq. (1) to the BCS Hamiltonian in a Zeeman field with field $h_Z = \mu$ and fixed BCS chemical potential $\mu_{\rm BCS} = -E_G/2$. When $E_G < 0$ (semimetal) the mean-field solution of K maps exactly to the BCS Hamiltonian in a Zeeman field [23,24]. Since $E_G > 0$ when the XL state is formed, the particle-hole transformation does not provide much further insights. However, we show that the instability is closely related to the Cooper-like pairing of interband particle-hole pairs at the Fermi surface.

Further analytical progress is possible by restricting our analysis to the *s*-wave pairing state. We make the standard approximation of a separable screened potential [18], $V_{\mathbf{k}\mathbf{k}'} = V\mathcal{A}(\mathbf{k})\mathcal{A}(\mathbf{k}')$, where $\mathcal{A}(\mathbf{k}) = 1$ for $|-\epsilon_{\mathbf{k}} - \mu| < \Lambda$ and zero otherwise (around the hole Fermi surface). The cutoff is of the order $\Lambda \sim O(E_G)$. This simplification allows the interaction

to be written as a product of bilinear operators,

$$H_{\rm int} = -\frac{V}{L^d} \sum_{\mathbf{q}} \hat{\Phi}^{\dagger}(\mathbf{q}) \hat{\Phi}(\mathbf{q}), \tag{2}$$

where $\hat{\Phi}(\mathbf{q}) = \sum_{\mathbf{k}}' \psi_{\mathbf{k}}^{\dagger} \tau^{+} \psi_{\mathbf{k}+\mathbf{q}} = \sum_{\mathbf{k}}' b_{\mathbf{k}}^{\dagger} a_{\mathbf{k}+\mathbf{q}}$, and τ^{+} is the band index raising operator. The prime on the k sum explicitly enforces the restriction on $\mathcal{A}(\mathbf{k})$. Thus we arrive at our simplified model Hamiltonian:

$$K = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^{\dagger} \left[\epsilon_{\mathbf{k}} \tau_3 - \mu \right] \psi_{\mathbf{k}} - \frac{V}{L^d} \sum_{\mathbf{q}} \hat{\Phi}^{\dagger}(\mathbf{q}) \hat{\Phi}(\mathbf{q}). \tag{3}$$

A. Fermi surface instability: Mean-field theory

We explore the possibility of a uniform XL ground state with a finite expectation value $V\langle \hat{\Phi}(\mathbf{q}) \rangle/L^d = \phi_0 \delta_{q,0}$. Such a state is anticipated from the behavior of the effective interaction, $\mathcal{U}(\mathbf{q}) = V\Gamma(\mathbf{q})$, which in the ladder-diagram approximation takes the general form

$$\Gamma(\mathbf{q}) = \frac{1}{1 - V \chi_0(\mathbf{q})}.\tag{4}$$

It follows from the form of K in Eq. (3) that χ_0 is the noninteracting interband susceptibility:

$$\chi_0(\mathbf{q}) = -\frac{1}{L^d} \sum_{\mathbf{k}}' \frac{f(\epsilon_{\mathbf{k}+\mathbf{q}}^+) - f(\epsilon_{\mathbf{k}}^-)}{\epsilon_{\mathbf{k}+\mathbf{q}}^+ - \epsilon_{\mathbf{k}}^-}.$$
 (5)

The energies $\epsilon_{\bf k}^{\pm}=\pm\epsilon_{\bf k}-\mu$ are the upper and lower band energies measured from μ . Since we assume hole doping, at T=0 the Fermi function $f(\epsilon_{\bf k}^+)=0$ for all ${\bf k}$, and $f(\epsilon_{\bf k}^-)=1$ for $|{\bf k}|>k_F$ and zero otherwise. k_F is the noninteracting Fermi wave vector that fixes the filling. Substituting for the Fermi functions in Eq. (5), we get $\chi_0(0)>0$ in the limit q=0. Hence the uniform $\Gamma(0)$ diverges at a critical V_c satisfying $1-V_c\chi_0(0)=0$, indicating a FL instability for the states at the chemical potential. The critical V_c that determines the QCP equals

$$\frac{1}{V_c} = \sum_{\mathbf{k}}^{"} \frac{1}{2\epsilon_{\mathbf{k}}}.$$
 (6)

The sum $\sum_{\mathbf{k}}'' = L^{-d} \sum_{|\mathbf{k}| > k_F}'$. [Remember that the single prime denotes the upper cutoff imposed by $\mathcal{A}(\mathbf{k})$.]

We show below, by using a more elementary quantum-mechanical calculation, that the above instability is related to the formation of Cooper-like pairs of interband particle-hole pairs with zero energy. This is done by writing the equation of motion for a single particle-hole pair in the background of a "rigid" Fermi sea of particles [7].

We assume a linear combination of pair wave functions $\varphi_{\mathbf{k}}$ of single particle-hole pairs created by annihilating an electron from inside of the Fermi surface $|FS\rangle$ of the partially filled valence band and recreating it at the same \mathbf{k} value in the empty conduction band

$$|\phi_0\rangle = \sum_{\mathbf{k}}^{"} \varphi_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} |\text{FS}\rangle.$$
 (7)

The sum extends from k_F to the upper cutoff.

The pair energy is obtained by solving the stationary Schrödinger equation

$$E \sum_{\mathbf{k}}^{"} \varphi_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} = \sum_{\mathbf{k}}^{"} \varphi_{\mathbf{k}} [K, b_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}]$$

$$= \sum_{\mathbf{k}}^{"} \left[2\epsilon_{\mathbf{k}} \varphi_{\mathbf{k}} - \frac{V}{L^{d}} \right]$$

$$\times \sum_{\mathbf{k}'}^{'} \varphi_{\mathbf{k}'} (a_{\mathbf{k}'}^{\dagger} a_{\mathbf{k}'} - b_{\mathbf{k}'}^{\dagger} b_{\mathbf{k}'}) b_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}.$$

$$(9)$$

The Cooper model assumes a rigid Fermi sea, which is equivalent to decoupling the interaction terms by averaging over the Fermi sea $\langle a^{\dagger}_{\mathbf{k}'}a_{\mathbf{k}'}-b^{\dagger}_{\mathbf{k}'}b_{\mathbf{k}'}\rangle=f(\epsilon^-_{\mathbf{k}'})-f(\epsilon^+_{\mathbf{k}'})$. One then obtains the Bethe–Goldstone equation:

$$E\varphi_{\mathbf{k}} = 2\epsilon_{\mathbf{k}}\varphi_{\mathbf{k}} - V \sum_{\mathbf{k}'}^{"} \varphi_{\mathbf{k}'}.$$
 (10)

Substituting $\phi_0 = V \sum_{\mathbf{k}}'' \varphi_{\mathbf{k}}$ and inverting the above equation gives the self-consistent equation

$$1 = -V \sum_{\mathbf{k}}^{"} \frac{1}{E - 2\epsilon_{\mathbf{k}}}.\tag{11}$$

Setting E = 0 gives Eq. (6). Since E is measured from the chemical potential, when $V > V_c$, it becomes favorable to create particle-hole pairs out of the Fermi sea, thus destabilizing the normal ground state.

A possible cure for this instability is to assume a new Hartree-Fock solution built of virtual excitons [2,3]. This is equivalent to assigning a nonzero expectation value to $\langle \hat{\Phi}(\mathbf{q}) \rangle \sim \phi_0 \delta_{q,0}$. We note that the order parameter is not invariant under a global U(1) rotation $e^{i\frac{v}{2}\tau_3}\psi_{\mathbf{k}}$ of the relative phase between the two bands. However, H_{int} in Eq. (2) conserves the particle number in each band separately and is therefore invariant. Hence the condensation spontaneously breaks the U(1) symmetry. The associated Goldstone mode is easily identified with the phase of the XL order parameter. We note, however, that the enhanced U(1) symmetry of H_{int} exists because terms such as $a^{\dagger}a^{\dagger}bb$ and $a^{\dagger}a^{\dagger}ab$ that do not conserve the particle number in each band are omitted in our model. It is therefore only an approximate symmetry in general and when spontaneously broken will give rise to a *massive* pseudo-Goldstone mode [25,26]. For the sake of generality, we suppress the gapless phase fluctuations in our simplified model by assuming ϕ_0 to be real.

We proceed to look for a mean-field solution by substituting ϕ_0 into Eq. (3). The mean-field Hamiltonian

$$K_{\rm MF} = \sum_{\mathbf{k}}' \psi_{\mathbf{k}}^{\dagger} \left[\epsilon_{\mathbf{k}} \tau_3 - \mu - \phi_0 \tau_1 \right] \psi_{\mathbf{k}} + \frac{L^d}{V} \phi_0^2. \tag{12}$$

Since ϕ_0 is assumed real, the linear terms in $K_{\rm MF}$ that originate upon decoupling the interaction terms are combined as $\phi_0[\hat{\Phi}^\dagger(0)+\hat{\Phi}(0)]=\phi_0\psi_{\bf k}^\dagger\tau_1\psi_{\bf k}$. [From Eq. (3), the q=0 component $\hat{\Phi}(0)=\sum_{\bf k}'\psi_{\bf k}^\dagger\tau^+\psi_{\bf k}=\sum_{\bf k}'b_{\bf k}^\dagger a_{\bf k}$.] Diagonalizing $K_{\rm MF}$, we obtain $\xi_{\bf k}^\pm=\pm E_{\bf k}-\mu$, where the energy $E_{\bf k}=(\epsilon_{\bf k}^2+\phi_0^2)^{1/2}$. When $E_G>0$, the levels never cross and all states up to the noninteracting Fermi wave vector k_F are filled. This point is worth emphasizing again, which is that, because $K_{\rm MF}$ commutes with the individual number operator $\hat{n}_{\bf k}=a_{\bf k}^\dagger a_{\bf k}+b_{\bf k}^\dagger b_{\bf k}$, every $\bf k$ state up to the noninteracting k_F

remains occupied as V is tuned through the QCP. It implies the Fermi wave vector k_F is not renormalized and a sharp Fermi surface exists in the condensed phase.

The most suggestive way to write the XL wave function, $|\mathrm{XL}\rangle$, so that k_F and the exciton nature are both apparent is $|\mathrm{XL}\rangle = \prod_{\mathbf{k}} [u_{\mathbf{k}} + v_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}] |\mathrm{FS}\rangle$. The "vacuum" is the noninteracting Fermi surface $|\mathrm{FS}\rangle = \prod_{|\mathbf{k}|>k_F} a_{\mathbf{k}}^{\dagger} |0\rangle$ corresponding to the partially filled valence band. Despite the formal similarity with the BCS wave function, it can be shown explicitly that $|\mathrm{XL}\rangle$ does not possess off-diagonal long-range order (ODLRO) [7] due to the sharp cutoff at k_F . In standard notation, the hybridized states are written as $c_{\mathbf{k}+} = u_{\mathbf{k}} b_{\mathbf{k}} - v_{\mathbf{k}} a_{\mathbf{k}}$ and $c_{\mathbf{k}-} = u_{\mathbf{k}} a_{\mathbf{k}} + v_{\mathbf{k}} b_{\mathbf{k}}$, corresponding to $\pm E_{\mathbf{k}}$, respectively. The coefficients are found by minimizing the free energy. Setting all the phases to zero, which is justified when ϕ_0 is real, we get

$$u_{\mathbf{k}}^2 = \frac{1}{2} \left(1 + \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} \right), \quad v_{\mathbf{k}}^2 = \frac{1}{2} \left(1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} \right).$$
 (13)

B. Order-parameter fluctuations

The existence of a sharp Fermi surface in the XL phase implies that gapless particle-hole excitations exists at the Fermi surface, which can couple to the fluctuations of the order parameter of the XL. The fluctuations about the mean-field solution are most easily calculated by using the standard functional integral method [27,28]. Briefly, the partition function is written as an imaginary time integral $Z = \int D[\bar{\psi},\psi]e^{-\int_0^\beta d\tau \mathcal{L}}$, where the Lagrangian $\mathcal{L} = \sum_{\mathbf{k}} \bar{\psi}_{\mathbf{k}}(\tau)\partial_\tau\psi_{\mathbf{k}}(\tau) + K$. Substituting for K from Eq. (3), we get $\mathcal{L} = \sum_{\mathbf{k}} \bar{\psi}_{\mathbf{k}}(\tau)(\partial_\tau - \mu + \epsilon_{\mathbf{k}}\tau_3)\psi_{\mathbf{k}}(\tau) - \frac{V}{L^d}\sum_{\mathbf{q}}\bar{\Phi}(\mathbf{q},\tau)\Phi(\mathbf{q},\tau)$. Next, Hubbard–Stratonovich fields $\phi(\mathbf{q},\tau)$ are introduced to decouple the quartic $\bar{\Phi}(\mathbf{q},\tau)\Phi(\mathbf{q},\tau)$ term. The resulting action is quadratic in the fermionic fields and can therefore be integrated out to give $Z = \int D[\phi^*]D[\phi]e^{-S_{\mathrm{eff}}[\phi^*,\phi]}$, where

$$S_{\text{eff}}[\phi^*, \phi] = -\text{Tr} \ln G^{-1} + \frac{L^d}{\beta V} \sum_{q} |\phi(q)|^2,$$
 (14)

$$G^{-1}(k,k') = (-i\epsilon_n - \mu + \epsilon_k \tau_3)\delta_{k,k'} - \frac{1}{\beta}\phi^*(k'-k)\tau^+ - \frac{1}{\beta}\phi(k-k')\tau^-.$$
 (15)

The shorthand notations $k \equiv (\mathbf{k}, ik_n)$ and $k' - k = q \equiv (\mathbf{q}, iq_m)$, where k_n (q_m) are the odd (even) Matsubara frequencies, are used throughout. The Fourier transform is defined as $\phi(x) = \beta^{-1} \sum_m L^{-d} \sum_{\mathbf{q}} e^{-iq_m \tau + i\mathbf{q} \cdot \mathbf{r}} \phi(q)$. Since only real $\phi(x)$ is considered, $\phi(q) = \phi^*(-q)$.

The mean-field solution corresponds to the saddle point $\phi(q) = \beta \delta_{m,0} \delta_{\mathbf{q},0} \phi_0$. The magnitude of ϕ_0 is obtained by minimizing the action $\delta S_{\rm eff}[\phi_0]/\delta \phi_0 = 0$. The saddle-point condition at T=0 generalizes Eq. (6) to

$$\frac{1}{V} = \sum_{k}^{"} \frac{1}{2E_{k}}.$$
 (16)

The mean-field scaling $\phi_0 \propto \sqrt{V - V_c}$ is recovered close to the QCP. Next, we investigate the stability of the saddle-point solution by analyzing the Gaussian fluctuations around ϕ_0 .

This is done by expanding the action to quadratic order in the deviation $\delta \phi(x) = \phi(x) - \phi_0$.

To this end, we first separate the ϕ_0 and the $\delta\phi$ contributions in G in Eq. (15) as $G^{-1}=G_0^{-1}(1-\Sigma G_0)$, where

$$G_0(k,k') = -\frac{(i\epsilon_n + \mu) + \epsilon_k \tau_3 - \phi_0 \tau_1}{(i\epsilon_n - \xi_k^+)(i\epsilon_n - \xi_k^-)} \delta_{k,k'}, \qquad (17)$$

$$\Sigma(k,k') = \frac{1}{\beta} \delta \phi(k - k') \tau_1. \tag{18}$$

The trace in Eq. (14) is then expanded in the standard way using the formula $\operatorname{Tr} \ln G^{-1} = \operatorname{Tr} \ln G_0^{-1} - \sum_n \frac{1}{n} \operatorname{Tr} (G_0 \Sigma)^n$. The order n=2 terms are collected to derive the $|\delta \phi|^2$ corrections. The first-order correction, n=1, vanishes since the saddle point is an extremum. We write the expansion to quadratic order of $S_{\rm eff}$ as $S_{\rm eff}^{(2)} = S_{\rm eff}[\phi_0] + L^d \sum_q [V\Gamma(q)]^{-1} |\delta \phi(q)|^2$, where $\Gamma^{-1}(q) = 1 - V \chi(q)$ is the generalization of Eq. (4).

The susceptibility $\chi(q)$ in the ordered phase equals

$$\chi(q) = -\frac{1}{2\beta L^d} \sum_{k} \text{Tr} \left[G_0(k+q) \tau_1 G_0(k) \tau_1 \right].$$
 (19)

Note that the Green's function G_0 as defined in Eq. (17) is a 2×2 matrix written in the original FL basis (b,a) and is therefore not diagonal due to the hybridization of the bands in the XL phase. Also note that the τ_1 in the trace originates from $\Sigma \sim \delta \phi \tau_1$ [see Eq. (18)]. The diagrams corresponding to the various terms from the expansion of the trace are shown in Fig. 2. Compared to the interband FL susceptibility χ_0 [see Eq. (5)], there are two new contributions in the XL phase that originate from the off-diagonal terms of G_0 . They are shown in the last line of Fig. 2; they vanish as $\sim \phi_0^2$.

In the mean-field basis $c_{\mathbf{k},\pm}$ defined in Eq. (13) (the XL basis) $\chi(q)$ separates into inter- and intraband contributions,

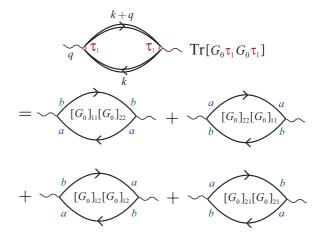


FIG. 2. (Color online) The diagrammatic expansion of the trace in the definition of $\chi(q)$ in Eq. (19) is shown. The new off-diagonal diagrams (last line) exist only in the XL phase; they vanish for ϕ_0^2 close to the QCP. The interaction of the bosonic propagator, corresponding to the amplitude fluctuations of the order parameter, with the gapless fermions at the chemical potential, generates a bosonic mass $\sim \phi_0^2$. The sign of the mass is derived in the main text and is shown to be negative.

which we write as $\chi(q) = \chi_{\perp}(q) + \chi_{\parallel}(q)$. After summing over the internal energy sums, we get

$$\chi_{\perp}(q) = \frac{1}{2L^d} \sum_{\mathbf{k}}' \mathcal{F}_{\perp}(\mathbf{k}, \mathbf{q}) [\Pi_{+-}(\mathbf{k}, q) + \Pi_{-+}(\mathbf{k}, q)], \quad (20)$$

$$\chi_{\parallel}(q) = \frac{1}{2L^{d}} \sum_{\mathbf{k}}' \mathcal{F}_{\parallel}(\mathbf{k}, \mathbf{q}) [\Pi_{++}(\mathbf{k}, q) + \Pi_{--}(\mathbf{k}, q)]. \quad (21)$$

The form factors $\mathcal{F}_{\perp}(\mathbf{k},\mathbf{q}) = (u_{\mathbf{k}}u_{\mathbf{k}+\mathbf{q}} - v_{\mathbf{k}}v_{\mathbf{k}+\mathbf{q}})^2$ and $\mathcal{F}_{\parallel}(\mathbf{k},\mathbf{q}) = (u_{\mathbf{k}}v_{\mathbf{k}+\mathbf{q}} + v_{\mathbf{k}}u_{\mathbf{k}+\mathbf{q}})^2$, where $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are defined in Eq. (13). The polarization functions

$$\Pi_{ss'}(\mathbf{k},q) = \frac{f\left(\xi_{\mathbf{k}+\mathbf{q}}^{s}\right) - f\left(\xi_{\mathbf{k}}^{s'}\right)}{iq_{m} - \left(\xi_{\mathbf{k}+\mathbf{q}}^{s} - \xi_{\mathbf{k}}^{s'}\right)},\tag{22}$$

where s,s'=+ (–) are the upper (lower) band indices. Note that the polarization operator, Π_{--} , corresponds to the intraband particle-hole bubble in the XL phase, i.e., the energies $\xi_{\bf k}^{\pm}$ correspond to the XL bands. (At T=0, the upper band is empty, hence $\Pi_{++}=0$.)

The hybridization of the bands in the XL phase couples the order parameter to the gapless fermions at the Fermi surface. The intraband polarization Π_{--} represents this coupling; it vanishes as $\mathcal{F}_{\parallel} \sim \phi_0^2$ close to the QCP. Physically, it generates an additional "mass" for the bosonic propagator. Depending on the sign of the mass, the condensate may or may not be stable. To determine the sign, we expand both $\chi_{\perp}(q)$ and $\chi_{\parallel}(q)$ for small q and take the static limit (mass term) of $\chi(q)$.

Since $E_G > 0$, the interband terms $\Pi_{+-/-+}$ in χ_{\perp} have a regular expansion in q. After analytical continuation, $iq_m = \omega + i0^+$, we get at T = 0 to $O(q^2, \phi_0^2)$:

$$\chi_{\perp}(q) = \sum_{\mathbf{k}}^{"} \frac{1}{2E_{\mathbf{k}}} - \gamma_{\perp} \left[4\phi_0^2 - \omega^2 + c|\mathbf{q}|^2 / (2m) \right]. \quad (23)$$

From the self-consistent equation derived in Eq. (16), the first term equals 1/V at the saddle point and cancels the constant in $\Gamma^{-1}(q) = 1 - V\chi(q)$. The remaining contributions of $O(\phi_0^2, q^2)$ to the bosonic propagator equal

$$[V\Gamma(q)]^{-1} = \gamma_{\perp} \left[4\phi_0^2 - \omega^2 + c|\mathbf{q}|^2/(2m) \right] - \chi_{\parallel}(q). \quad (24)$$

The occurrence of the pole $\omega^2 = (2\phi_0)^2 + c|\mathbf{q}|^2/(2m)$, starting at $\omega = 2\phi_0$, is identified with the collective excitations of the transverse-field Ising model [29,30]. To elucidate this further, we rewrite the fermionic bilinears in the Hamiltonian K in Eq. (3) in terms of pseudospin operators [31] $\sigma_i(\mathbf{k}) = \psi_{\mathbf{k}}^{\dagger} \tau_i \psi_{\mathbf{k}}$. They obey the usual SU(2) commutation relations $[\sigma_i(\mathbf{k}), \sigma_j(\mathbf{k}')] = 2i\epsilon_{ijk}\sigma_k(\mathbf{k})\delta_{\mathbf{k},\mathbf{k}'}$. The dynamics of the uniform state is described by the q=0 term of K. The reduced Hamiltonian K_0 equals

$$K_0 = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \sigma_3(\mathbf{k}) - \frac{V}{L^d} \sum_{\mathbf{k}, \mathbf{k}'} \sigma^{-}(\mathbf{k}) \sigma^{+}(\mathbf{k}'). \tag{25}$$

(The constant μ is suppressed here, it plays a crucial role only when the scattering at the Fermi surface involving $\mathbf{q} \neq 0$ is included.) As V increases, a transition occurs from the paramagnetic state in which all states point down (occupied valence band) to a correlated Ising ferromagnetic state with spins pointing in the x-y plane (hybridized states). Our choice of a real order parameter, $\langle \hat{\Phi}(0) \rangle = \langle \hat{\Phi}^{\dagger}(0) \rangle \propto \phi_0$, breaks

the symmetry in the x direction, i.e., $\sum_{\mathbf{k}} \langle \sigma_1(\mathbf{k}) \rangle \neq 0$ [see Eq. (12)]. The key point is that this Ising symmetry is lost when the finite $\mathbf{q} \neq 0$ terms involving particle-hole scattering at the Fermi surface are included. The scattering is represented by $\chi_{\parallel}(q)$, which appears as a self-energy correction to the bosonic propagator in Eq. (24). We show next that the static limit of $\chi_{\parallel}(q) \sim \phi_0^2$ is positive [implying a negative mass contribution to $\Gamma(q)$] and therefore has the potential to destabilize the condensate. Note that at half filling $\chi_{\parallel}=0$, hence the condensate is always stable.

First we show that the condensate is stable when χ_{\parallel} is suppressed. This requires that the constants γ_{\perp} and c>0 are positive in Eq. (24). The integral for γ_{\perp} is ultraviolet (Λ) convergent in dimensions d<6 and hence we set $\Lambda\to\infty$ and restrict ourselves to d<6. In the limit $\phi_0,q=0$, only two parameters remain, the dimension d and the hole-doping factor $x=1-E_G/(2\epsilon_F)$.

Separating the factor $\nu(\epsilon) = \nu_d (\epsilon - E_G/2)^{d/2-1}$ where $\nu_d = (m/2\pi)^{d/2}/\Gamma(d/2)$, corresponding to the density of states, the constant γ_\perp can be written as

$$\gamma_{\perp} = \sum_{\mathbf{k}}^{"} \frac{1}{(2\epsilon_{\mathbf{k}})^3} = \frac{1}{8} \nu_d \epsilon_F^{d/2 - 3} R_{\perp}^{(d)}(x).$$
 (26)

Restricting ourselves to d = 2, 3, and 4, we get

$$\{R_{\perp}^{(2)}, R_{\perp}^{(3)}, R_{\perp}^{(4)}\} = \left\{\frac{1}{2}, \frac{\pi}{8} \left(1 + \frac{3x}{2}\right), \frac{1}{2}(1+x)\right\}. \tag{27}$$

Only the leading O(x) correction is shown in d=3. We find that the constant $c=2E_G/(4-d)+O(x)$, which is ultraviolet convergent only for d<4. (The derivation of c is not shown here because it is not crucial to the discussion.) We therefore restrict our analysis to below d=4.

Finally, the effect of the self-energy correction χ_{\parallel} in Eq. (24) is derived. From Eq. (13) it follows that the form factor $\mathcal{F}_{\parallel} \sim (u_{\bf k}v_{\bf k})^2 \sim [\phi_0/(2E_{\bf k})]^2$. Hence to ϕ_0^2 order, it is sufficient to set $\phi_0=0$ in the polarization function: $\chi_{\parallel}(q)=\phi_0^2\sum_{\bf k}''\Pi_0(q)/(2\epsilon_{\bf k}^2)$, where $\Pi_0(q)=\Pi_{--}(q)|_{\phi_0=0}$ is the standard Lindhard-type function. It has the well-known FL singularities

$$\Pi^{0}(q) \approx -\frac{\partial f(\xi_{\mathbf{k}}^{-})}{\partial \xi_{\mathbf{k}}^{-}} \left(\frac{-\mathbf{q} \cdot \nabla_{\mathbf{k}} \xi_{\mathbf{k}}^{-}}{\omega - \mathbf{q} \cdot \nabla_{\mathbf{k}} \xi_{\mathbf{k}}^{-}} \right), \tag{28}$$

with different limiting values [32] when $\omega, |\mathbf{q}| \to 0$: the dynamic limit $\Pi_0^\omega = \lim_{\omega \to 0} \Pi_0(\mathbf{q} = 0, \omega) = 0$, and the static limit $\Pi_0^q = \lim_{|\mathbf{q}| \to 0} \Pi_0(\mathbf{q}, \omega = 0) = -\partial f(\xi_{\mathbf{k}}^-)/\partial \xi_{\mathbf{k}}^-$. Importantly, this FL singularity induces a singularity in $\chi_{\parallel}(q)$ which in turn induces a singularity in $\Gamma(q)$. Keeping the same notation for the static and dynamic limits, we get $\chi_{\parallel}^q = -\gamma_{\parallel}(2\phi_0)^2$, where

$$\gamma_{\parallel} = \frac{1}{8} \nu_d \epsilon_F^{d/2 - 3} R_{\parallel}^{(d)}(x).$$
 (29)

The function $R_{\parallel}^{(d)}(x) = -x^{d/2-1}$ derives its form from the density of states at the chemical potential.

We now combine the two contributions $\gamma_{\perp} + \gamma_{\parallel}$ to determine the sign of the mass term. To this end, we write the static limit Γ^q in Eq. (24) as

$$[V\Gamma^q]^{-1} \equiv \gamma (2\phi_0)^2 = \frac{1}{8} \nu_d \epsilon_F^{d/2 - 3} R^{(d)}(x) (2\phi_0)^2.$$
 (30)

From Eqs. (26) and (29) we obtain the following expressions for the leading x dependence for $R^{(d)} = R_{\perp}^{(d)} + R_{\parallel}^{(d)}$ in dimensions d = 2, 3, and 4:

$$\{R^{(2)}, R^{(3)}, R^{(4)}\} = \left\{ -\frac{1}{2}, \left(\frac{\pi}{8} - \sqrt{x}\right), \frac{1}{2}(1-x) \right\}. \tag{31}$$

Note that the filling factor x < 1 away from half filling. Hence for all d < 4 the function $R^{(d)}(x)$ becomes negative (and correspondingly γ becomes negative) beyond some critical doping x_c . In particular, $x_c = 0$ in d = 2, and $x_c = (\pi/8)^2 \approx 0.15$ in d = 3 (the exact value is slightly higher at ≈ 0.2 corresponding to a hole Fermi energy $\sim E_G/8$). A negative γ in Eq. (30) implies an instability of the XL phase (negative mass).

This is our main result in this section; namely, the uniform XL obtained self-consistently at the mean-field level is mostly unstable in d < 4 (small doping) and is always unstable in d = 2.

III. EXCITONIC-LIQUID PHASE WITH BROKEN \mathcal{T} SYMMETRY

In the last section, we demonstrated that the uniform XL phase with s-wave pairing in a two-band system with quadratic dispersions is unstable in d=2. We extend this analysis to study the stability of the XL phase in an interacting system in which \mathcal{T} symmetry is spontaneously broken in the ground state. To this end, we consider the extended Hubbard model of spinless electrons on a honeycomb lattice with next-nearest-neighbor (nnn) repulsion. The Hamiltonian is defined as

$$H = -t \sum_{nn} (A_i^{\dagger} B_j + B_i^{\dagger} A_j) + V \sum_{nnn} (n_i^A n_j^A + n_i^B n_j^B).$$
(32)

The operators A_i^{\dagger} (A_i) and B_i^{\dagger} (B_i) are the on-site electron creation (annihilation) operators on the respective sublattices and n_i^A and n_i^B are the number operators. The spin degrees of freedom are suppressed to avoid any spin-related \mathcal{T} -symmetry-breaking effects [33].

The noninteracting spectrum with nearest-neighbor (nn) tunneling is a semimetal with two inequivalent degeneracy points $\pm \mathbf{k}_D$, called Dirac points, located at the corners of the Brillouin zone. At the mean-field level, beyond a critical interaction strength V_c , the interaction lifts the degeneracy at the Dirac points and opens a gap to stabilize a topological Mott insulator [17] (TMI) phase at half filling. Unlike the conventional Mott phase, the TMI breaks both chirality (C) and T symmetries but is invariant under the combined CT transformation. It is therefore a type-II state according to the classification in Ref. [15]. (See Fig. 3 for a physical description of these states.) The properties of the TMI phase are insensitive to the nn repulsion U when $U/V_c \ll 1$. We therefore neglect U in our model. (Further details about the interplay of U and V can be found in Ref. [17].)

The methods developed in the last section are applied here to study the stability of the broken \mathcal{T} phase away from half filling. We first write the Hamiltonian (32) in \mathbf{k} space (we set

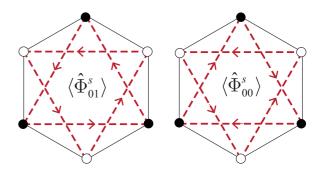


FIG. 3. (Color online) The ordered states can be pictured as two separate current-carrying loops running along the sides of the two triangular sublattices composed of A (white vertices) and B (black vertices) sites that form the honeycomb lattice. (The atoms at A and B are assumed identical.) The current loops break the \mathcal{T} symmetry [16]. Since the total moment in a unit cell is zero, they generate translationally invariant patterns when extended over the whole lattice. The pattern generated by $\langle \hat{\Phi}_{01}^{s\dagger}(\mathbf{q}=0) \rangle$ has C_6 symmetry, while $\langle \hat{\Phi}_{00}^{s\dagger}(\mathbf{q}=0) \rangle$ has only a reduced C_{3v} symmetry that breaks inversion symmetry.

t = 1 and use N for the number of sites):

$$H = -\sum_{\mathbf{k}} \epsilon_{\mathbf{k}} e^{-i\theta_{\mathbf{k}}} A_{\mathbf{k}}^{\dagger} B_{\mathbf{k}} - \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} e^{i\theta_{\mathbf{k}}} B_{\mathbf{k}}^{\dagger} A_{\mathbf{k}}$$

$$-\frac{V}{N} \sum_{\mathbf{k}, \mathbf{p}; \mathbf{q}} g(\mathbf{k} - \mathbf{p}) A_{\mathbf{k} + \frac{\mathbf{q}}{2}}^{\dagger} A_{\mathbf{k} - \frac{\mathbf{q}}{2}} A_{\mathbf{p} - \frac{\mathbf{q}}{2}}^{\dagger} A_{\mathbf{p} + \frac{\mathbf{q}}{2}}$$

$$-\frac{V}{N} \sum_{\mathbf{k}, \mathbf{p}; \mathbf{q}} g(\mathbf{k} - \mathbf{p}) B_{\mathbf{k} + \frac{\mathbf{q}}{2}}^{\dagger} B_{\mathbf{k} - \frac{\mathbf{q}}{2}} B_{\mathbf{p} - \frac{\mathbf{q}}{2}}^{\dagger} B_{\mathbf{p} + \frac{\mathbf{q}}{2}}. \quad (33)$$

The real part of the kinetic term $\epsilon_{\mathbf{k}}e^{i\theta_{\mathbf{k}}} = \sum_{l} \exp(i\mathbf{k}\cdot\mathbf{d}_{l})$ gives the energy $\epsilon_{\mathbf{k}} = [3+2\sum_{l}\cos(\mathbf{k}\cdot\mathbf{t}_{l})]^{1/2}$; it vanishes at the Dirac points, i.e., $\epsilon_{\pm\mathbf{k}_{D}} = 0$. The \mathbf{d}_{l} vectors connect the nearest-neighbor atoms and \mathbf{t}_{l} 's are the basis vectors of the hexagonal Bravais lattice (l=1,2, and 3). In the following, we transform to the basis in which the kinetic term is diagonal; namely,

$$\psi_{\mathbf{k}} = \begin{pmatrix} b_{\mathbf{k}} \\ a_{\mathbf{k}} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -e^{\frac{i}{2}\theta_{\mathbf{k}}} e^{-\frac{i}{2}\theta_{\mathbf{k}}} \\ e^{\frac{i}{2}\theta_{\mathbf{k}}} e^{-\frac{i}{2}\theta_{\mathbf{k}}} \end{pmatrix} \begin{pmatrix} B_{\mathbf{k}} \\ A_{\mathbf{k}} \end{pmatrix}. \tag{34}$$

The various interaction-induced symmetry-breaking possibilities consistent with the lattice symmetries can be gleaned by expressing $g(\mathbf{k} - \mathbf{p}) = \sum_{l} \cos[(\mathbf{k} - \mathbf{p}) \cdot \mathbf{t}_{l}]$ in terms of the distinct irreducible representations (irreps) of the underlying lattice. One possible decomposition involving separable irreps of the planar C_{6v} symmetry group of the honeycomb lattice is shown below:

$$g(\mathbf{k} - \mathbf{p}) = \sum_{\nu=0}^{2} \mathcal{A}_{\nu}^{s*}(\mathbf{k}) \mathcal{A}_{\nu}^{s}(\mathbf{p}) + \mathcal{A}_{\nu}^{c*}(\mathbf{k}) \mathcal{A}_{\nu}^{c}(\mathbf{p}).$$
(35)

Here, \mathcal{A}_0^s and \mathcal{A}_0^c belong to the one-dimensional representations B_1 and A_1 , while $(\mathcal{A}_1^s, \mathcal{A}_2^s)$ and $(\mathcal{A}_1^c, \mathcal{A}_2^c)$ form the basis for the two-dimensional representations E_1 and E_2 . (See, e.g., Ref. [34] for the notation used here.) Explicitly, the functions $\mathcal{A}_{\nu}^s(\mathbf{k}) = \frac{1}{\sqrt{3}}[\sin(\mathbf{k} \cdot \mathbf{t}_1) + e^{i\frac{2\nu\pi}{3}}\sin(\mathbf{k} \cdot \mathbf{t}_2) + e^{i\frac{4\nu\pi}{3}}\sin(\mathbf{k} \cdot \mathbf{t}_3)]$, and the $\mathcal{A}_{\nu}^c(\mathbf{k})$ functions have sines replaced by cosines.

We first note that in order to have the closed-loop configurations shown in Fig. 3, it is necessary that the order parameter has a minimum of C_3 symmetry. The two-dimensional irreps E_1 and E_2 have characters -1 under C_3 and therefore cannot form closed loops. Furthermore, since under a time-reversal operation an arbitrary function $\mathcal{A}(\mathbf{k})$ transforms as $\mathcal{T}\mathcal{A}(\mathbf{k})\mathcal{T}^{-1} = \mathcal{A}^*(-\mathbf{k})$, only the B_1 representation, or \mathcal{A}_0^s , breaks the \mathcal{T} symmetry. (\mathcal{A}_0^s does not break \mathcal{T} symmetry.) \mathcal{A}_0^s has a reduced C_6 symmetry and hence breaks the C_{6v} symmetry to C_6 .

In the ladder approximation, the interactions in the A_0^s channel diverge near the QCP and hence the other channels can be neglected. This simplifies the interaction part of the Hamiltonian (33) to just two terms:

$$H_{\text{int}} = -\frac{V}{2N} \sum_{\mathbf{q}} \hat{\Phi}_{01}^{s\dagger}(\mathbf{q}) \hat{\Phi}_{01}^{s}(\mathbf{q}) + \hat{\Phi}_{00}^{s\dagger}(\mathbf{q}) \hat{\Phi}_{00}^{s}(\mathbf{q}).$$
(36)

The bilinear operators are obtained by combining the A_k and B_k operators as ψ_k [see Eq. (34)]:

$$\hat{\Phi}_{0j}^{s}(\mathbf{q}) = \sum_{\mathbf{k}} S_{\mathbf{k}} \psi_{\mathbf{k} + \frac{\mathbf{q}}{2}}^{\dagger} e^{\frac{i}{2}\theta_{\mathbf{k} + \frac{\mathbf{q}}{2}}\tau_{1}} \tau_{j} e^{-\frac{i}{2}\theta_{\mathbf{k} - \frac{\mathbf{q}}{2}}\tau_{1}} \psi_{\mathbf{k} - \frac{\mathbf{q}}{2}}.$$
 (37)

For notational simplicity, we define $S_{\bf k} \equiv \mathcal{A}_0^{\sigma}({\bf k})$. Note that our choice of the basis in Eq. (34) introduces phases in the interaction. The indices j=0,1 label the Pauli matrices τ_0 (identity) and τ_1 . Physically, they correspond to adding or subtracting the two loop currents on each sublattice as described in Fig. 3. Mean-field analysis [17] of the two patterns favors the condensation of $\langle \hat{\Phi}_{01}^{s\dagger}({\bf q}=0) \rangle$. We therefore neglect $\hat{\Phi}_{00}$ and arrive at our minimal model

$$K_T = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^{\dagger} [\epsilon_{\mathbf{k}} \tau_3 - \mu] \psi_{\mathbf{k}} - \frac{V}{2N} \sum_{\mathbf{q}} \hat{\Phi}_{01}^{s\dagger}(\mathbf{q}) \hat{\Phi}_{01}^{s}(\mathbf{q}). \quad (38)$$

The Hamiltonian K_T is a generalization of K derived in Eq. (3) and the mean-field analysis and the fluctuation calculations follow exactly as detailed in the last section. To avoid repetition we present only the main steps below.

A. Mean-field theory

We note that since $\hat{\Phi}_{01}^{s\dagger}(\mathbf{q}) = \hat{\Phi}_{01}^{s}(-\mathbf{q})$, the order parameter $\phi_T = \frac{V}{N} \langle \hat{\Phi}_{01}^{s}(0) \rangle$ is real. Hence, the mean-field Hamiltonian reads

$$K_{T,\text{MF}} = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^{\dagger} \left[\epsilon_{\mathbf{k}} \tau_3 - \mu - \phi_T S_{\mathbf{k}} \tau_1 \right] \psi_{\mathbf{k}} + \frac{N}{2V} \phi_T^2.$$
 (39)

It follows that the energies $\xi_{\mathbf{k}}^{\pm} = \pm E_{\mathbf{k}} - \mu$, where $E_{\mathbf{k}} = (\epsilon_{\mathbf{k}}^2 + \phi_T^2 S_{\mathbf{k}}^2)^{1/2}$. Thus, a gap $\sim \phi_T |S_{\mathbf{k}_D}|$ opens at $\pm \mathbf{k}_D$. However, since $S_{\mathbf{k}}$ is an odd function, the sign of the gaps is in opposite directions at the two Dirac points. This is the origin of the anomalous quantum Hall effect as described by Haldane [16]. A nonzero ϕ_T breaks \mathcal{T} symmetry but does not break inversion symmetry [35].

Minimizing the action we obtain the self-consistent equation at T=0 as $1/V=\frac{1}{N}\sum_{BZ}'S_{\mathbf{k}}^2/E_{\mathbf{k}}$. As before, we consider hole doping, i.e., $\mu<0$. At T=0, all states $|\mathbf{k}|>k_F$ measured from $\pm\mathbf{k}_D$ are filled, leaving small hole pockets at the Dirac points. The lower cutoff k_F is denoted by the prime

on the summation. Since it is a convergent integral no upper cutoff is required and the summation extends over the whole Brillouin zone (BZ).

Finally, as before we write the eigenfunctions in the form $c_{\mathbf{k}+} = u_{\mathbf{k}}b_{\mathbf{k}} - v_{\mathbf{k}}a_{\mathbf{k}}$ and $c_{\mathbf{k}-} = u_{\mathbf{k}}a_{\mathbf{k}} + v_{\mathbf{k}}b_{\mathbf{k}}$, corresponding to $\pm E_{\mathbf{k}}$. After minimizing the free energy, we get for $u_{\mathbf{k}}^2$ and $v_{\mathbf{k}}^2$ the same relations as in Eq. (13) with an additional phase for $v_{\mathbf{k}}$ given as $(\phi_T > 0$ is assumed)

$$v_{\mathbf{k}} = \sqrt{v_{\mathbf{k}}^2 \frac{S_{\mathbf{k}}}{|S_{\mathbf{k}}|}} = \sqrt{v_{\mathbf{k}}^2} \operatorname{sgn}(S_{\mathbf{k}}).$$
 (40)

This additional phase does not appear in the calculation of the static susceptibility as shown below.

B. Order-parameter fluctuations

Since only the stability of the condensate is under question, we only examine the static limit of the susceptibilities below. We follow the same steps as in the previous section. First, the matrices in Eqs. (17) and (18) are modified for the honeycomb lattice as

$$G_0(k,k') = -\frac{(i\epsilon_n + \mu)\tau_0 + \epsilon_k \tau_3 - \phi_T S_k \tau_1}{(i\epsilon_n - \xi_k^+)(i\epsilon_n - \xi_k^-)} \delta_{k,k'}, \quad (41)$$

$$\Sigma(k,k') = \frac{1}{\beta} \delta \phi(k-k') S_{\mathbf{k}_{+}} e^{\frac{i}{2}(\theta_{\mathbf{k}} - \theta_{\mathbf{k}'})\tau_{1}} \tau_{1}. \tag{42}$$

The momentum $\mathbf{k}_{+} = (\mathbf{k} + \mathbf{k}')/2$. Second, the form factors in Eqs. (20) and (21) are modified to include the structure factor $S_{\mathbf{k}}$ as $\mathcal{F}_{\perp}(\mathbf{k}, \mathbf{q} = 0) = S_{\mathbf{k}}^{2}(u_{\mathbf{k}}^{2} - v_{\mathbf{k}}^{2})$ and $\mathcal{F}_{\parallel}(\mathbf{k}, \mathbf{q} = 0) = 4S_{\mathbf{k}}^{2}u_{\mathbf{k}}^{2}v_{\mathbf{k}}^{2}$. As noted below Eq. (40), only the squares of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ appear in these expressions.

Finally, to $O(\phi_T^2)$, we get $[V\Gamma^q]^{-1} = \gamma \phi_T^2$ for the static limit of the interaction amplitude [equivalent to Eq. (30)]:

$$\gamma = \frac{1}{N} \sum_{\mathbf{k}}' \frac{S_{\mathbf{k}}^4}{\epsilon_{\mathbf{k}}^2} \left[\frac{f(\xi_{\mathbf{k}}^-)}{\epsilon_{\mathbf{k}}} + \frac{\partial f(\xi_{\mathbf{k}}^-)}{\partial \xi_{\mathbf{k}}^-} \right]. \tag{43}$$

It includes contributions from the inter- and intraband susceptibility, i.e., $\gamma = \gamma_{\perp} + \gamma_{\parallel}$, as explained in Eqs. (26) and (29). Since $S_{\bf k}^4$ is a sharply peaked function around ${\bf k}_D$, the integrals can be evaluated by linearizing the spectrum around ${\bf k}_D$ as $\epsilon_{\bf k} \sim \alpha |{\bf k} - {\bf k}_D|$, where $\alpha = 3/2$ (in units of lattice spacing). The lower cutoff is from k_F and hence there is no divergence away from half filling and an expansion in ϕ_T^2 is possible (unlike at half filling [17]).

After linearizing, we get $\gamma_{\parallel} = -2\nu_0 S_{k_F}^4/\epsilon_F$. The negative sign originates from the derivative of the Fermi function. The density of states around each \mathbf{k}_D equals $\nu_0 = 1/(\sqrt{3}\pi)$ and the factor 2 accounts for the contributions from $\pm \mathbf{k}_D$. The interband contribution is easily shown to satisfy $\gamma_{\perp} < |\gamma_{\parallel}|$, implying that $\gamma < 0$ in Eq. (43). Hence, we conclude that the uniform \mathcal{T} broken state on the honeycomb lattice, which is stable at half filling [17], is unstable to infinitesimal doping.

IV. DISCUSSION

We have shown that the mean-field solution for the interband particle-hole condensate with a sharp Fermi surface, which we call an excitonic liquid (XL) in this paper, is unstable in the presence of the gapless fermions at the Fermi

surface. The origin of the instability is closely related to the singularity of the FL polarization function in Eq. (28). We demonstrate this destabilization in two models, both of which stabilizes an uniform XL phase at the mean-field level. Our results therefore suggest that a uniform condensate of virtual excitons, with or without spontaneous time-reversal symmetry breaking, is an unstable phase at T=0. We arrive at this conclusion by analyzing the static limit of the effective interaction in the particle-hole channel and showing it to be negative. It follows that a Ginzburg–Landau-type description of the ordered phase [15] is in general not possible.

Finally, a few remarks about the relevance of the higherorder terms in the expansion of the action $S_{\rm eff}$ in Eq. (14). In general, the bosonic action can be expanded as

$$S_{\text{eff}} = S_{\text{eff}}^{(2)} + \sum_{n=2}^{\infty} \int (d\omega d^2 \mathbf{q})^{2n-1} b_{2n} [\delta \phi(q)]^{2n}. \tag{44}$$

The coefficients b_{2n} were calculated in Ref. [11] and shown to contain universal singular contributions that makes the coefficients anomalously large in the dynamic limit $\omega \to 0$ and q = 0, leading to the general conclusion that the Hertz theory is incomplete. (The corresponding dynamical corrections in $S_{\rm eff}^{(2)}$ is the familiar Landau damping term.) In the opposite limit, i.e., the static limit, no such anomalous contributions exists and the Hertz assumption that the vertices are local is restored, allowing for a controlled expansion in powers

of $\delta\phi$. To establish the stability of the mean-field ground state, it is necessary that the static susceptibilities for all possible perturbations of the ground state are positive. For the order-parameter fluctuations, this translates to the sign of the coefficient of the $(\delta\phi)^2$ term in a finite field ϕ_0 . Close to the transition, we calculate the contributions to order ϕ_0^2 , which are shown in Fig. 2. Note that there are no vertex corrections in this order.

Our results suggest that XL condensates with a sharp Fermi surface tends to be unstable in d=2. Of course, any condensate can be stabilized if a gap opens, however, the mechanism to open a gap in the XL condensate is unclear at the moment [36]. Another possible cure for this instability might be to assume a nonuniform $(q \neq 0)$ mean-field state similar to the spin-bag models proposed in the case of doped antiferromagnetism [37,38]. This possibility is not analyzed in this paper.

ACKNOWLEDGMENTS

We acknowledge insightful conversations with J. Birman (CCNY), R. Matheus (IFT), A.R. Rocha (IFT), and C. M. Varma (UCR). We would like to thank the C.M.B. and the Physics Departments at Tulane University for their kind hospitality where part of this work was done. Partial support was provided by PSC-CUNY Award 41.

- [1] N. F. Mott, Philos. Mag. 6, 287 (1961).
- [2] R. S. Knox, in *Solid State Physics* Supplemental 5, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1963), Vol. 5, p. 100.
- [3] J. des Cloizeaux, J. Phys. Chem. Solids 26, 259 (1965).
- [4] I. Pomeranchuk, Sov. Phys.-JETP 8, 361 (1958).
- [5] L. V. Keldysh and Yu. V. Kopaev, Sov. Phys.-Solid State 6, 2219 (1965).
- [6] A. N. Kozlov and L. A. Maksimov, Sov. Phys.-JETP 21, 790 (1965).
- [7] D. Jerome, T. M. Rice, and W. Kohn, Phys. Rev. 158, 462 (1967).
- [8] B. I. Halperin and T. M. Rice, Rev. Mod. Phys. 40, 755 (1968).
- [9] C. Comte and P. Nozières, J. Phys. (Paris) 43, 1069 (1982).
- [10] J. A. Hertz, Phys. Rev. B 14, 1165 (1976).
- [11] A. Abanov and A. Chubukov, Phys. Rev. Lett. 93, 255702 (2004).
- [12] H. v. Löhneysen, A. Rosch, M. Vojta, and P. Wölfle, Rev. Mod. Phys. 79, 1015 (2007).
- [13] C. M. Varma, Z. Nussinov, and W. van Saarloos, Phys. Rep. 361, 267 (2002).
- [14] C. M. Varma, Phys. Rev. B 55, 14554 (1997).
- [15] K. Sun and E. Fradkin, Phys. Rev. B 78, 245122 (2008).
- [16] F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988).
- [17] S. Raghu, X.-L. Qi, C. Honerkamp, and S.-C. Zhang, Phys. Rev. Lett. 100, 156401 (2008).
- [18] J. Gavoret, P. Nozières, B. Roulet, and M. Combescot, J. Phys. (Paris) 30, 987 (1969).
- [19] P. Nozières and C. Comte, J. Phys. (Paris) 43, 1083 (1982).
- [20] R. Côté and A. Griffin, Phys. Rev. B 37, 4539 (1988).

- [21] C. A. R. Sá de Melo, M. Randeria, and J. R. Engelbrecht, Phys. Rev. Lett. **71**, 3202 (1993).
- [22] V. M. Loktev, R. M. Quick, and S. G. Sharapov, Phys. Rep. **349**, 1 (2001).
- [23] L. Balents and C. M. Varma, Phys. Rev. Lett. 84, 1264 (2000).
- [24] V. Barzykin and L. P. Gorkov, Phys. Rev. Lett. 84, 2207 (2000).
- [25] Y. Nambu and G. Jona-Lasinio, Phys. Rev. 122, 345 (1961).
- [26] Y. Nambu and G. Jona-Lasinio, Phys. Rev. 124, 246 (1961).
- [27] V. N. Popov, Functional Integrals and Collective Excitations (Cambridge University Press, Cambridge, 1987).
- [28] H. Kleinert, Fortsch. Phys. 26, 565 (1978).
- [29] P. G. de Gennes, Solid State Commun. 1, 132 (1963).
- [30] R. Brout, K. A. Müller, and H. Thomas, Solid State Commun. 4, 507 (1966).
- [31] H. J. Lipkin, *Lie Groups for Pedestrians* (Dover Publications, New York, 2002).
- [32] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Dover Publications, New York, 1975).
- [33] B. A. Volkov, Yu. V. Kopaev, and A. I. Rusinov, Sov. Phys.-JETP **41**, 952 (1976).
- [34] M. Tinkham, *Group Theory and Quantum Mechanics* (Dover Publications, New York, 1992).
- [35] J. L. Mañes, F. Guinea, and M. A. H. Vozmediano, Phys. Rev. B **75**, 155424 (2007).
- [36] C. M. Varma, Phys. Rev. Lett. 83, 3538 (1999).
- [37] A. Singh and Z. Tešanović, Phys. Rev. B 41, 614 (1990).
- [38] A. Singh, Z. Tešanović, and J. H. Kim, Phys. Rev. B 44, 7757 (1991).