Berezinskii-Kosterlitz-Thouless transition in the time-reversal-symmetric Hofstadter-Hubbard model

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Assuming that two-component Fermi gases with opposite artificial magnetic fields on a square optical lattice are well-described by the so-called time-reversal-symmetric Hofstadter-Hubbard model, we explore the thermal superfluid properties along with the critical Berezinskii-Kosterlitz-Thouless (BKT) transition temperature in this model over a wide-range of its parameters. In particular, since our self-consistent BCS-BKT approach takes the multi-band butterfly spectrum explicitly into account, it unveils how dramatically the inter-band contribution to the phase stiffness dominates the intra-band one with an increasing interaction strength for any given magnetic flux.

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I. INTRODUCTION

The phase stiffness, also known as the helicity modulus, measures the response of a system in an ordered phase to a twist of the order parameter \( |\Delta|^2 \), and it is directly linked to the superfluid (SF) density of the superconducting systems [2–4]. In its most familiar form, the conventional expression for the elements of the phase stiffness tensor can be written as

\[
D_{\mu\nu} = \frac{1}{V_d} \sum_k \left\{ \frac{\partial^2 \xi_k}{\partial k_\mu \partial k_\nu} \left[ 1 - \frac{\xi_k}{E_k} \tanh \left( \frac{E_k}{2k_BT} \right) \right] - \frac{1}{2k_BT} \left( \frac{\partial \xi_k}{\partial k_\mu} \frac{\partial \xi_k}{\partial k_\nu} \right) \text{sech}^2 \left( \frac{E_k}{2k_BT} \right) \right\},
\]

where \( V_d \) is the volume element and \( k \) is the wave vector in \( d \) spatial dimensions, \( k_\nu \) with \( \nu \equiv \{x, y, \ldots\} \) is the projection of \( k \), \( \xi_k = \varepsilon_k - \mu \) is the single-particle dispersion relation shifted by the chemical potential, \( E_k = \sqrt{\varepsilon_k^2 + |\Delta_k|^2} \) is the quasi-particle dispersion relation with the order parameter \( \Delta_k \), \( k_B \) is the Boltzmann constant, and \( T \) is the temperature. Here, \( \xi_k \) is assumed to be quite general, and not limited with the usual quadratic dependence on \( k_\nu \). In particular, this tensor plays a special role in two dimensions for which it appears explicitly in the universal BKT relation determining the critical SF transition temperature \( T_{BKT} \) [2,4]. This is a topological phase transition characterized by the binding (unbinding) of two vortices with opposite circulations, i.e., the so-called vortex-antivortex pairs, below (above) \( T_{BKT} \) with algebraically (exponentially) decaying spatial correlations [5,7]. For instance, one of the immediate manifestations of Eq. (1) is that it rules out the possibility of superfluidity in systems with a nearly flat \( k \)-space dispersion, i.e., the SF density/current is identically zero since the particles are strictly immobile in a flat-band with \( \xi_k \approx \xi_0 \) for all \( k \).

Motivated by the experimental advances with cold Fermi gases, the calculation of \( D_{\mu\nu} \) have recently been extended to a class of multi-band Hamiltonians that are characterized by a single mean-field order parameter \( \Delta \) with a uniform spread in real space, and that exhibit time-reversal (T) symmetry [5,11]. It has been found that, in addition to the intra-band contribution to \( D_{\mu\nu} \) that has exactly the same form as the one given in Eq. (1) for each single-particle band, the inter-band contribution may also be necessary for a proper description of the multi-band systems. For instance, in marked contrast with the single flat-band systems, it turns out that superfluidity may prevail in a flat-band in the presence of other bands as a result of the inter-band tunnelings [8,9]. See also the related discussion on two-band superconductivity in graphene for a resolution of the ‘superconductivity without supercurrent’ controversy in the vicinity of its Dirac points [12–15].

In view of the recent realization of the Hofstadter-Hubbard model with \( T \) symmetry [14–15], and the forthcoming experiments, here we study \( T_{BKT} \) in this model and address the interplay between the intra-band and inter-band contributions to the phase stiffness in the presence of a multi-band butterfly spectrum. Despite our naive expectations, we find that the maximum \( T_{BKT} \approx 0.25 \) for \( k_B \mu \approx 0 \) when the interaction strength is around \( U \approx 3.75 \). Here, \( t \) is the hopping strength. In addition, one of the highlights of this paper is that increasing the interaction strength always shifts the relative importance of the intra-band and inter-band contributions in an overwhelming favor of the latter, and that the proper description of the Cooper molecules requires an indiscriminate account of both contributions in the strong-coupling limit.

The remainder of this paper is organized as follows. After a short overview of the Hofstadter model with \( T \) symmetry in Sec. [1A], first we introduce the self-consistent BCS-BKT formalism in Sec. [1B] together with the multi-band generalization of the phase stiffness detailed in Sec. [1C]. Then we discuss the analytically-tractable strong-coupling or molecular limit in Sec. [1D] as a warm-up for our numerical results presented in Sec. [1E]. We end the paper with a brief summary of our conclusions in Sec. [1V].
II. THEORETICAL FRAMEWORK

Assuming that the tight-binding approximation is a viable description of the kinematics of a two-component Fermi gas on an optical lattice, we start with the single-particle Hamiltonian \( H_0 = -\sum_{ij} t_{ij} c_{ij}^\dagger c_j \), where \( c_i^\dagger \) (\( c_i \)) creates (annihilates) a spinless fermion at site \( i \) so that \( t_{ij} = t^*_{ji} \) is the element of the hopping matrix from site \( j \) to \( i \). This model also offers a convenient way to incorporate the effects of additional gauge fields, e.g., an external magnetic field \( B(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r}) \) may be taken into account via the minimal coupling, i.e., \( t_{ij} \rightarrow t_{ij} e^{i 2\pi \phi_{ij}/\phi_0} \), leading to an additional phase factor \( \phi_{ij} = (1/\phi_0) \int_{r_i}^{r_j} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{r} \) in the hopping matrix. Here, \( \phi_0 \) is the flux quantum and \( \mathbf{A}(\mathbf{r}) \) is the magnetic vector potential. In a broader context, \( \mathbf{A}(\mathbf{r}) \) could be any gauge field, including the artificial ones created in atomic systems.

In this paper, we are interested in a square lattice lying in the entire \((x, y)\) plane, that is under the influence of a spatially-uniform magnetic field \( B(\mathbf{r}) = B \) pointing along the perpendicular \( z \) axis. Such a setting can be represented by \( \mathbf{A}(\mathbf{r}) = (0, Bx, 0) \) in the Landau gauge without losing generality. Thus, for a given flux quanta per unit cell \( \alpha = B a^2/\phi_0 \) with \( a \) the lattice spacing, the particle gains an Aharonov-Bohm phase \( e^{2i\pi \alpha} \) after traversing a loop around the unit cell. Next we consider the original Hofstadter model [16] and allow the particle to hop back and forth between only the nearest-neighbor sites, which by itself gives rise to one of the most fascinating single-particle energy spectra in nature.

A. Hofstadter Butterfly

When the flux \( \alpha = p/q \) corresponds precisely to a ratio of two relatively prime numbers \( p \) and \( q \), one can simplify the single-particle problem considerably by switching to the reciprocal \((k)\) space representation and making use of the new translational symmetry [16]. That is, since the \( B \) field enlarges the unit cell by a factor of \( q \) in the \( x \) direction, the first magnetic Brillouin zone (MBZ) is reduced to \(-\pi/(qa) \leq k_x < \pi/(qa) \) and \(-\pi/a < k_y < \pi/a\). This not only splits the tight-binding \( \mathbf{s}\)-band of the flux-free system, i.e., \( \varepsilon_k = -2t \cos(k_x a) - 2t \cos(k_y a) \), into \( q \) sub-bands for a given \( \alpha = p/q \), but the competition between the magnetic length scale, i.e., the cyclotron radius, and the periodicity of the lattice potential also produces a very complicated energy \( \varepsilon \) versus \( p/q \) landscape with an underlying fractal pattern. As the overall landscape bears a resemblance to the shape of a butterfly, the spectrum is usually referred to as the Hofstadter butterfly in the literature [16].

For a given \( \alpha = p/q \), the multi-band spectrum can be obtained by solving the Schrödinger equation \( E_{\mathbf{k}}|n\mathbf{k}\rangle = \varepsilon_{\mathbf{k}}|n\mathbf{k}\rangle \) in \( \mathbf{k} \) space, where \( n = 0, \ldots, q-1 \) labels the sub-bands starting from the lowest-energy branch. This leads to \( \sum_{j=0}^{q-1} H_{\mathbf{k}}^{(j)} g_{\mathbf{k}j} = \varepsilon_{\mathbf{k}} g_{\mathbf{k}0} \), where \( g_{\mathbf{k}n} \) is the \( n \)-th component of the \( \mathbf{k} \)-vector.

The butterfly spectrum exhibits a number of symmetries. First of all, it preserves the inversion symmetry in \( \mathbf{k} \) space, i.e., \( \varepsilon_{-\mathbf{k}} = \varepsilon_{\mathbf{k}} \), as a direct manifestation of the gauge invariance in a uniform flux. In addition, it is not only symmetric around \( \varepsilon = 0 \) for a given flux, i.e., \( \varepsilon_{\mathbf{k}}(\alpha) = -\varepsilon_{\mathbf{q}+\mathbf{k}}(\alpha) \), due to the particle-hole symmetry of \( H_0 \) on a biparticle lattice, but it is also mirror-symmetric around \( \alpha = 1/2 \) for a given \( |\mathbf{n}\rangle \) k state, i.e., \( \varepsilon_{\mathbf{k}}(\alpha) = \varepsilon_{\mathbf{n}+\mathbf{k}}(1-\alpha) \) for \( 0 \leq \alpha \leq 1 \). The latter relation suggests that the flux-free \( \alpha = 0 \) system is exactly equivalent to the \( \alpha = 1 \) case, and hence, \( \alpha = 1/2 \) corresponds to the maximally attainable flux [16]. Furthermore, when \( q \) is an even denominator, combination of the inversion and particle-hole symmetries implies the condition \( \varepsilon_{q/2-1, \mathbf{k}} = -\varepsilon_{q/2, \mathbf{k}} \), from which we infer that the centrally-symmetric bands \( n = q/2-1 \) and \( n = q/2 \) have degenerate \( \mathbf{k} \) states with \( \varepsilon = 0 \). It turns out that these central bands contain \( q \) Dirac cones with \( q \) zero-energy touching points in the first MBZ, and therefore, are not separated by a bulk energy gap. For example, setting \( p/q = 1/2 \), we obtain \( \varepsilon_{\mathbf{n}k} = (-1)^{n+1} 2t \sqrt{\cos^2(k_x a) + \cos^2(k_y a)} \) for the \( n = 0 \) and \( n = 1 \) bands, where \( g^0_{\mathbf{k}n}/g^1_{\mathbf{k}n} = -\cos(k_y a)/|\cos(k_y a)| + (-1)^{n+1} \cos^2(k_x a) + \cos^2(k_y a) \) together with \( |g^0_{\mathbf{k}n}|^2 + |g^1_{\mathbf{k}n}|^2 = 1 \). The locations of the Dirac points are \( k_x = -\pi/(2a) \) and \( k_y = \pm \pi/(2a) \).

Our primary interest in this paper is the superfluidity of a spin-1/2 Fermi gas on a square lattice that is experiencing an equal but opposite magnetic fields for its spin components [17, 19], i.e., \( \alpha_{\uparrow} = -\alpha_{\downarrow} = \alpha \). This restores the \( T \) symmetry into the system in such a way that the solutions of the Hofstadter model for a single particle can be written in terms of the \( \uparrow \) ones (given above) as follows:
\(\varepsilon_{\uparrow n k} = \varepsilon_{\downarrow n,-k}\) and \(g^g_{\uparrow n k} = g^g_{\downarrow n,-k}\). More importantly, the self-consistent mean-field theory of such a time-reversal-symmetric Hofstadter-Hubbard model \[18, 19\] turns out to be dramatically simpler to implement than that of the usual Hofstadter-Hubbard model \[20, 21\], as we discuss next.

### B. Self-consistent BCS-BKT Theory

Having an equal number of \(\uparrow\) and \(\downarrow\) particles that are interacting with on-site and attractive interactions in mind, we have recently shown that the mean-field Hamiltonian can be simply written as \[18, 19\]

\[
H = \sum_{\sigma n k} \xi_{\sigma n k} d_{\sigma n k}^\dagger d_{\sigma n k} - \Delta \sum_{n, k} \left( d_{\uparrow n k}^\dagger d_{\downarrow n,-k} + \text{H.c.} \right), \tag{3}
\]

in \(k\) space. Here, \(H\) is given up to a constant \(M\Delta^2/U\) term, where \(M = A/a^2\) is the number of lattice sites with \(A\) the area of the system, \(\xi_{\sigma n k} = \varepsilon_{\sigma n k} - \mu\) is the butterfly spectrum \(\varepsilon_{\sigma n k}\) shifted by the chemical potential \(\mu\), and \(\Delta = (U/M) \sum_{n,k} (d_{\uparrow n,-k} d_{\downarrow n k})\) is the order parameter characterizing a uniformly-atomic SF phase. In addition, \(U \geq 0\) is the strength of the inter-particle interactions, \(\langle \ldots \rangle\) denotes the thermal average, \(\text{H.c.}\) is the Hermitian conjugate, and \(\Delta\) is assumed to be real without losing generality.

In contrast to the usual Hofstadter-Hubbard model where the competing vortex-lattice like SF phases involve both intra- and inter-band Cooper pairings with nontrivial sets of finite center of mass momenta \(K\), and hence, require \(q \times q\) order parameters \[20, 21\], here the energetically more favorable mean-field solution boils down to the superfluidity of intra-band Cooper pairs with \(K = 0\) only \[18, 19\]. This is simply because, as the \(T\) symmetry guarantees the existence of a \(\downarrow\) partner in state \(|n,-k\rangle\) for every \(\uparrow\) fermion in state \(|n,k\rangle\), the spatially-uniform SF solution allows all particles to take advantage of the attractive potential by making \(\uparrow\downarrow\) Cooper pairs with \(K = 0\). We also emphasize that the disappearance of all of the inter-band pairing terms from the mean-field Hamiltonian is a direct consequence of the uniform SF phase with \(T\) symmetry.

Given the quadratic Hamiltonian, minimization of the corresponding thermodynamic potential with respect to \(\Delta\), together with the number equation \(N = \sum_{\sigma n k} \langle d_{\sigma n k}^\dagger d_{\sigma n k} \rangle\) that is controlled by \(\mu\), leads to a closed set of self-consistency equations that are analytically tractable. For instance, a compact way to express these mean-field equations is \[18, 19, 22\]

\[
1 = \frac{U}{2M} \sum_{n, k} \frac{\xi_{\uparrow n k}}{F_{\uparrow n k}}, \tag{4}
\]

\[
F = 1 - \frac{1}{M} \sum_{n, k} \frac{\xi_{\uparrow n k}}{F_{\uparrow n k}}, \tag{5}
\]

where \(\chi_{\uparrow n k} = \text{tanh} [E_{\uparrow n k} / (2k_B T)]\) is a thermal factor with \(k_B\) the Boltzmann constant and \(T\) the temperature, \(E_{\uparrow n k} = \sqrt{\xi_{\uparrow n k}^2 + \Delta^2}\) is the energy spectrum of the quasiparticles arising from band \(n\), and the particle filling \(0 \leq F = N/M \leq 2\) corresponds to the total number of particles per site. Thus, we use Eqs. \(4\) and \(5\) to determine \(\Delta\) and \(\mu\) for any given set of \(U, F, T\) and \(\alpha\) parameters.

Since neither the amplitude nor the phase fluctuations of the SF order parameter are included in the mean-field theory, while the self-consistent solutions of Eqs. \(4\) and \(5\) is a reliable description of the ground state at \(T = 0\) for all \(U\) values, the theory works reasonably well at finite temperatures \(T \lesssim T_{BCS} \ll t/k_B\) as long as \(U \lesssim t\) is weak \[24\]. Here, \(T_{BCS}\) is the critical BCS transition temperature that is determined by setting \(\Delta \to 0\). However, as the role played by the temporal phase fluctuations increases dramatically with stronger \(U \gtrsim t\) values, the mean-field theory becomes gradually insufficient, failing eventually at capturing the finite temperature correlations of the SF phase in the strong-coupling or molecular limit even though \(T \ll T_{BCS}\) \[26, 27\]. In the \(U \gg t\) limit, we note that the mean-field \(T_{BCS}\) is directly proportional to the binding energy \(U\) of the two-body bound state in vacuum, and therefore, it characterizes the pair formation temperature of the Cooper molecules. Thus, away from the weak-coupling limit, \(T_{BCS}\) has obviously nothing to do with the critical SF transition temperature of the system, for which the phase coherence is known to be established at a much lower temperature.

Taking only the phase fluctuations into account in our two dimensional model characterized by a single SF order parameter, the critical SF transition temperature is determined by the universal BKT relation \[4, 7, 23\]

\[
k_B T_{BKT} = \frac{\pi}{8} D_0(T_{BKT}), \tag{6}
\]

where \(D_0\) is the isotropic measure of the \(2 \times 2\) phase stiffness tensor, i.e., \(D_{\mu \nu} = D_0 \delta_{\mu \nu}\) with \((\mu, \nu) \equiv \{x, y\}\). Similar to the usual Hubbard model with a single SF order parameter \[4\], and thanks to the time-reversal symmetry of the current model, the elements \(D_{\mu \nu}\) are identified by making an analogy with the effective phase-only XY Hamiltonian \[8, 10\], where \(H_{XY} = (1/8) \int dx \int dy \sum_{\mu, \nu} \partial_\mu \chi \partial_\nu \chi\) under the assumption that \(\Delta_F = \Delta e^{i\phi}\). Setting \(\chi = K \cdot r\) for a spatially-uniform condensate density with \(hK\) the pair momentum, we note that \(H_{XY} = D_0 AK^2 / 4 = m_0 A \rho_s v^2 / 2\), where \(v = hK / (2m_0)\) is the velocity of the SF pairs with \(m_0\) the mass of the particles, and \(\rho_s = m_0 D_0 / h^2\) is the density of the SF particles. Thus, the phase stiffness of a SF is essentially equivalent to its SF density. Here, the factor \(m_0 \rho_s\) is often called the SF mass density of the system.

We note that since \(T_{BCS}\) is determined by the BCS condition \(\Delta \to 0\) and a finite \(T_{BKT}\) requires a finite \(\Delta\) by definition, Eq. \(6\) already puts \(T_{BCS}\) as the upper bound on \(T_{BKT}\) for any \(U \neq 0\). It turns out that while \(T_{BKT} \sim t^2 / (k_B U) \ll T_{BCS}\) in the \(U/t \gg 1\) limit \[20, 27\], \(T_{BKT} \rightarrow T_{BCS}\) in the opposite \(U/t \ll 1\) limit where the rate \(D_0 / t \rightarrow 0\) is the same as \(\Delta / t \rightarrow 0\) only when \(U/t \rightarrow \infty\).
0. In fact, we find in Sec. 111 that the maximum $T_{BKT} \approx 0.253t/k_B$ is attained for $\xi = 1$ at $\mu = 0$ when $U \sim 3.75t$.

Next we justify that the self-consistent solutions of Eqs. 11-21 for $\Delta$, $\mu$ and $T_{BKT}$, along with the proper multiband generalization 10 of $D_{\mu\nu}$ given below, is a reliable description of the SF transition temperature $T_{BKT}$ for any given set of $U$, $F$ and $\alpha$ parameters. We note in passing that the self-consistent BCS-BKT approach amounts to be the simultaneous solutions of BCS mean-field equations and the universal BKT relation, i.e., the phase fluctuations are taken only into account by the latter via the analogy with the underlying XY model. While this simple description is known to be quite accurate for the weak-coupling BCS and strong coupling molecular limits, it provides a qualitative but reliable picture of the crossover regime.

C. Phase Stiffness

As an alternative to the expression given in Ref. 10, a compact way to write the elements of the phase stiffness tensor is

$$D_{\mu\nu} = \frac{\Delta^2}{A} \sum_{nmk} \left( \frac{<x_{nk}}{E_{nk} - \xi_{nk}} - \frac{<x_{mk}}{E_{mk} - \xi_{mk}} \right) \times \frac{2Q_{\mu\nu}^{nmk}}{E_{mk}(E_{nk} + E_{mk})}, \tag{7}$$

where the independent $n$ and $m$ summations run over all bands, $<x_{nk} = \text{tan}[E_{nk}/(2k_BT)]$ is the thermal factor, and the coefficient $Q_{\mu\nu}^{nmk} = \text{Re}[(<n|\partial\Phi_{nk}/\partial k_\nu)|<m|\partial\Phi_{mk}/\partial k_\mu]|<n)]$ is directly related to the details of the band geometry of the single-particle problem 11. For instance, since $D_{\mu\nu}$ is isotropic in space for spatially-uniform SFs, we have $Q_{\mu\nu}^{nmk} = Q_{\mu\nu}^{mnk}$. Furthermore, by denoting $D_{\mu\nu} = D_{\mu\nu}^{\text{intra}} + D_{\mu\nu}^{\text{inter}}$, we distinguish the intra-band contribution of the phase stiffness from the inter-band contribution, that is based, respectively, on whether $n = m$ or not in Eq. (7). Such an association proves to be illuminating in some of our analysis given below.

First, let us show that the intra-band contribution of Eq. (7) corresponds precisely to the conventional expression given in Eq. (1). Setting $n \to m$ for the intra-band contribution, the second term in the parenthesis implies a derivative such that $d\text{tan}(ax)/dx = \text{sec}^2(ax)$, and the coefficient $Q_{\mu\nu}^{nmk} = (\partial\xi_{nk}/\partial k_\mu)(\partial\xi_{mk}/\partial k_\nu)$ depends only on the spectrum. After plugging them into Eq. (7), we rearrange the intra-band contribution into two pieces as

$$D_{\mu\nu}^{\text{intra}} = \left(1/A\right) \sum_{nk} \partial\xi_{nk}/\partial k_\mu \partial\xi_{nk}/\partial k_\nu \frac{E_{nk}}{E_{mk}(E_{nk} + E_{mk})}$$

$$- [1/(2Ak_BT)] \sum_{nk} \text{sech}^2(\xi_{nk}/(2k_BT)) \partial\xi_{nk}/\partial k_\mu \partial\xi_{nk}/\partial k_\nu.$$  

Since the latter piece already appears in the conventional expression, next we re-arrange the first piece into two summations as $(1/A) \sum_{nk} \delta(\partial\xi_{nk}/\partial k_\mu) \xi_{nk}/(E_{nk}/\partial k_\mu) \partial\xi_{nk}/\partial k_\nu - \left[1/(2Ak_BT)\right] \sum_{nk} \text{sech}^2(\xi_{nk}/(2k_BT))(\partial\xi_{nk}/\partial k_\mu)(\partial\xi_{nk}/\partial k_\nu).$

To be exact, this expression is precisely the $T = 0$ limit of Eq. (7). However, it is also valid for all $T \leq T_{BKT}$ in the molecular limit, since $k_BT_{BKT} \sim U/\alpha$ when $U/\alpha \gg 1$, and hence, $k_BT_{BKT} \ll t \ll \Delta$ is well-founded.
In the Δ ≫ t or equivalently U ≫ t limit of tightly-bound Cooper molecules [26, 27], Eqs. (4) and (5) give
\[ \Delta = \frac{\langle U(2) \rangle}{\sqrt{F(2 - F)}} \] and μ = −(U/2)(1 − F), so that
\[ \sqrt{\mu^2 + 2^2} = U/2 \] is independent of T. Therefore, both of these mean-field parameters are not only proportional to the binding energy U of the two-body bound state in vacuum, but are also independent of α as the T symmetry ensures that the center of mass of the Cooper pairs are neutral against the flux. In other words, the only mechanism that allows a Cooper molecule to hop from one site to another is via the virtual breaking of its ↑ ↓ constituents [26, 27]. Since the cost for breaking the bound state is \( E_{\text{sm}} \), the molecule effectively hops from site j to site i with \( t_{\text{niij}} = 2t_{\text{ij}}t_{\text{ij}}/U \). Thus, for our nearest-neighbor lattice model, we identify \( t_m = 4t^2/U \) as the hopping amplitude of the molecules, and \( \alpha_m = \alpha_1 + \alpha_2 = 0 \) as their flux.

In addition, this intuition further suggests that the SF density, and hence the SF phase stiffness, must be independent of α in the molecular limit. We prove this physical expectation by first approximating Eq. (8) as,
\[ D_{\mu \nu} = \{\Delta^2/[A(\mu^2 + 2^2)]\} \sum_{mnk} Q_{\mu \nu}^{mnk}, \]
and noting that the summations over \( n \) and \( m \) is equivalent to \( \sum_{mnk} Q_{\mu \nu}^{mnk} = \text{Tr}[(\partial \mathcal{H}_{\text{sm}}/\partial k_2)(\partial \mathcal{H}_{\text{sm}}/\partial k_2)] \), for any given \( k \). In particular to our Hamiltonian given in Eq. (2), we immediately get
\[ 4t^2 \sum_{ \mathbf{k} \in \text{BZ}} \sum_{\mu \nu} \sum_{n \neq m} \sin^2(k_\mu a + 2\pi \alpha) \]
for the \( \mu = y, y \) element, and this summation is exactly equivalent to that of the flux-free system, i.e.,
\[ 4t^2 \sum_{ \mathbf{k} \in \text{BZ}} \sum_{\mu} \sum_{n \neq m} \sin^2(k_\mu a) = M/2, \]
since the interval \( -\pi \leq k_\mu a < \pi \) remains unchanged in both Brillouin zones. Thus, we conclude that \( D_0 = 4F(2 - F)t^2/U \) is independent of both α and T ≤ \( T_{\text{BKT}} \) in the molecular limit. It is worth highlighting that, given the indiscriminate account of both the intra-band and inter-band contributions in recovering the desired \( D_0 \) of the Cooper molecules, our proof offers an indirect yet an impartial support of the recent results. In fact, our numerical calculations presented in Sec. III reveal that \( D_0^{\text{int}} \) eventually dominates over \( D_0^{\text{tra}} \) with increasing \( U/t \) for any \( q \geq 2 \). While this domination is substantial even for the simplest two-band and three-band (\( q = 2 \) and 3) cases, it is already quite dramatic for \( q > 3 \) as the butterfly bands get more flattened.

In addition, to make an analogy with the molecular limit of a continuum Fermi gas that is discussed at length in Sec. IIIC, we first recall that the expression \( D_0 = \hbar^2 e_s/n_0 \) is derived for all \( \Delta \neq 0 \) including the molecular limit. Second, we rewrite \( D_0 \) in terms of the SF density of the continuum molecules \( \rho_{\text{sm}} = \rho_s/2 \) and their mass \( m_{\text{sm}} = 2m_0 \) as \( D_0 = 4\hbar^2 \rho_{\text{sm}}/m_{\text{sm}} \). Then, by plugging the effective mass \( m_{\text{sm}} = \hbar^2/(2t_0^2 a^2) \) of the lattice molecules into this continuum expression, we identify \( F_{\text{sm}} = a^2 \rho_{\text{sm}} = UD_0/(16t^2) = (F/2)(1 - F/2) \) as the filling of SF molecules. It is pleasing to confirm that \( F_{\text{sm}} \) is independent of α, which need not be the case for the filling of SF particles \( F_s = a^2 \rho_s = D_0/(2t) \) in the weak-coupling limit.

On the other hand, by adapting the definition of the number of condensed particles for our model [28],
\[ F_c = \frac{\Delta^2}{2M} \sum_{\mathbf{n} \mathbf{k}} \frac{\Lambda^2_{\mathbf{n} \mathbf{k}}}{E_{\mathbf{n} \mathbf{k}}^2}, \]
and taking the molecular limit, we obtain \( F_{\text{sm}} = \Delta^2/[4(\mu^2 + 2^2)] = (F/2)(1 - F/2) \) as the filling of condensed molecules, which is also independent of α. Thus, we conclude that all of the SF molecules are condensed with a fraction of \( 2F_{\text{sm}}/F = 2F_{\text{sm}}/F = 1 - F/2 \). In perfect agreement with the continuum model where we find that the entire Fermi gas is condensed and become SF in the dilute \( (F \rightarrow 0) \) limit, half of the Fermi gas is not condensed at half-filling \((F \rightarrow 1)\). This difference between the dilute continuum and finite-filling lattice has to do with the fact that Cooper molecules are intrinsically hardcore by their composite nature, which is strictly dictated by the Pauli exclusion principle in the \( U/t \rightarrow \infty \) limit. For this reason, whether a site is almost empty or singly occupied by one of the Cooper molecules gives rise to a notable outcome in lattice models.

III. NUMERICAL RESULTS

To illustrate the numerical accuracy of our analysis given in the previous Sec. IIIC, next we present the self-consistent solutions of Eqs. (4)–(6) for two sets of \( \alpha = 1/q \), the even \( q \in \{2, 4, 6\} \) set is shown in Fig. 1 and the odd \( q \in \{3, 5, 7\} \) is shown in Fig. 2. Here, we primarily focus on the evolution of \( T_{\text{BKT}} \) together with the corresponding \( \Delta \), \( D_0^{\text{tra}} \), and \( F_c \) in the \( \mu \) versus \( U \) plane. The trivial \( q = 1 \) case is included as App. A for the sake of completeness. Thanks to the particle-hole symmetry of the model Hamiltonian, we restrict numerics to \( \mu \leq 0 \) or equivalently \( F \leq 1 \), as the solutions are mirror-symmetric around \( \mu = 0 \) or the half-filling \( F = 1 \).

First of all, since \( T_{\text{BKT}}/t \rightarrow T_c/t_0 \) as \( \Delta/t \rightarrow 0 \) or \( U \rightarrow U_c \), where the value of the critical interaction threshold \( U_c \) for SF pairing depends strongly on the energy density \( D(\varepsilon) \) of single-particle states, e.g., \( U_c/t_0 > 0 \) when \( \mu \) lies within the butterfly gaps or at \( \mu = 0 \) when \( q \) is even, the top two rows in Figs. 1 and 2 recover the overall structure of the ground-state \((T \rightarrow 0)\) phase diagrams [19]. We recall that the multi-band butterfly spectrum gives rise to a number of insulating lobes that are reminiscent of the well-known Mott-insulator transitions of the Bose-Hubbard model. This is because while \( \Delta \), and therefore, \( T_{\text{BKT}} \) grows exponentially \( e^{-1/[U(\mu)]} \) slow with \( U \neq 0 \) and \( D(\varepsilon) \) wherever \( \mu \) lies within any of the butterfly bands, it grows linearly \( U - U_c \) fast from the semi-metal when \( \mu = 0 \) and \( q \) is even, and with a square root \( \sqrt{U - U_c} \) from the insulators in general [18, 19].

Even though \( \Delta \) and \( T_{\text{BKT}} \) must, in theory, vanish strictly at \( U = 0 \) whenever \( \mu \) lies within any of the butterfly bands, this appears not to be the case in any of
FIG. 1: (color online) The critical SF transition temperature \( k_B T_{BKT}/t \) is shown in the first row together with the corresponding SF order parameter \( \Delta/t \) in the second row, relative weight of the intra-band and inter-band contributions to the phase stiffness \( (D_0^{\text{intra}} - D_0^{\text{inter}})/D_0 \) in the third row, and condensate fraction \( F_c/F \) in the last row.

Figs. 1 and 2, e.g., \( U \to 0 \) regions appear white instead of black. This is due to a lack of our numerical resolution as the non-linear solver fails to converge once the relative accuracy of two consecutive \( \Delta \) iterations reduces below the order of \( 10^{-5} \). We checked that using a \( 10^{-6} \) resolution does not improve the phase diagrams, i.e., the minor corrections are indistinguishable to the eye. On the other hand, this shortage makes the general structure of \( D(\varepsilon) \) visible on the periphery of the white regions. In contrast, the insulating lobes are determined quite accurately, since \( \Delta \) and \( T_{BKT} \) vanish very rapidly as \( U \to U_c \neq 0 \).

The top rows in Figs. 1 and 2 show that the maximum critical temperatures are always attained at \( \mu = 0 \) for some intermediate \( U \sim 3.75t - 5.5t \), and are all of the order of \( k_B T_c^{\max} \sim 0.19t - 0.25t \) for any given \( \alpha \). In particular, we approximately determine the following \( (k_B T_c^{\max}/t, U/t) \) values in our numerics: (0.1917, 5.45) for \( q = 2 \), (0.2027, 4.70) for \( q = 3 \), (0.2181, 4.25) for \( q = 4 \), (0.2260, 4.10) for \( q = 5 \), (0.2321, 4.00) for \( q = 6 \), and (0.2363, 3.95) for \( q = 7 \). Thus, increasing \( q \) from 2 not only enhances \( k_B T_{c}^{\max}/t \) quite monotonously, but it also occurs at a lower \( U/t \). In comparison, we find (0.2528, 3.75) for \( q = \infty \) or equivalently \( q = 1 \) corresponding to the usual no-flux model presented in App. [A]. Assuming that the monotonic trend continues for larger \( q \), we suspect that the result of \( q = \infty \) case is an ultimate upper bound for \( T_{c}^{\max} \) in the entire parameter range of the model Hamiltonian given in Eq. (3). In the molecular limit when \( U \gg t \), we verify that \( k_B T_{BKT}/t \) decreases as \( \pi F(2 - F)t/(2U) \) in all figures, which is in perfect agreement with the analysis given above in Sec. [II D].

In addition, we present the relative \( D_0^{\text{intra}} - D_0^{\text{inter}} \) weights of the intra-band and inter-band contributions to \( D_0 \) in the third rows of Figs. 1 and 2. Together with the \( T_{BKT} \) figures shown in the top rows which are directly
proportional to the sum $D_{0}^{\text{intra}} + D_{0}^{\text{inter}}$, these results reveal that $D_{0}^{\text{inter}}$ eventually dominates over $D_{0}^{\text{intra}}$ with increasing $U/t$ for any $q \geq 2$. While this domination is substantial even for the simplest two-band and three-band ($q = 2$ and 3) cases, it becomes sheer dramatic for $q > 3$ once the butterfly bands get more flattened. Thus, our numerical results unveil and highlight the relative importance of $D_{0}^{\text{inter}}$ contribution without a doubt.

Lastly, the condensate fractions $F_{c}/F$ are shown in the bottom rows of Figs. 1 and 2. These results show that $F_{c}/F \rightarrow 0$ is directly controlled by $\Delta$ in the weak-coupling limit when $\Delta/t \rightarrow 0$. On the other hand, $F_{c}/F$ saturates to $1 - F/2$ in the molecular limit, which is again in perfect agreement with the ground-state analysis given above in Sec. II D. This is because $k_{B}T_{\text{BKT}}/t \rightarrow 0$ in both $U \rightarrow U_{c}$ and $U \gg t$ limits. Having achieved the primary objectives of this paper, next we are ready to end it with a brief summary of our conclusions.

### IV. CONCLUSIONS

In summary, by studying the thermal SF properties along with the critical SF transition temperature in the Hofstadter-Hubbard model with $T$ symmetry, here we analyzed the competition between the intra-band and inter-band contributions to the phase stiffness in the presence of a multi-band butterfly spectrum. For instance, one of the highlights of this paper is that increasing the interaction strength always shifts the relative importance of the two in favor of the inter-band contribution. In marked contrast with the two-band and three-band cases for which the shift takes place gradually, our numerical results showed an extremely striking shift for the higher-band ones. Last but not least, we also showed analytically that the proper description of the Cooper molecules requires an indiscriminate account of both contributions in the strong-coupling limit.
Given our convincing evidence that the inter-band effects are absolutely non-negligible in a typical multi-band butterfly spectrum, we hope to see further studies along this direction in other models and/or contexts as well. Presumably, similar to the resolution of the ‘two-band superconductivity without supercurrent’ controversy near the Dirac points in graphene [12, 13], such effects may already be playing a part in the multi-band family of high-$T_c$ superconductors that are waiting to be uncovered and characterized.

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Appendix A: Usual Hubbard Model

For the sake of completeness, here we included the self-consistent solutions of Eqs. (4)-(6) for $\alpha = 0$ or equivalently $\alpha = 1/1$, where $\varepsilon_k = -2t \cos(k_x a) - 2t \cos(k_y a)$. As we noted in Sec. III, even though $\Delta$ and $T_{BKT}$ must, in theory, vanish strictly at $U = 0$ wherever $\mu$ lies within the band, i.e., $-4t < \mu < 4t$, this appears not to be the case in Fig. 3 as well, e.g., $U \rightarrow 0$ regions appear white instead of black. This is again due to a lack of our numerical resolution as the non-linear solver fails to converge once the relative accuracy of two consecutive $\Delta$ iterations reduces below the order of $10^{-5}$. Despite this shortage, we find $k_B T_{\text{max}} \approx 0.2528t$ at $\mu = 0$ when $U = 3.75t$, which is in very good agreement with an earlier estimate [1].

![Image](317x266 to 643x511)

FIG. 3: (color online) The critical SF transition temperature $k_B T_{\text{BKT}}/t$ is shown in the first row together with the corresponding SF order parameter $\Delta/t$ in the second row, and condensate fraction $F_c/F$ in the last row.

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