



Geometric superfluid weight of composite bands in multiorbital superconductorsGuodong Jiang ^{1,2} and Yafis Barlas ¹¹*Department of Physics, University of Nevada, Reno, Reno, Nevada 89502, USA*²*Department of Applied Physics, Aalto University School of Science, FI-00076 Aalto, Finland*

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The superfluid weight of an isolated flat band in multiorbital superconductors contains contributions from the band's quantum metric and a lattice geometric term that depends on the orbital positions in the lattice. Since the superfluid weight is a measure of the superconductor's energy fluctuation, it is independent of the lattice geometry, leading to the minimal quantum metric of a band [Phys. Rev. B **106**, 014518 (2022)]. Here, a perturbation approach is developed to study the superfluid weight and its lattice geometric dependence for composite bands. When all orbitals exhibit uniform pairing, the quantum geometric term contains each band's contribution and an interband contribution between every pair of bands in the composite. Based on a band representation analysis, they provide a topological lower bound for the superfluid weight of an isolated composite of flat bands. Using this perturbation approach, an analytical expression of the lattice geometric contribution is obtained. It is expressed in terms of Bloch functions, providing a convenient formula to calculate the superfluid weight for multiorbital superconductors.

DOI: [10.1103/PhysRevB.109.214518](https://doi.org/10.1103/PhysRevB.109.214518)**I. INTRODUCTION**

The discovery of superconductivity in twisted two-dimensional (2D) crystals [1–14] has brought focus to the nature of superconductivity in flat or weakly dispersive bands [15–32]. While the pairing mechanism remains unresolved, the superconducting fluctuations in flat bands are exotic enough to warrant a complete understanding [33–50]. A particular focus is on the question of superfluid weight (SW) in flat-band superconductors, which serves as an essential criterion to distinguish superconductors from metals [51,52]. The SW in conventional superconductors, irrespective of the order-parameter symmetry, is inversely proportional to the effective mass [53,54], ruling out flat-band superconductivity. However, in multiorbital superconductors, band geometry rescues superconductivity by providing a finite SW, which is proportional to the quantum metric of the band [16–25,27–29]. This quantum geometric SW dominates in flat-band superconductors like twisted 2D crystals [22,23,55]. Moreover, geometric effects can result in transitions to exotic superconducting states [56–58], which necessitates the need for a further understanding of the role of band geometry in multiorbital superconductors.

Up to now, most studies of the geometric SW have been restricted to a single isolated band [16,18–25,27–29]. This is valid when the pairing potential is comparable with the bandwidth of the active band near the Fermi level but much smaller than the band gap of other remote bands. However, many examples exist where multiple bands lie within or close to the pairing interaction window, violating this single-band projection. In these cases, the interband geometric effects [17,26,59,60] can be significant. In addition, quantum geometric quantities like the Berry curvature and quantum metric are usually large near the local \mathbf{k} -points where the remote bands are energetically close to the active band. Therefore,

it is essential to study the geometric SW when a composite of bands is within or near the interaction range.

In this paper, we employ a band projection formalism to study the SW of composite bands. This projection to the composite transforms the orbital basis to band basis but projects to a few bands most relevant to the interaction energy scale determined by the pairing Hamiltonian. We then develop a perturbation approach to calculate the SW, which is similar to the $\mathbf{k} \cdot \mathbf{p}$ method of calculating the effective-mass tensor of bands in solids. This approach provides an alternative derivation of the general results in Refs. [16,19] and identifies each term of the quantum geometric SW from transitions between Bogoliubov bands. The quantum geometric SW of composite bands contains each band's contribution and an interband contribution between every pair of bands in the composite. This separation of SW emphasizes the role of interband quantum metric, which originates from the derivative of interband pairing functions. Although the interband geometric terms are negative semidefinite and reduce the SW, the total SW is always positive semidefinite, implying the local stability of the zero center-of-mass momentum (CMM) state in the uniform pairing channel.

Analyzing the reduction of superfluid weight due to the interband pairing, we derive a topological lower bound for the SW of an isolated composite of flat bands (ICFB), Eq. (19). The necessity of such a lower bound arises from a very fundamental question, as in realistic materials the scenario of a single isolated flat band is rare. Instead, many flat or weakly dispersive bands can coexist in the interaction window. In the simplest case, one can ask if there is a topological lower bound for the SW when two flat bands of opposite Chern numbers ± 1 are both within the pairing interaction window.

An analysis of this case from the perspective of band representation (BR) turns out to be illuminating. If the two bands

are constructed from the same set of Wannier orbital bases of an elementary band representation (EBR) [61,62], their topological lower bounds tend to cancel, $|+1 + (-1)| = 0$. In contrast, when they belong to different EBRs, their topological lower bounds will add, $|+1| + |-1| = 2$. The latter is due to a suppression of the reduction effect by interband pairings. This suggests that a larger SW can be achieved if a multiorbital superconductor is doped to a set of bands that contain multiple incomplete EBRs.

In the second half of this paper, we study the relation between lattice geometry and SW for multiorbital superconductors. Recently, it was shown that an additional contribution encoding the modification of order parameters with orbital positions in a unit cell must be included in the calculation of SW [30,31]. This lattice geometric term, combined with the quantum geometric term, makes the total SW invariant with the choice of orbital positions [31], therefore it is lattice-geometry-independent [63]. Using the perturbation method, we derive an analytical expression of the lattice geometric term in terms of Bloch functions, Eq. (35). This expression provides a convenient way of computing the lattice geometric term numerically without solving gap equations.

The rest of this paper is organized as follows. In Sec. II, we develop the projection procedure for composite bands, and we present the quantum geometric SW calculated from the perturbation method. Section III contains an analysis of the interband effect on the geometric SW, and it establishes a topological lower bound for an ICFB. Section IV studies the derivative of the gap equation with respect to CMM using the perturbation method, thereby obtaining the second derivative of the grand potential with order parameters and analyzing its properties. In Sec. V, we show the geometry independence of the SW, and we provide a convenient formula for computing the lattice geometric term. Finally, we conclude our findings in Sec. VI.

II. SUPERFLUID WEIGHT OF COMPOSITE BANDS

We start from the tight-binding lattice Hamiltonian with intraorbital attractive interactions ($U_\alpha > 0$):

$$\hat{\mathcal{H}} = \sum_{ij,\alpha\beta,\sigma} t_{ij,\alpha\beta}^\sigma c_{i\alpha\sigma}^\dagger c_{j\beta\sigma} - \sum_{i,\alpha} U_\alpha \hat{n}_{i\alpha\uparrow} \hat{n}_{i\alpha\downarrow}, \quad (1)$$

where i, j label the unit cell, $\alpha, \beta = 1, \dots, s$ label the orbitals in a unit cell, and $\sigma = \uparrow, \downarrow$ labels the spin. The tight-binding matrix elements $t_{ij,\alpha\beta}^\sigma$ encode the hopping pattern and amplitudes from orbital (j, β) to (i, α) . This hopping graph determines the band dispersion and topology. The second term is the on-site density-density interaction, with $\hat{n}_{i\alpha\sigma} = c_{i\alpha\sigma}^\dagger c_{i\alpha\sigma}$ the number operator. We assume time-reversal symmetry (TRS) with zero spin-orbit coupling, thereby restricting to singlet pairing.

For attractive pairing interactions, we assume a BCS-type ground state and perform the usual mean-field decoupling of Eq. (1) to arrive at the mean-field Hamiltonian $\hat{\mathcal{H}}_{\text{MF}}$. Throughout this paper, we focus on an orbital-independent pairing matrix $\hat{\Delta} = \Delta \hat{\mathcal{I}}_s$, referred to as the uniform pairing condition (UPC) in the literature [16,17,19]. Here $\hat{\mathcal{I}}_s$ is the s -dim identity matrix in orbital space. This choice of pairing channel can always be made for any intraorbital interactions obeying

TRS by tuning parameters U_α . It corresponds to a particular solution channel to the BCS gap equation, which always leads to a positive-semidefinite SW tensor.

The superconducting fluctuations to finite CMM can be described within the same framework by a reduced mean-field Hamiltonian (see Appendix A),

$$\hat{\mathcal{H}}_{\text{MF}}(\mathbf{q}) = \sum_{\mathbf{k}} \mathbf{C}_{\mathbf{k},\mathbf{q}}^\dagger H_{\text{BdG},\mathbf{k}}(\mathbf{q}) \mathbf{C}_{\mathbf{k},\mathbf{q}} + N \sum_{\alpha=1}^s \frac{|\Delta_{\mathbf{q},\alpha}|^2}{U_\alpha} + \sum_{\mathbf{k}} \text{Tr}\{h_{-\mathbf{k}+\mathbf{q}}^\downarrow - \mu_{\mathbf{q}}\}, \quad (2)$$

where $\mathbf{C}_{\mathbf{k},\mathbf{q}} = (c_{\mathbf{k}+\mathbf{q},\alpha\uparrow}, c_{-\mathbf{k}+\mathbf{q},\alpha\downarrow}^\dagger)^T$ denotes the Nambu spinor, with \mathbf{q} half of the CMM, N denotes the number of unit cells, and

$$H_{\text{BdG},\mathbf{k}}(\mathbf{q}) = \begin{pmatrix} h_{\mathbf{k}+\mathbf{q}}^\uparrow - \mu_{\mathbf{q}} & \hat{\Delta}_{\mathbf{q}} \\ \hat{\Delta}_{\mathbf{q}}^\dagger & -(h_{-\mathbf{k}+\mathbf{q}}^{\downarrow T} - \mu_{\mathbf{q}}) \end{pmatrix} \quad (3)$$

is the Bogoliubov–de Gennes (BdG) matrix. TRS imposes that $h_{-\mathbf{k}}^{\downarrow T} = h_{\mathbf{k}}^\uparrow$. The chemical potential $\mu_{\mathbf{q}}$ and pairing matrix $\hat{\Delta}_{\mathbf{q}}$ are attained self-consistently. The pairing matrix $\hat{\Delta}_{\mathbf{q}} = \text{diag}\{\Delta_{\mathbf{q},1}, \dots, \Delta_{\mathbf{q},s}\}$ in general has its entries complex and \mathbf{q} -dependent.

To compute the SW, we adopt the grand potential method [16]. SW is the second total derivative of the superconducting free energy $F(\mathbf{q})$ with respect to \mathbf{q} ,

$$D_{s,\mu\nu} = \frac{1}{A} \frac{d^2 F}{dq_\mu dq_\nu} \Big|_{\mathbf{q}=\mathbf{0}}. \quad (4)$$

For simplicity, we set the area $A = 1$. The free energy $F(\mathbf{q}) = \Omega(\mathbf{q}, \mu_{\mathbf{q}}, \hat{\Delta}_{\mathbf{q}}, \hat{\Delta}_{\mathbf{q}}^*) + \mu_{\mathbf{q}} N_e$, where the grand potential

$$\Omega(\mathbf{q}, \mu_{\mathbf{q}}, \hat{\Delta}_{\mathbf{q}}, \hat{\Delta}_{\mathbf{q}}^*) = -\frac{1}{\beta} \ln \text{Tr}\{e^{-\beta \hat{\mathcal{T}}_{\text{MF}}(\mathbf{q})}\} \quad (5)$$

is a function of $\mathbf{q}, \mu_{\mathbf{q}}, \hat{\Delta}_{\mathbf{q}}, \hat{\Delta}_{\mathbf{q}}^*$ explicitly. N_e is the fixed average number of electrons. In the presence of TRS, $D_{s,\mu\nu}$ can be related to partial derivatives of the grand potential [16,30,31]:

$$D_{s,\mu\nu} = \left[\frac{\partial^2 \Omega}{\partial q_\mu \partial q_\nu} - \frac{d\Delta_{\mathbf{q},\alpha}^I}{dq_\mu} \frac{\partial^2 \Omega}{\partial \Delta_{\mathbf{q},\alpha}^I \partial \Delta_{\mathbf{q},\beta}^I} \frac{d\Delta_{\mathbf{q},\beta}^I}{dq_\nu} \right] \Big|_{\mathbf{q}=\mathbf{0}}, \quad (6)$$

where $\Delta_{\mathbf{q},\alpha}^I$ is the imaginary part of $\Delta_{\mathbf{q},\alpha}$, and we have employed the Einstein summation rule for $\alpha, \beta = 1, \dots, s$. $U(1)$ symmetry allows one to fix $\Delta_{\mathbf{q},1}$ to be real and positive for all \mathbf{q} , so the sum over α, β above can be reduced as from 2 to s [31]. However, we assume an arbitrary global phase to keep the discussion general.

The first term of Eq. (6) ($D_s^{(1)}$) contains two contributions to the SW of multiorbital superconductors—the conventional contribution, which is inversely proportional to the effective mass, and the quantum geometric contribution. This quantum geometric SW is proportional to an integral of the quantum metric [16], which is lattice-geometry-dependent [63]. However, as expected from general considerations, this geometry dependence is canceled by the second term of Eq. (6) (the lattice geometric term, $D_s^{(2)}$), which encodes the order parameter's variation with orbital positions [30–32].

We consider the scenario in which $n \leq s$ bands are energetically within or close to the interaction window [64] around

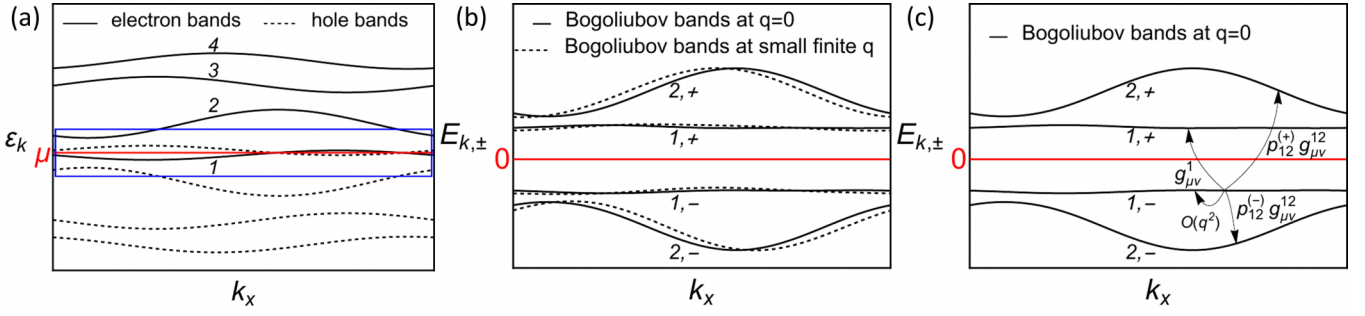


FIG. 1. Interpretation of the band projection, composite, and geometric terms of Eq. (9) from Bogoliubov band transitions (see Appendix D for details). (a) Two electronic bands (1,2) energetically close to the interaction scale are projected from a four-orbital model, defining the composite. The blue rectangle indicates the interaction window of 2Δ around the Fermi level. (b), (c) Zoom-in picture of the composite. (b) Electronic bands mix with hole bands to form four Bogoliubov bands ($1, \pm$ and $2, \pm$). At $\mathbf{q} = \mathbf{0}$, these bands are particle-hole symmetric (PHS); at $\mathbf{q} \neq \mathbf{0}$, the dispersion is deformed and particle-hole symmetry is broken. SW measures the second derivative of energy with respect to \mathbf{q} . (c) For small \mathbf{q} , the deformation can be treated with perturbation, which enables transitions between Bogoliubov bands. Here, only the transitions from band $1, -$ are indicated by arrows. The $O(q^2)$ transition amplitude to band $1, -$ itself, combined with the $O(q)$ amplitude to band $1, +$, gives the intraband geometric SW $\propto g_{\mu\nu}^1$; the $O(q)$ transition amplitudes to band $2, \pm$ give the interband terms $\propto p_{12}^{(\pm)} g_{\mu\nu}^{12}$, respectively.

the Fermi level [the case of $n = 2$ is shown in Fig. 1(a)]. We refer to the group of n flat or dispersive bands, whether connected or disconnected from each other, as a “composite,” and denote it by \mathcal{C} . We perform a projection of the full Hamiltonian Eq. (2) to the composite, a generalization of the single-band projection in an earlier paper [58]. The projected mean-field Hamiltonian at finite \mathbf{q} , involving the kinetic energy of the n bands and pairing interactions between them, reads

$$\hat{\mathcal{H}}_{\mathcal{C}}(\mathbf{q}) = \sum_{\mathbf{k}} \sum_{l \in \mathcal{C}} [\xi_{l,\mathbf{k}+\mathbf{q}}^{\uparrow} c_{l,\mathbf{k}+\mathbf{q}\uparrow}^{\dagger} c_{l,\mathbf{k}+\mathbf{q}\uparrow} - \xi_{l,-\mathbf{k}+\mathbf{q}}^{\downarrow} c_{l,-\mathbf{k}+\mathbf{q}\downarrow}^{\dagger} c_{l,-\mathbf{k}+\mathbf{q}\downarrow}] + \sum_{\mathbf{k}} \sum_{l \in \mathcal{C}} \xi_{l,-\mathbf{k}+\mathbf{q}}^{\downarrow} + \sum_{\mathbf{k}} \sum_{l,l' \in \mathcal{C}} [\Delta_{ll',\mathbf{k}}(\mathbf{q}) c_{l,\mathbf{k}+\mathbf{q}\uparrow}^{\dagger} c_{l',-\mathbf{k}+\mathbf{q}\downarrow}^{\dagger} + \text{H.c.}] + N \sum_{\alpha=1}^s \frac{|\Delta_{\mathbf{q},\alpha}|^2}{U_{\alpha}}, \quad (7)$$

where $\xi_{l,\mathbf{k}+\mathbf{q}}^{\uparrow} = \varepsilon_{l,\mathbf{k}+\mathbf{q}}^{\uparrow} - \mu_{\mathbf{q}}$, $\xi_{l,-\mathbf{k}+\mathbf{q}}^{\downarrow} = \varepsilon_{l,-\mathbf{k}+\mathbf{q}}^{\downarrow} - \mu_{\mathbf{q}}$ are the band energies measured from the fluctuated chemical potential. By TRS we have defined $\xi_{l\mathbf{k}} \equiv \xi_{l\mathbf{k}}^{\uparrow} = \xi_{l,-\mathbf{k}}^{\downarrow}$. Projection to the composite naturally defines the interband gap functions

$$\Delta_{ll',\mathbf{k}}(\mathbf{q}) \equiv \langle u_{l,\mathbf{k}+\mathbf{q}} | \hat{\Delta}_{\mathbf{q}} | u_{l',\mathbf{k}-\mathbf{q}} \rangle, \quad (8)$$

where l, l' are band indices restricted in the composite, and $u_{l\mathbf{k}}$ is the periodic part of the Bloch function of the l th spin- \uparrow band. For the case $l = l'$, $\Delta_{ll',\mathbf{k}}(\mathbf{q})$ is just the intraband gap function $\Delta_{l,\mathbf{k}}(\mathbf{q})$ [58]. Under the UPC, the interband gap functions ($l \neq l'$) vanish at $\mathbf{q} = \mathbf{0}$ by the orthogonality of Bloch functions but are nonvanishing at $\mathbf{q} \neq \mathbf{0}$. After projection to the composite, the projected order parameter has equal pairing on the orbitals that make up the composite. In addition, our projection formalism also applies to a general case of intraorbital pairing when the pairing matrix takes the

form $\hat{\Delta} = \text{diag}\{\Delta_1, \dots, \Delta_1, \Delta_2, \dots, \Delta_2, \dots\}$ (i.e., uniform among subsets of orbitals). By definition of the gap functions, Eq. (8), the pairing between band l and l' in the composite can be viewed as uniform if they are spanned by orbitals in a single subset. Therefore, we only require equal pairing on the orbitals of the composite bands.

We developed a stationary state perturbation method to diagonalize the quadratic Hamiltonian of composite bands, Eq. (7). The perturbation method has been commonly used to simplify Kubo formula results [65] but is mainly restricted to the single-band case without considering band geometry. Here, it not only reproduces the first term of Eq. (6), $D_s^{(1)}$, which agrees with the general results in Refs. [16,19], but gives each contribution the meaning of transitions between Bogoliubov bands.

The first term of Eq. (6) is (see Appendix D for details)

$$D_{s,\mu\nu}^{(1)} = \sum_{\mathbf{k}} \sum_{l \in \mathcal{C}} \frac{\Delta^2}{E_{l\mathbf{k}}^3} \left(\tanh \frac{\beta E_{l\mathbf{k}}}{2} - \frac{\beta E_{l\mathbf{k}}}{2} \text{sech}^2 \frac{\beta E_{l\mathbf{k}}}{2} \right) \partial_{\mu} \xi_{l\mathbf{k}} \partial_{\nu} \xi_{l\mathbf{k}} + \sum_{\mathbf{k}} \sum_{l \in \mathcal{C}} \tanh \frac{\beta E_{l\mathbf{k}}}{2} \left\{ \frac{4\Delta^2}{E_{l\mathbf{k}}} g_{\mu\nu}^l(\mathbf{k}) + \sum_{l' \in \mathcal{C}, l' \neq l} 8\Delta^2 \left[\frac{p_{ll'}^{(+)}(\mathbf{k})}{E_{l\mathbf{k}} + E_{l'\mathbf{k}}} + \frac{p_{ll'}^{(-)}(\mathbf{k})}{E_{l\mathbf{k}} - E_{l'\mathbf{k}}} \right] g_{\mu\nu}^{ll'}(\mathbf{k}) \right\}, \quad (9)$$

where Δ is the uniform pairing order parameter at finite temperature $T = 1/\beta$, and $E_{l\mathbf{k}} = \sqrt{\xi_{l\mathbf{k}}^2 + \Delta^2}$ is the $\mathbf{q} = \mathbf{0}$ quasiparticle energy. The first line of Eq. (9) corresponds to the conventional contribution to SW, and the two separate pieces in the second line correspond to the intra- and interband geometric contributions. The different transition processes represented by these geometric contributions can be interpreted from stationary state perturbations and are illustrated in Fig. 1 (see Appendix D for details). We have introduced functions

$$p_{ll'}^{(\pm)}(\mathbf{k}) \equiv \frac{1}{2} \left(1 \pm \frac{\xi_{l\mathbf{k}} \xi_{l'\mathbf{k}} + \Delta^2}{E_{l\mathbf{k}} E_{l'\mathbf{k}}} \right), \quad l \neq l', \quad (10)$$

which can be termed as the $\mathbf{q} = \mathbf{0}$ *interband coherence factors* [66], in contrast to the intraband coherence factors ($l = l'$) in conventional BCS theory [53,65]. $g_{\mu\nu}^l = \text{Re} R_{\mu\nu}^l$, $g_{\mu\nu}^{l'} = \text{Re} R_{\mu\nu}^{l'}$ are the real parts of the intra- and interband component of the quantum geometric tensor $R_{\mu\nu}^l$, $R_{\mu\nu}^{l'}$, respectively, with

$$\begin{aligned} R_{\mu\nu}^l(\mathbf{k}) &= \langle \partial_\mu u_{l\mathbf{k}} | (1 - |u_{l\mathbf{k}}\rangle \langle u_{l\mathbf{k}}|) | \partial_\nu u_{l\mathbf{k}} \rangle, \\ R_{\mu\nu}^{l'}(\mathbf{k}) &= -\langle \partial_\mu u_{l\mathbf{k}} | u_{l'\mathbf{k}} \rangle \langle u_{l'\mathbf{k}} | \partial_\nu u_{l\mathbf{k}} \rangle, \quad l \neq l'. \end{aligned} \quad (11)$$

Together they constitute the quantum geometric tensor of the composite bands,

$$R_{\mu\nu}^C(\mathbf{k}) = \sum_{l \in C} R_{\mu\nu}^l(\mathbf{k}) + \sum_{l, l' \in C, l \neq l'} R_{\mu\nu}^{ll'}(\mathbf{k}), \quad (12)$$

where $R_{\mu\nu}^C(\mathbf{k}) = \text{Tr}\{\hat{P}_C(\mathbf{k}) \partial_\mu \hat{P}_C(\mathbf{k}) \partial_\nu \hat{P}_C(\mathbf{k})\}$, and $\hat{P}_C(\mathbf{k}) = \sum_{l \in C} |u_{l\mathbf{k}}\rangle \langle u_{l\mathbf{k}}|$ is the projection operator.

Tensor $g_{\mu\nu}^{ll'}(\mathbf{k})$ measures small distances between Bloch functions of different bands in the momentum space,

$$|\langle u_{l\mathbf{k}} | u_{l', \mathbf{k}+\mathbf{q}} \rangle|^2 \approx -q_\mu q_\nu g_{\mu\nu}^{ll'}(\mathbf{k}). \quad (13)$$

With our convention Eq. (11), $g_{\mu\nu}^{ll'}(\mathbf{k})$ is *negative* semidefinite, indicating that the interband geometric contributions in Eq. (9) are negative and reduce the total SW. However, in Appendix E we show that the total SW, which is the sum of the conventional, intra-, and interband geometric terms, is always positive semidefinite. This implies that the $\mathbf{q} = \mathbf{0}$ BCS state locally minimizes the free energy at any temperature whenever the UPC is valid for the composite bands.

In addition to the first term $D_s^{(1)}$, the perturbation method also gives an analytical expression of the Hessian matrix $\partial^2 \Omega / \partial \Delta_{\mathbf{q}, \alpha}^I \partial \Delta_{\mathbf{q}, \beta}^I |_{\mathbf{q}=0}$, thereby putting the lattice geometric term $D_s^{(2)}$ into a computationally convenient form. We address this in Secs. IV and V.

III. TOPOLOGICAL LOWER BOUND FOR AN ISOLATED COMPOSITE OF FLAT BANDS

The interband geometric terms in Eq. (9) are negative semidefinite and reduce the SW. In this section, we use this reduction effect along with the relative topology of the bands in the composite to establish a topological lower bound for the SW of composite bands. For a single isolated flat band, the absolute value of the Chern number provides a weak lower bound for the geometric SW [16]. These bounds stem from

the relation

$$\text{Tr} g^m(\mathbf{k}) \geq |B^m(\mathbf{k})| \quad (14)$$

for an isolated band m , with B^m the Berry curvature of the band, and the fact that the gauge-invariant part of the Wannier localization functional (WLF) is related to the trace of the quantum metric. Additional lower bounds due to Wilson loop winding numbers or real space invariants in other topological classifications have also been established [18,23,67]. One might ask for composite bands whether there is a lower bound for the SW, and what are the possible generalizations of Eq. (14)?

To answer these questions, we restrict our discussion to the zero-temperature limit in the following. At $T = 0$, the problem is simplified and Eq. (9) reads

$$\begin{aligned} D_{s,\mu\nu}^{(1)} &= \sum_{\mathbf{k}} \sum_{l \in C} \left[\frac{\Delta^2}{E_{l\mathbf{k}}^3} \partial_\mu \xi_{l\mathbf{k}} \partial_\nu \xi_{l\mathbf{k}} + \frac{4\Delta^2}{E_{l\mathbf{k}}} g_{\mu\nu}^l(\mathbf{k}) \right] \\ &+ \sum_{\mathbf{k}} \sum_{l, l' \in C, l' > l} \frac{16\Delta^2}{E_{l\mathbf{k}} + E_{l'\mathbf{k}}} p_{ll'}^{(+)}(\mathbf{k}) g_{\mu\nu}^{ll'}(\mathbf{k}). \end{aligned} \quad (15)$$

Here, coherence factors $p_{ll'}^{(-)}$ are canceled because they describe Bogoliubov transitions between two quasiparticle bands or two quasihole bands [Fig. 1(c)], which are suppressed at $T = 0$, a ‘‘Pauli blocking’’ effect. Following a similar procedure described in Appendix E, we break the intraband quantum metric g^l into interband ones, and the geometric part of Eq. (15) splits into two terms,

$$\begin{aligned} D_{s,\mu\nu}^{(1)\text{geo}} &= - \sum_{\mathbf{k}} \sum_{l \in C, l' \neq C} \frac{4\Delta^2}{E_{l\mathbf{k}}} g_{\mu\nu}^{ll'}(\mathbf{k}) \\ &- \sum_{\mathbf{k}} \sum_{l, l' \in C, l' > l} \frac{4\Delta^2 (\xi_{l\mathbf{k}} - \xi_{l'\mathbf{k}})^2}{E_{l\mathbf{k}} E_{l'\mathbf{k}} (E_{l\mathbf{k}} + E_{l'\mathbf{k}})} g_{\mu\nu}^{ll'}(\mathbf{k}). \end{aligned} \quad (16)$$

In this expression, the first term contains the interband quantum metric between bands inside and outside the composite, while the second term contains these between bands inside the composite only.

To establish a topological lower bound, we consider a *special class* of composite bands, where each band in the composite is within the interaction window, and these bands are energetically close to each other—we call this an ‘‘isolated composite of flat bands’’ (ICFB). Hereafter, our definition of flat bands encompasses weakly dispersive bands. This requires that the bandwidth of each band, $\delta \xi_l = \max\{|\xi_{l\mathbf{k}} - \xi_{l'\mathbf{k}}|\}$, and the band gaps between them, $\delta \xi_{ll'} = \max\{|\xi_{l\mathbf{k}} - \xi_{l'\mathbf{k}}|\}$ ($l, l' \in C$), are all much smaller than the uniform order parameter Δ . This notion of ICFB gives the separation in Eq. (16) a well-defined physical meaning.

In Eq. (16), the first term depends on the overall topology of the composite since it contains the quantum metric between bands inside and outside the composite, whereas the second term depends on the relative topology between bands inside the composite. For an ICFB, as long as the first term is nonzero, it is of order Δ and dominates over the second term, which is of order $\delta \xi^2 / \Delta$.

Furthermore, we assume that the ICFB contains an incomplete set of n disconnected bands ($n < s$), each with Chern

number C_l ($1 \leq l \leq n$). When a few bands are connected, the Chern numbers will be generalized to the integrals of non-Abelian Berry curvature over the Brillouin zone [68]. The total Chern number of an ICFB, $C = \sum_{l=1}^n C_l$, is always an integer.

With these clarifications, it is important to note that the inequality Eq. (14) holds for composite bands also [16,23,60,69,70], which reads

$$\text{Tr}g^C(\mathbf{k}) \geq |B^C(\mathbf{k})|, \quad (17)$$

where g^C and B^C are the quantum metric and Berry curvature of the composite. Following the definition Eq. (12), we write the quantum metric of composite bands as

$$g_{\mu\nu}^C = \sum_{l \in C} g_{\mu\nu}^l + \sum_{l,l' \in C, l' \neq l} g_{\mu\nu}^{ll'} = - \sum_{l \in C, l' \notin C} g_{\mu\nu}^{ll'}. \quad (18)$$

This is proportional to the leading term of Eq. (16), since Δ^2/E_{lk} is approximately a constant for an ICFB. As a result, the total SW is lowered bounded by $|C|$ (besides a proportional constant), with C the total Chern number of the composite. Exceptional cases may exist, e.g., when the composite is complete ($n = s$), such that $C = 0$ and the first term of Eq. (16) vanishes. In these cases, the SW will rely on the second term of Eq. (16) and the conventional term, which depends on the dispersion details; then, a simple topological lower bound cannot be obtained. We will see examples below when the composite has $C = 0$ but still provides a nonzero topological bound.

The result $D_s \geq |C|$ can be compared to the single isolated band case. If we add the lower bound $|C_l|$ of each band, it would give $D_s \geq \sum_{l=1}^n |C_l|$ for a composite. Therefore, we deduce that by the reduction effect of the interband geometric SW, the lower bound shrinks from the sum of absolute values to the absolute value of the sum, $|C| = |\sum_{l=1}^n C_l|$. This poses a contrast between composites with $\{C_l\}$ of uniform signs and different signs, e.g., $+, +, \dots$ and $+, -, \dots$, which can be further explained by analyzing the WLF [16,69].

The absolute value of the Chern number of the composite bands, $|C|$, is a lower bound for the WLF of Wannier orbitals of the composite, providing a measure of Wannier obstruction. If the composite is Wannier representable, then the bands inside and outside the composite can be constructed from disjoint sets of Wannier orbitals. In the language of “topological quantum chemistry” [61,62,71,72], such a composite is said to form a BR. In this case, the interband terms of Eq. (15) cancel the intraband terms altogether, giving a zero lower bound for the leading term of Eq. (16). On the contrary, in the presence of Wannier obstruction, the composite has to form a BR with some bands outside the composite. Then the interband terms of Eq. (15) partially cancel the intraband terms, leaving a finite lower bound for the leading term of Eq. (16).

However, the lower bound by $|C|$ in some cases is too weak, and a stronger lower bound can be derived. Suppose the s bands formed by the s atomic orbitals are divided into a few EBRs [61,62], which are constructed from disjoint sets of Wannier basis. For each EBR, it might be that only part of the bands belong to the composite. By making an induction from BR to EBR, one can immediately deduce that the interband geometric terms of Eq. (15) can only reduce the SW

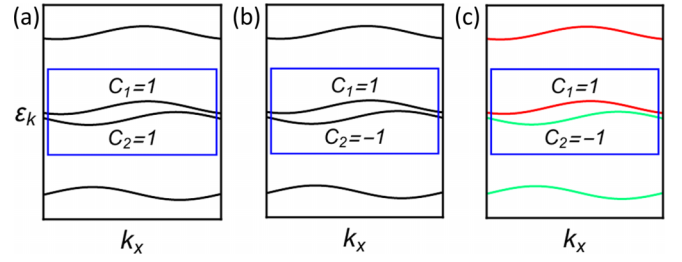


FIG. 2. An isolated composite of two weakly dispersive bands near the Fermi level (only spin-up bands are shown), with the blue rectangle indicating the interaction window of 2Δ . (a) The two bands in the composite have Chern number $C_1 = C_2 = 1$. The SW is lower bounded by $|C| = 2$. (b) The two bands have $C_1 = 1$ and $C_2 = -1$, and the SW is lower bounded by $|C| = 0$. (c) Same as (b), but the two bands belong to different EBRs (shown in red and green), thus the lower bound can be improved to $|C_1| + |C_2| = 2$.

substantially within an EBR, and not between two EBRs [73]. As a result, the topological lower bound can be improved, with $|C|$ replaced by

$$\left| \sum_{l_1=1}^{n_1} C_{l_1}^{(1)} \right| + \dots + \left| \sum_{l_j=1}^{n_j} C_{l_j}^{(j)} \right| = \sum_{j=1}^J \left| \sum_{l_j=1}^{n_j} C_{l_j}^{(j)} \right|, \quad (19)$$

where J is the number of EBRs formed by the s atomic orbitals, n_j is the number of bands in the composite that is from the j th EBR (with the sum $\sum_{j=1}^J n_j = n$), and $C_{l_j}^{(j)}$ is the Chern number of the l_j th band of the j th EBR. In the extreme case when each band of the composite belongs to a different EBR, there is no substantial reduction of SW by the interband terms, so the improved lower bound is $\sum_{l=1}^n |C_l|$. This simple idea of reducing the topological lower bound within individual EBRs is illustrated in Fig. 2 using the example of a two-band composite. Similar arguments can be generalized to systems with nonzero Chern numbers to attain stronger bounds based on real-space invariants [67].

IV. SUPERFLUID WEIGHT AND LATTICE GEOMETRY

We now study the relationship between SW and lattice geometry using the perturbation method. Here “lattice geometry” refers to the position of atomic orbitals in a unit cell of non-Bravais lattices. It was shown in Ref. [31] that when the atomic orbitals occupy some optimal positions, the second term of SW $D_s^{(2)}$ vanishes and the geometric part of $D_s^{(1)}$ becomes the minimal quantum metric (MQM). Typically, the optimal positions are high-symmetry points in the real space lattice.

However, if the symmetry of the tight-binding Hamiltonian is lower than that of the underlying Bravais lattice, the optimal positions can shift along high-symmetry lines [31]. Since Bravais lattice symmetries no longer protect them, the optimal positions can be sensitive to temperature, interaction, and the tight-binding graph $t_{ij,\alpha\beta}^\sigma$. This observation suggests that instead of seeking the optimal positions of MQM, it would be more straightforward to work with some general positions and find an explicit expression of the second term $D_s^{(2)}$. Notice in Eq. (6) one has to either numerically compute the

derivative of order parameters $d_\mu \Delta_\alpha^I$ (a short-hand notation of $d \Delta_{\mathbf{q},\alpha}^I / d q_\mu |_{\mathbf{q}=0}$) or vary the first term $D_s^{(1)}$ with respect to orbital positions to achieve MQM, both of which may require a large number of calculations.

In this section, we derive an explicit expression of the Hessian matrix $\partial^2 \Omega / \partial \Delta_\alpha^I \partial \Delta_\beta^I$ (similarly, it denotes $\partial^2 \Omega / \partial \Delta_{\mathbf{q},\alpha}^I \partial \Delta_{\mathbf{q},\beta}^I |_{\mathbf{q}=0}$) in Eq. (6) for general composite bands. It also contains an analysis of its rank and semidefiniteness, which allows us to write $D_s^{(2)}$ in a convenient form in Sec. V.

Before we proceed, it is essential to clarify and distinguish between geometry-independent and -dependent quantities [63]. Electronic band energies and topological properties, such as Chern numbers, are determined by the hopping integrals $t_{ij,\alpha\beta}^\sigma$, therefore they are geometry-independent. Geometry-dependent quantities, like the quantum metric and Berry curvature, instead depend on the orbital positions. Following Ref. [63], we adopt the convention that the atomic orbitals are pointlike, therefore the periodic part of the Bloch function, $u_{l\mathbf{k}}$, depends on the orbital positions through a componentwise phase, $u_{l\mathbf{k}\alpha} = e^{-i\mathbf{k}\cdot\mathbf{x}_\alpha} u_{l\mathbf{k}\alpha}^0$. Here $u_{l\mathbf{k}\alpha}^0$ are the Bloch components of gauge choice at some arbitrary reference positions in the unit cell, and \mathbf{x}_α are the orbital positions measured from these reference points. This explains the origin of the geometric dependence of $D_s^{(1)}$, Eq. (9).

According to the spirit of Ref. [31], the MQM can be defined in two ways, which are precisely given below:

Definition 1. MQM corresponds to the orbital positions that make the second term of Eq. (6), $D_s^{(2)}$, vanish.

Definition 2. MQM corresponds to the orbital positions that extremize (in fact, minimize) some geometric functional of the quantum metric tensor, which in general takes the form

$$I = \sum_{\mathbf{k}} \left[\sum_{l \in \mathcal{C}} f_l(\mathbf{k}) \text{Tr} g^l(\mathbf{k}) + \sum_{l, l' \in \mathcal{C}, l \neq l'} f_{ll'}(\mathbf{k}) \text{Tr} g^{ll'}(\mathbf{k}) \right]. \quad (20)$$

I is a function of orbital positions $\mathbf{x}_1, \dots, \mathbf{x}_s$ because the quantum metrics $g_{\mu\nu}^l(\mathbf{k})$, $g_{\mu\nu}^{ll'}(\mathbf{k})$ depend on them explicitly. $f_l(\mathbf{k})$ and $f_{ll'}(\mathbf{k})$ are a set of intra- and interband geometry-independent functions. For finite-temperature SW calculations, they are

$$f_l(\mathbf{k}) = \frac{1}{E_{l\mathbf{k}}} \tanh \frac{\beta E_{l\mathbf{k}}}{2}, \quad (21)$$

$$f_{ll'}(\mathbf{k}) = \left[\frac{2p_{ll'}^{(+)}(\mathbf{k})}{E_{l\mathbf{k}} + E_{l'\mathbf{k}}} + \frac{2p_{ll'}^{(-)}(\mathbf{k})}{E_{l\mathbf{k}} - E_{l'\mathbf{k}}} \right] \tanh \frac{\beta E_{l\mathbf{k}}}{2}, \quad (22)$$

such that the functional I is proportional to the trace of the geometric part of $D_s^{(1)}$. Notice that the quasiparticle energy and coherence factors depend on the band energy only, therefore they are geometry-independent.

The equivalence of the two definitions above relies on an assumption made in Ref. [31] about the rank and semidefiniteness of matrix $\partial^2 \Omega / \partial \Delta_\alpha^I \partial \Delta_\beta^I$ (see Appendix H). Below, we prove this assumption by computing the matrix explicitly.

It was argued in Ref. [31] that the order parameter minimizes the superconducting free energy. Therefore, the matrix $\partial^2 \Omega / \partial \Delta_\alpha^I \partial \Delta_\beta^I$ has to be positive semidefinite. However, this statement may not be true for a general pairing matrix $\hat{\Delta}$ as a solution to the gap equation of multiorbital superconductors.

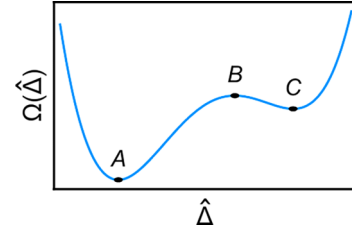


FIG. 3. Schematic plot of the grand potential in the space of components of $\hat{\Delta}$, at $\mathbf{q} = \mathbf{0}$. Multiorbital superconductors may have multiple solution channels, A, B, C , etc., to some fixed interaction parameters. A solution channel $\hat{\Delta}$ satisfies the gap equation $\partial \Omega / \partial \hat{\Delta} = 0$, so it extremizes Ω , but the minimization is not guaranteed. A ground-state channel (point A) ensures the global minimum, but there may also exist “unstable” solutions (e.g., point B). This instability is irrelevant to convergence for numerically solving the gap equation.

As a solution channel, it guarantees that the first derivative of grand potential Ω with respect to $\hat{\Delta}$ is zero (see Appendix B), but in general it cannot imply information about the second derivative. The second derivative instead is related to the “stability” of the channel.

A multiorbital superconductor can have multiple channels that are solutions to some fixed interaction parameters, an example of which can be seen in the supplementary material of Ref. [58]. If some channel corresponds to the superconducting ground state, it should be the global minimum of free energy. Therefore, its Hessian matrix needs to be positive semidefinite (Fig. 3). However, for solutions that are not the ground state, the Hessian matrix may not be positive semidefinite. For instance, in Appendix J we show that for two-orbital models when the order parameter matrix takes the form $\hat{\Delta} = \text{diag}\{\Delta_1, \Delta_2\}$ with Δ_1, Δ_2 both real, $\partial^2 \Omega / \partial \Delta_\alpha^I \partial \Delta_\beta^I$ is positive semidefinite if and only if $\text{sgn}(\Delta_1 \Delta_2) = 1$. For this reason, obtaining an explicit expression of this matrix for the uniform pairing channel is necessary. To achieve this goal, we study the gap equation for composite bands at finite \mathbf{q} and extract the Hessian matrix from its derivative with respect to \mathbf{q} .

Let us define the finite- \mathbf{q} mean-field order parameter as

$$\Delta_{\mathbf{q},\alpha} = -U_\alpha \langle c_{i\alpha\downarrow} c_{i\alpha\uparrow} \rangle_{\mathbf{q}} e^{-2i\mathbf{q}\cdot(\mathbf{R}_i + \mathbf{x}_\alpha)}, \quad (23)$$

where $\langle \rangle_{\mathbf{q}}$ is the average over the fluctuated pairing state $\Psi_{\mathbf{q}}$, and the phase factor $e^{-2i\mathbf{q}\cdot(\mathbf{R}_i + \mathbf{x}_\alpha)}$ gets rid of the superficial \mathbf{q} -dependence from $\Delta_{\mathbf{q},\alpha}$. Taking the total derivative of Eq. (23) with respect to q_μ at $\mathbf{q} = \mathbf{0}$, it yields a matrix equation [30,31]

$$M_{\alpha\beta} d_\mu \Delta_\beta = V_{\alpha,\mu}, \quad (24)$$

where $d_\mu \Delta_\alpha = i d_\mu \Delta_\alpha^I$ by TRS. After choosing a proportional constant, it is easy to show that (see Appendix C)

$$M_{\alpha\beta} = \frac{1}{2} \frac{\partial^2 \Omega}{\partial \Delta_{\mathbf{q},\alpha}^I \partial \Delta_{\mathbf{q},\beta}^I} \Big|_{\mathbf{q}=\mathbf{0}}, \quad (25)$$

$$V_{\alpha,\mu} = - \frac{\partial^2 \Omega}{\partial \Delta_{\mathbf{q},\alpha}^* \partial q_\mu} \Big|_{\mathbf{q}=\mathbf{0}}, \quad (26)$$

so the problem of computing matrix $\partial^2 \Omega / \partial \Delta_\alpha^I \partial \Delta_\beta^I$ is reduced to determining the gap equation (23).

For example, the zero-temperature gap equation for a single isolated band m can be expressed as [58]

$$\Delta_{\mathbf{q},\alpha} = \frac{U_\alpha}{N} \sum_{\mathbf{k}} u_{m,\mathbf{k}-\mathbf{q},\alpha}^* u_{m,\mathbf{k}+\mathbf{q},\alpha} \times \frac{\Delta_{m,\mathbf{k}}(\mathbf{q})}{\sqrt{(\xi_{m,\mathbf{k}+\mathbf{q}} + \xi_{m,\mathbf{k}-\mathbf{q}})^2 + 4|\Delta_{m,\mathbf{k}}(\mathbf{q})|^2}}, \quad (27)$$

from which the derivative can be easily calculated. Here $\Delta_{m,\mathbf{k}}(\mathbf{q}) = \langle u_{m,\mathbf{k}+\mathbf{q}} | \hat{\Delta}_{\mathbf{q}} | u_{m,\mathbf{k}-\mathbf{q}} \rangle$ is the projected intraband gap function. Unfortunately, for general composite bands, a closed form like Eq. (27) does not exist since one needs to diagonalize the $2n$ -dim mean-field Hamiltonian Eq. (7) to get the

pairing state $\Psi_{\mathbf{q}}$. However, the perturbation method allows us to expand $\Psi_{\mathbf{q}}$ and the gap equation in powers of \mathbf{q} . Thus, Eq. (24) as its first derivative can be exactly calculated.

To proceed, we transform the gap equation (23) from orbital to band basis and project to the composite, reading

$$\Delta_{\mathbf{q},\alpha} = -\frac{U_\alpha}{N} \sum_{\mathbf{k}} \sum_{l,l' \in \mathcal{C}} u_{l',\mathbf{k}-\mathbf{q},\alpha}^* u_{l,\mathbf{k}+\mathbf{q},\alpha} \langle c_{l',-\mathbf{k}+\mathbf{q}\downarrow} c_{l,\mathbf{k}+\mathbf{q}\uparrow} \rangle_{\mathbf{q}}. \quad (28)$$

Then we use the standard perturbation method to calculate the pairing amplitude $\langle c_{l',-\mathbf{k}+\mathbf{q}\downarrow} c_{l,\mathbf{k}+\mathbf{q}\uparrow} \rangle_{\mathbf{q}}$ (see Appendix F). Taking the total derivative of Eq. (28) with q_μ , we finally obtain Eq. (24) with

$$M_{\alpha\beta} = \sum_{\mathbf{k}} \sum_{l \in \mathcal{C}} |u_{l\mathbf{k}\alpha}|^2 \delta_{\alpha\beta} \frac{\tanh(\beta E_{l\mathbf{k}}/2)}{2E_{l\mathbf{k}}} - \frac{1}{2} \sum_{\mathbf{k}} \sum_{l,l' \in \mathcal{C}} u_{l'\mathbf{k}\alpha}^* u_{l\mathbf{k}\alpha} u_{l\mathbf{k}\beta}^* u_{l'\mathbf{k}\beta} \times \left[\frac{p_{l'l'}^{(+)}(\mathbf{k})}{E_{l\mathbf{k}} + E_{l'\mathbf{k}}} \left(\tanh \frac{\beta E_{l\mathbf{k}}}{2} + \tanh \frac{\beta E_{l'\mathbf{k}}}{2} \right) + \frac{p_{l'l'}^{(-)}(\mathbf{k})}{E_{l\mathbf{k}} - E_{l'\mathbf{k}}} \left(\tanh \frac{\beta E_{l\mathbf{k}}}{2} - \tanh \frac{\beta E_{l'\mathbf{k}}}{2} \right) \right] \quad (29)$$

and

$$V_{\alpha,\mu} = \sum_{\mathbf{k}} \sum_{l \in \mathcal{C}} (u_{l\mathbf{k}\alpha}^* \partial_\mu u_{l\mathbf{k}\alpha} - \partial_\mu u_{l\mathbf{k}\alpha}^* u_{l\mathbf{k}\alpha}) \frac{\Delta}{2E_{l\mathbf{k}}} \tanh \frac{\beta E_{l\mathbf{k}}}{2} - \sum_{\mathbf{k}} \sum_{l,l' \in \mathcal{C}} u_{l'\mathbf{k}\alpha}^* u_{l\mathbf{k}\alpha} \langle u_{l\mathbf{k}} | \partial_\mu u_{l'\mathbf{k}} \rangle \times \left[\frac{\Delta p_{l'l'}^{(+)}(\mathbf{k})}{E_{l\mathbf{k}} + E_{l'\mathbf{k}}} \left(\tanh \frac{\beta E_{l\mathbf{k}}}{2} + \tanh \frac{\beta E_{l'\mathbf{k}}}{2} \right) + \frac{\Delta p_{l'l'}^{(-)}(\mathbf{k})}{E_{l\mathbf{k}} - E_{l'\mathbf{k}}} \left(\tanh \frac{\beta E_{l\mathbf{k}}}{2} - \tanh \frac{\beta E_{l'\mathbf{k}}}{2} \right) \right]. \quad (30)$$

Although matrix $M_{\alpha\beta}$ and vector $V_{\alpha,\mu}$ take a complicated form, they have some simple properties we shall discuss now. We assume that the composite \mathcal{C} contains all the s orbitals of the lattice model; therefore, $M_{\alpha\beta}$ is an s -dim square matrix. This assumption may not hold for some exceptional cases, e.g., the atomic limit of the single-band projection of two-orbital models (Appendix I) and the isolated flat-band limit of the Lieb lattice, which will be discussed in Sec. V.

From Eqs. (29) and (30) above, one first notices that $M_{\alpha\beta}$ is a real symmetric matrix, while $V_{\alpha,\mu}$ is a purely imaginary vector. Moreover, $M_{\alpha\beta}$ contains factors $|u_{l\mathbf{k}\alpha}|^2$, $u_{l'\mathbf{k}\alpha}^* u_{l\mathbf{k}\alpha}$, and quasiparticle energy $E_{l\mathbf{k}}$, which are all geometry-independent quantities, therefore it is geometry-independent, whereas $V_{\alpha,\mu}$ is geometry-dependent. These properties are all governed by Eq. (24).

One can also notice that $M_{\alpha\beta}$ of Eq. (29) is not invertible, since $\sum_{\beta=1}^s M_{\alpha\beta} = 0$ (similarly, $\sum_{\alpha=1}^s V_{\alpha,\mu} = 0$), which implies that it has an eigenvector $\mathbf{v}_0 = (1, 1, \dots, 1)^T$ with eigenvalue zero. Physically, this is associated with the $U(1)$ symmetry of the order parameter. The existence of such a kernel vector implies that the rank of $M_{\alpha\beta}$ cannot exceed $s - 1$. In general, one can prove that under the UPC if the composite bands contain all the s orbitals, then $\text{Rank}(M) = s - 1$. We prove this for two special cases in Appendix G.

Nevertheless, one can imagine a process in which some orbitals are removed from the composite, which may arise from topological phase transitions or changes in the interaction scale. Whenever an r th orbital is removed ($1 \leq r \leq s$), $\mathbf{e}_r = (\dots, 0, 1, 0, \dots)^T$ (with the r th component nonzero only) becomes an additional kernel vector of $M_{\alpha\beta}$, lowering

$\text{Rank}(M)$ by 1. The reason is that the physics will no longer depend on its position as the r th orbital becomes irrelevant to the composite.

In addition, one can show that $M_{\alpha\beta}$ is positive semidefinite, which means it has one zero eigenvalue and $s - 1$ positive eigenvalues (see Appendix G). This vital property, as a consequence of UPC, reveals that the uniform pairing channel belongs to these ‘‘stable’’ solutions to the gap equation like points A and C in Fig. 3.

V. GEOMETRY INDEPENDENCE AND THE LATTICE GEOMETRIC TERM IN TERMS OF BLOCH FUNCTIONS

With the expression of matrix $M_{\alpha\beta}$ and vector $V_{\alpha,\mu}$, it is not difficult to show that each component of the SW tensor is geometry-independent. For this, we write the second term of Eq. (6) as

$$D_{s,\mu\nu}^{(2)} = 2M_{\alpha\beta} d_\mu \Delta_\alpha d_\nu \Delta_\beta, \quad (31)$$

where $d_\mu \Delta_\alpha = id_\mu \Delta_\alpha^l$. Under a geometric transformation that translates orbital positions from \mathbf{x}_α^0 to $\mathbf{x}_\alpha = \mathbf{x}_\alpha^0 + \delta \mathbf{x}_\alpha$ [74], it is changed by

$$\delta D_{s,\mu\nu}^{(2)} = 2M_{\alpha\beta} (\delta d_\mu \Delta_\alpha d_\nu \Delta_\beta^0 + d_\mu \Delta_\alpha^0 \delta d_\nu \Delta_\beta + \delta d_\mu \Delta_\alpha \delta d_\nu \Delta_\beta), \quad (32)$$

where $d_\mu \Delta_\alpha^0$ is $d_\mu \Delta_\alpha$ evaluated at the initial positions and $\delta d_\mu \Delta_\alpha^0$ is the change due to such a transformation. Equation (32) can be further simplified using Eq. (H8) in Appendix H. Similarly, the change of the quantum geometric

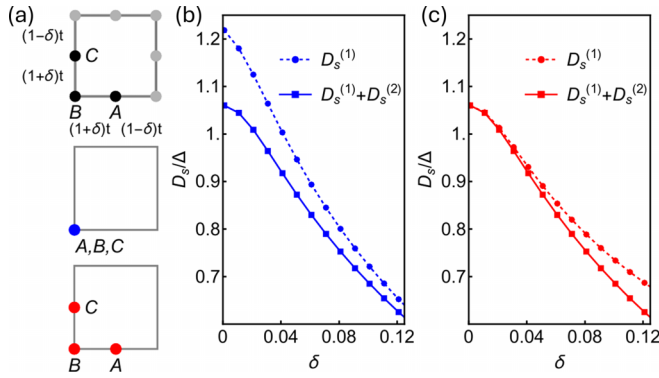


FIG. 4. SW calculation of the Lieb lattice model. (a) The gray square indicates the unit cell of the Lieb lattice and the three orbitals A, B, C . Top: the tight-binding hoppings can be tuned to $(1 \pm \delta)t$ to open a gap $2\sqrt{2}t\delta$ between the flat and dispersive bands. Middle: lattice geometry assuming the three orbitals sitting on the same site. Bottom: assuming the orbitals sitting on the regular sites of the Lieb lattice. (b),(c) SW computed using Eqs. (9) and (35) at $T = 0$, $t/\Delta = 10$, $\mu = 0$. Part (b) assumes the geometry of (a), middle while (c) assumes the geometry of (a), bottom.

term of SW, $\delta D_s^{(1)}$, can be evaluated by inserting Eq. (H2) into Eq. (9). Then, one can immediately check the geometry independence of the total SW,

$$\delta D_s = \delta D_s^{(1)} + \delta D_s^{(2)} = 0, \quad (33)$$

therefore we have finished establishing the relation between SW and lattice geometry.

As mentioned at the beginning of Sec. IV, a shortcoming of Eq. (6) to compute the SW is that one needs to either solve the gap equation at a few \mathbf{q} points to get the derivative $d_\mu \Delta_\alpha$, or vary the orbital positions in the whole geometric space to find the MQM positions. However, since we have treated the gap equation perturbatively to get Eqs. (29) and (30), the total SW can be computed using simple integrals of Bloch functions and their derivatives without following these procedures.

In fact, as pointed out in Refs. [30,31], once we are convinced that $\text{Rank}(M) = s - 1$, it would be convenient to partially project [75] the matrix $M_{\alpha\beta}$, vector $V_{\alpha,\mu}$, and $d_\mu \Delta_\alpha$ into an $(s - 1)$ -dim subspace, in which the matrix M becomes invertible, so one can write

$$\widetilde{d}_\mu \widetilde{\Delta}_\alpha = (\widetilde{M}^{-1})_{\alpha\beta} \widetilde{V}_{\beta,\mu}, \quad (34)$$

where a tilde denotes the projected quantities. This finally yields a simple expression for the lattice geometric term:

$$D_{s,\mu\nu}^{(2)} = 2(\widetilde{M}^{-1})_{\alpha\beta} \widetilde{V}_{\alpha,\mu} \widetilde{V}_{\beta,\nu}. \quad (35)$$

In this expression, the projected \widetilde{M} and \widetilde{V} are not unique but can be taken as eliminating the first row and column from matrix M and eliminating the first component from vector V in Eqs. (29) and (30). This corresponds to restricting to the geometric space spanned by the $s - 1$ orbitals.

To show the utility of Eq. (35), we take the Lieb lattice model [17,31] as an example. A unit cell of the Lieb lattice is shown at the top of Fig. 4(a), where parameters t and δ completely determine the tight-binding matrix elements. Remember that the hopping graph does not specify the positions

of orbital A, B , and C , which leaves the degree of freedom for writing the Bloch Hamiltonian $h_{\mathbf{k}}^c$. Since the hopping integrals are usually defined from a given lattice structure, in this case one can still imagine the underlying Bravais lattice as a square lattice with C_{4v} symmetry.

When $\delta \neq 0$, the hopping graph breaks C_4 symmetry, making the tight-binding model acquire a lower symmetry than the imagined square lattice. Then it was found that the optimal positions of MQM of atoms A and C no longer sit at the midpoint of the side but shift towards the B atom [31]. As a contrast, in our calculations using Eqs. (9) and (35), we can place the orbitals at any general positions in the unit cell. In Fig. 4(b), we imagine the three orbitals sitting on the same site, while Fig. 4(c) assumes they are sitting on the regular sites of the Lieb lattice. Since we make no approximations and take into account all the interband and lattice geometric effects, the total SW data of the two geometries [two solid curves in (b) and (c)] completely match, showing the geometry independence of the SW. One also notices that in Fig. 4(b) the $D_s^{(1)}$ curve converges to $D_s^{(1)} + D_s^{(2)}$ in the large δ limit, whereas in Fig. 4(c) they converge in the $\delta = 0$ limit. This exhibits how the actual MQM geometry approaches the two geometries in the two limits.

Finally, we address two possible issues of applying Eq. (35) for numerical calculations. The first regards the definition of composite for the Lieb lattice. For most parameter ranges, one can take all three bands of the Lieb lattice as the composite, which contains three orbitals; then matrix \widetilde{M} and vector \widetilde{V} are 2-dim. However, in the isolated flat-band limit, $\mu \sim 0$ and $\Delta \ll t\delta$, the composite effectively contains just the flat band, which comprises only two orbitals. Then as $\text{Rank}(M)$ is lowered to 1, we need to project M to a 1-dim subspace to make \widetilde{M} invertible. This gives a 1-dim matrix \widetilde{M} and vector \widetilde{V} , which means for Eqs. (29) and (30) we only need to evaluate the integral for orbital A or C .

The second is about the differentiability of Bloch functions in calculating vector $V_{\alpha,\mu}$. For systems with nontrivial topology, the Bloch functions may not be differentiable everywhere in the momentum space. Although the derivative of Bloch functions can be locally singular in some cases, one can argue on general grounds that the lattice geometric term $D_s^{(2)}$ is finite. Since the total SW $D_s^{(1)} + D_s^{(2)}$ is geometry-independent and positive finite under the UPC, it implies that $D_s^{(2)}$ is bounded: $-D_s^{(1)} < D_s^{(2)} < 0$. Here, we have used the fact that $D_s^{(1)}$, which contains integrals of the quantum metric, is always finite, which can be understood from two generic cases. For gapped insulating states, the interband quantum metric can be written in terms of velocity operators, $\langle u_{l\mathbf{k}} | \partial_\mu u_{l\mathbf{k}} \rangle = \langle u_{l\mathbf{k}} | \partial_\mu h_{\mathbf{k}} | u_{l\mathbf{k}} \rangle / (E_{l\mathbf{k}} - E_{l\mathbf{k}})$. Therefore, the derivatives are shifted to the Bloch Hamiltonian, usually a continuous and smooth function of \mathbf{k} . In the case of a band degeneracy, the quantum metric can diverge, giving a $1/k^2$ divergence near the isolated band degeneracy points, leading to a logarithmic divergence of the intraband contributions to $D_s^{(1)}$. However, this divergence is canceled by the inter-band geometric contributions due to the reduction effect, giving a finite total $D_s^{(1)}$ [76]. In summary, even though the nondifferentiability of Bloch functions may cause singularities at some local \mathbf{k} -points, it does not affect the numerical convergence for calculations of both $D_s^{(1)}$ and $D_s^{(2)}$.

VI. CONCLUSION AND OUTLOOK

We developed a perturbation approach to treat multiorbital superconductors' center-of-mass momentum (phase) fluctuation. This approach naturally separates the superfluid weight of composite bands into intra- and interband contributions from Bogoliubov band transitions. Based on the reduction by the interband geometric terms, a topological lower bound was derived for the superfluid weight of isolated composite flat bands. Applying the theory of band representation, we found that the elementary band representations should be considered the minimum "block" for deriving a stronger lower bound.

In studying the geometry independence of the superfluid weight, we emphasized the role of the derivative of gap equations in getting the Hessian matrix $\partial^2 \Omega / \partial \Delta_\alpha^l \partial \Delta_\beta^l$. The perturbation method facilitated the calculation as we expanded the gap equation in powers of \mathbf{q} . We analyzed the properties of this Hessian matrix in detail and showed how the positive semidefiniteness and rank information stem from the uniform pairing condition. We finally rewrote the superfluid weight formula into a convenient form suitable for numerical calculations of any general tight-binding model.

Since the superfluid weight is the stiffness of the Meissner effect, it naturally encodes the information about fluctuation to a finite-momentum pairing state within a given channel. Still, there is little information about competition between superconducting channels and other correlated states [77,78]. However, as pointed out, the Hessian matrix of the grand potential with respect to order parameters can be nonpositive definite for multiorbital superconductors, and it contains information about the stability of the channel. Whether this allows one to determine the ground state is left to future studies.

Note added. During the review process, we became aware of Ref. [79], which discusses the geometry independence of the superfluid weight for degenerate flat bands using the random phase approximation. On topics in which there is an overlap, our findings are consistent with theirs.

ACKNOWLEDGMENTS

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$$\begin{aligned} \hat{\mathcal{H}}_{\text{kin}} &= \sum_{\mathbf{k}, \alpha \beta} [c_{\mathbf{k}\alpha\uparrow}^\dagger (h_{\mathbf{k}}^\uparrow)_{\alpha\beta} c_{\mathbf{k}\beta\uparrow} + c_{-\mathbf{k}, \alpha\downarrow}^\dagger (h_{-\mathbf{k}}^\downarrow)_{\alpha\beta} c_{-\mathbf{k}, \beta\downarrow}] - \mu_{\mathbf{q}} \sum_{\mathbf{k}, \alpha} (c_{\mathbf{k}\alpha\uparrow}^\dagger c_{\mathbf{k}\alpha\uparrow} + c_{-\mathbf{k}, \alpha\downarrow}^\dagger c_{-\mathbf{k}, \alpha\downarrow}) \\ &= \sum_{\mathbf{k}, \alpha \beta} \{c_{\mathbf{k}+\mathbf{q}, \alpha\uparrow}^\dagger [(h_{\mathbf{k}+\mathbf{q}}^\uparrow)_{\alpha\beta} - \mu_{\mathbf{q}} \delta_{\alpha\beta}] c_{\mathbf{k}+\mathbf{q}, \beta\uparrow} - c_{-\mathbf{k}+\mathbf{q}, \alpha\downarrow}^\dagger [(h_{-\mathbf{k}+\mathbf{q}}^{\downarrow, T})_{\alpha\beta} - \mu_{\mathbf{q}} \delta_{\alpha\beta}] c_{-\mathbf{k}+\mathbf{q}, \beta\downarrow}\} + \sum_{\mathbf{k}} \text{Tr}\{h_{-\mathbf{k}+\mathbf{q}}^\downarrow - \mu_{\mathbf{q}}\}. \end{aligned} \quad (\text{A6})$$

In the last line above, $\sum_{\mathbf{k}} \text{Tr} h_{-\mathbf{k}+\mathbf{q}}^\downarrow = \sum_{l, \mathbf{k}} \varepsilon_{l, -\mathbf{k}+\mathbf{q}}^\downarrow$ is \mathbf{q} -independent because \mathbf{k} is summed over the entire Brillouin zone, whereas $\sum_{\mathbf{k}} \text{Tr} \mu_{\mathbf{q}} = \mu_{\mathbf{q}} s N$ with N the number of unit cells. Equations (A5) and (A6) together give Eq. (2).

APPENDIX A: INTERACTING HAMILTONIAN WITH CENTER-OF-MASS MOMENTUM FLUCTUATION

By the transformation $c_{i\alpha\sigma} = (1/\sqrt{N}) \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}_i + \mathbf{x}_\alpha)} c_{\mathbf{k}\alpha\sigma}$ (we chose this gauge for $c_{\mathbf{k}\alpha\sigma}$ if not otherwise specified), the on-site intraorbital interaction takes the form

$$\begin{aligned} \hat{\mathcal{H}}_{\text{int}} &= - \sum_{i, \alpha} U_\alpha c_{i\alpha\uparrow}^\dagger c_{i\alpha\downarrow}^\dagger c_{i\alpha\downarrow} c_{i\alpha\uparrow} \\ &= - \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}, \alpha} \frac{U_\alpha}{N} c_{\mathbf{k}+\mathbf{q}, \alpha\uparrow}^\dagger c_{-\mathbf{k}+\mathbf{q}, \alpha\downarrow}^\dagger c_{-\mathbf{k}'+\mathbf{q}, \alpha\downarrow} c_{\mathbf{k}'+\mathbf{q}, \alpha\uparrow}. \end{aligned} \quad (\text{A1})$$

The conventional BCS theory makes the ansatz that electron $\mathbf{k} \uparrow$ pairs with $-\mathbf{k} \downarrow$, therefore the reduced interaction $\hat{\mathcal{H}}_{\text{int}}^{(\text{red})}$ only keeps the $\mathbf{q} = \mathbf{0}$ term from above.

We now consider a pairing state of fluctuated CMM $2\mathbf{q}$ (i.e., phase fluctuation), so the reduced interaction keeps a term of fixed and finite \mathbf{q} , reading

$$\hat{\mathcal{H}}_{\text{int}}^{(\text{red})}(\mathbf{q}) = - \sum_{\mathbf{k}\mathbf{k}', \alpha} \frac{U_\alpha}{N} c_{\mathbf{k}+\mathbf{q}, \alpha\uparrow}^\dagger c_{-\mathbf{k}+\mathbf{q}, \alpha\downarrow}^\dagger c_{-\mathbf{k}'+\mathbf{q}, \alpha\downarrow} c_{\mathbf{k}'+\mathbf{q}, \alpha\uparrow}. \quad (\text{A2})$$

This form of interaction implies that in the fluctuated state electron $\mathbf{k} + \mathbf{q}, \uparrow$ pairs with $-\mathbf{k} + \mathbf{q}, \downarrow$. With the order parameter $\Delta_{\mathbf{q}, \alpha}$ defined by Eq. (23), Fourier transform gives

$$\Delta_{\mathbf{q}, \alpha} = - \frac{U_\alpha}{N} \sum_{\mathbf{k}} \langle c_{-\mathbf{k}+\mathbf{q}, \alpha\downarrow} c_{\mathbf{k}+\mathbf{q}, \alpha\uparrow} \rangle_{\mathbf{q}}. \quad (\text{A3})$$

To get Eq. (A3), we have used the fact that in the fluctuated state $\Psi_{\mathbf{q}}$ the electron $\mathbf{k} + \mathbf{q}, \uparrow$ pairs with $-\mathbf{k} + \mathbf{q}, \downarrow$. Using the transformation between orbital and band basis

$$c_{\mathbf{k}\alpha\uparrow} = \sum_l u_{l\mathbf{k}\alpha} c_{l\mathbf{k}\uparrow}, \quad c_{-\mathbf{k}, \alpha\downarrow} = \sum_l u_{l\mathbf{k}\alpha}^* c_{l, -\mathbf{k}\downarrow}, \quad (\text{A4})$$

one obtains Eq. (28) (the sum over l has been restricted to the composite due to projection).

With (A3), mean-field decoupling yields

$$\begin{aligned} \hat{\mathcal{H}}_{\text{int}}^{(\text{red})}(\mathbf{q}) &\simeq \sum_{\mathbf{k}, \alpha} (\Delta_{\mathbf{q}, \alpha} c_{\mathbf{k}+\mathbf{q}, \alpha\uparrow}^\dagger c_{-\mathbf{k}+\mathbf{q}, \alpha\downarrow}^\dagger + \text{H.c.}) \\ &\quad + N \sum_{\alpha=1}^s \frac{|\Delta_{\mathbf{q}, \alpha}|^2}{U_\alpha}. \end{aligned} \quad (\text{A5})$$

For the kinetic part, we shift the dummy momentum \mathbf{k} by $\pm\mathbf{q}$ for the spin- \uparrow, \downarrow sector, respectively,

APPENDIX B: SELF-CONSISTENCY EQUATIONS

For completeness, we derive the gap equation and electron number equation, and we study their properties under TRS, which is similar to Ref. [16]. With the grand potential Eq. (5),

we first derive the gap equation

$$\frac{\partial \Omega}{\partial \Delta_{\mathbf{q},\alpha}^*} = 0, \quad \forall \mathbf{q}, \alpha. \quad (\text{B1})$$

Using Eq. (2),

$$\begin{aligned} \frac{\partial \Omega}{\partial \Delta_{\mathbf{q},\alpha}^*} &= \frac{\text{Tr}\{e^{-\beta \hat{\mathcal{H}}_{MF}(\mathbf{q})} \sum_{\mathbf{k}} c_{-\mathbf{k}+\mathbf{q},\alpha\downarrow} c_{\mathbf{k}+\mathbf{q},\alpha\uparrow}\}}{\text{Tr}\{e^{-\beta \hat{\mathcal{H}}_{MF}(\mathbf{q})}\}} + \frac{N}{U_\alpha} \Delta_{\mathbf{q},\alpha} \\ &= \sum_{\mathbf{k}} \langle c_{-\mathbf{k}+\mathbf{q},\alpha\downarrow} c_{\mathbf{k}+\mathbf{q},\alpha\uparrow} \rangle_{\mathbf{q}} + \frac{N}{U_\alpha} \Delta_{\mathbf{q},\alpha}. \end{aligned} \quad (\text{B2})$$

This cancels by the definition of order parameter (A3); therefore, (B1) is proved.

Next, we look at the electron number equation:

$$\frac{\partial \Omega}{\partial \mu_{\mathbf{q}}} = -N_e, \quad \forall \mathbf{q}, \quad (\text{B3})$$

where the fixed average number of electrons N_e is a constraint for the system; condition $\forall \mathbf{q}$ means when we compare the fluctuated state $\Psi_{\mathbf{q}}$ of different \mathbf{q} , N_e is always fixed at the same value. Using Eq. (2) again, one obtains

$$\frac{\partial \Omega}{\partial \mu_{\mathbf{q}}} = -\frac{\text{Tr}\{e^{-\beta \hat{\mathcal{H}}_{MF}(\mathbf{q})} \sum_{\mathbf{k}\alpha\sigma} c_{\mathbf{k}\alpha\sigma}^\dagger c_{\mathbf{k}\alpha\sigma}\}}{\text{Tr}\{e^{-\beta \hat{\mathcal{H}}_{MF}(\mathbf{q})}\}}, \quad (\text{B4})$$

therefore Eq. (B3) is just

$$N_e = \sum_{\mathbf{k}\alpha\sigma} \langle c_{\mathbf{k}\alpha\sigma}^\dagger c_{\mathbf{k}\alpha\sigma} \rangle_{\mathbf{q}}. \quad (\text{B5})$$

The two self-consistency equations (A3) and (B5) determine all the properties of the fluctuated state $\Psi_{\mathbf{q}}$, and one can solve them for $\hat{\Delta}_{\mathbf{q}}, \mu_{\mathbf{q}}$. In the presence of TRS, one can show that whenever $\{\hat{\Delta}_{\mathbf{q}}, \mu_{\mathbf{q}}\}$ is a solution to the self-consistency equations of \mathbf{q} state, then $\{\hat{\Delta}_{-\mathbf{q}}, \mu_{-\mathbf{q}}\}$ is a solution to the equations for $-\mathbf{q}$ state (the single isolated band case was proved in Ref. [58]). Then for the case of diagonal $\hat{\Delta}_{\mathbf{q}}$ matrix, $\Delta_{-\mathbf{q},\alpha} = \Delta_{\mathbf{q},\alpha}^*$ and $\mu_{-\mathbf{q}} = \mu_{\mathbf{q}}$, so there are the following identities:

$$\left. \frac{d\mu_{\mathbf{q}}}{dq_\mu} \right|_{\mathbf{q}=\mathbf{0}} = 0, \quad (\text{B6})$$

$$\left. \frac{d\Delta_{\mathbf{q},\alpha}}{dq_\mu} \right|_{\mathbf{q}=\mathbf{0}} = -\left. \frac{d\Delta_{\mathbf{q},\alpha}^*}{dq_\mu} \right|_{\mathbf{q}=\mathbf{0}} = i \left. \frac{d\Delta_{\mathbf{q},\alpha}^I}{dq_\mu} \right|_{\mathbf{q}=\mathbf{0}}, \quad (\text{B7})$$

where $\Delta_{\mathbf{q},\alpha}^I$ is the imaginary part of $\Delta_{\mathbf{q},\alpha}$. The importance of TRS will be discussed further in Appendix C.

APPENDIX C: SUPERFLUID WEIGHT FORMULA, DERIVATIVE OF THE GAP EQUATION, AND TIME-REVERSAL SYMMETRY

In this Appendix, we derive the SW formula Eq. (6). We treat the free energy $F(\mathbf{q})$ as a function of \mathbf{q} only, while $\Omega(\mathbf{q}, \mu_{\mathbf{q}}, \Delta_{\mathbf{q},\alpha}, \Delta_{\mathbf{q},\alpha}^*)$ is a function of $\mathbf{q}, \mu_{\mathbf{q}}, \Delta_{\mathbf{q},\alpha}, \Delta_{\mathbf{q},\alpha}^*$ explicitly.

Using $F(\mathbf{q}) = \Omega(\mathbf{q}, \mu_{\mathbf{q}}, \Delta_{\mathbf{q},\alpha}, \Delta_{\mathbf{q},\alpha}^*) + \mu_{\mathbf{q}} N_e$, we have the first derivative

$$\begin{aligned} \frac{dF}{dq_\mu} &= \frac{\partial \Omega}{\partial q_\mu} + \left(\frac{\partial \Omega}{\partial \mu_{\mathbf{q}}} + N_e \right) \frac{d\mu_{\mathbf{q}}}{dq_\mu} \\ &+ \sum_{\alpha} \left(\frac{\partial \Omega}{\partial \Delta_{\mathbf{q},\alpha}} \frac{d\Delta_{\mathbf{q},\alpha}}{dq_\mu} + \text{c.c.} \right). \end{aligned} \quad (\text{C1})$$

The second term cancels by the electron number equation, and the third term cancels by the gap equation; therefore,

$$\frac{dF}{dq_\mu} = \frac{\partial \Omega}{\partial q_\mu}, \quad \forall \mathbf{q}. \quad (\text{C2})$$

An important consequence of TRS is that $F(\mathbf{q})$ is an even function of \mathbf{q} , so

$$\left. \frac{dF}{dq_\mu} \right|_{\mathbf{q}=\mathbf{0}} = \left. \frac{\partial \Omega}{\partial q_\mu} \right|_{\mathbf{q}=\mathbf{0}} = 0. \quad (\text{C3})$$

Caution is needed if one wants to prove this like Eqs. (B2) and (B4). The derivative should not act on $c_{\mathbf{k}+\mathbf{q},\uparrow}$ and $c_{-\mathbf{k}+\mathbf{q},\downarrow}$ operators since they form the Nambu basis. At the same time, the grand potential depends only on the eigenvalues of the BdG Hamiltonian. One can calculate $\partial \Omega / \partial q_\mu$ directly using an explicit form like Eq. (D5), and then show that Eq. (C3) holds as long as $\hat{\Delta}_{\mathbf{q}=\mathbf{0}}$ is a Hermitian matrix up to a $U(1)$ phase, which TRS imposes. The case of a single isolated band has been proved in Ref. [58]. If TRS is broken, SW being the second derivative of free energy at $\mathbf{q} = \mathbf{0}$ will lose its meaning as a stiffness tensor, since the first derivative of free energy is already nonzero.

In the presence of TRS, the second derivative of free energy is

$$\begin{aligned} \frac{d^2 F}{dq_\mu dq_\nu} &= \frac{\partial^2 \Omega}{\partial q_\mu \partial q_\nu} + \frac{\partial^2 \Omega}{\partial q_\mu \partial \mu_{\mathbf{q}}} \frac{d\mu_{\mathbf{q}}}{dq_\nu} \\ &+ \sum_{\alpha} \left(\frac{\partial^2 \Omega}{\partial q_\mu \partial \Delta_{\mathbf{q},\alpha}} \frac{d\Delta_{\mathbf{q},\alpha}}{dq_\nu} + \text{c.c.} \right). \end{aligned} \quad (\text{C4})$$

To simplify this, we take the total derivative of gap equation (B1) with respect to q_μ , yielding

$$\begin{aligned} \frac{\partial^2 \Omega}{\partial \Delta_{\mathbf{q},\alpha}^* \partial q_\mu} + \frac{\partial^2 \Omega}{\partial \Delta_{\mathbf{q},\alpha}^* \partial \mu_{\mathbf{q}}} \frac{d\mu_{\mathbf{q}}}{dq_\mu} \\ + \sum_{\beta} \left(\frac{\partial^2 \Omega}{\partial \Delta_{\mathbf{q},\alpha}^* \partial \Delta_{\mathbf{q},\beta}} \frac{d\Delta_{\mathbf{q},\beta}}{dq_\mu} + \text{c.c.} \right) = 0. \end{aligned} \quad (\text{C5})$$

Changing variables $\Delta_{\mathbf{q},\alpha}, \Delta_{\mathbf{q},\alpha}^* \rightarrow \Delta_{\mathbf{q},\alpha}^R, \Delta_{\mathbf{q},\alpha}^I$ ($\Delta_{\mathbf{q},\alpha} \equiv \Delta_{\mathbf{q},\alpha}^R + i\Delta_{\mathbf{q},\alpha}^I$), evaluating at $\mathbf{q} = \mathbf{0}$, and using TRS properties Eqs. (B6) and (B7), one can verify that $d^2 F / dq_\mu dq_\nu |_{\mathbf{q}=\mathbf{0}}$ gives the SW formula Eq. (6).

Moreover, Eq. (C5) at $\mathbf{q} = \mathbf{0}$ gives

$$\frac{1}{2} \left. \frac{\partial^2 \Omega}{\partial \Delta_{\mathbf{q},\alpha}^I \partial \Delta_{\mathbf{q},\beta}^I} \right|_{\mathbf{q}=\mathbf{0}} d_\mu \Delta_\beta + \left. \frac{\partial^2 \Omega}{\partial \Delta_{\mathbf{q},\alpha}^* \partial q_\mu} \right|_{\mathbf{q}=\mathbf{0}} = 0, \quad (\text{C6})$$

which exactly maps to $M_{\alpha\beta} d_\mu \Delta_\beta - V_{\alpha,\mu} = 0$ and the total derivative of Eq. (B2). Therefore, we get Eqs. (25) and (26) in the main text.

APPENDIX D: PERTURBATION APPROACH TO CALCULATE THE SUPERFLUID WEIGHT

In this Appendix, we provide the steps of using the perturbation method to calculate $D_s^{(1)}$, Eq. (9).

$$H_{\mathbf{k}}(\mathbf{q}) = \begin{pmatrix} \xi_{1,\mathbf{k}+\mathbf{q}} & \Delta_{1,\mathbf{k}}(\mathbf{q}) & & & & & & & & & \Delta_{1n,\mathbf{k}}(\mathbf{q}) \\ \Delta_{1,\mathbf{k}}(\mathbf{q})^* & -\xi_{1,\mathbf{k}-\mathbf{q}} & \Delta_{21,\mathbf{k}}(\mathbf{q})^* & & & & & & & & \\ & \Delta_{21,\mathbf{k}}(\mathbf{q}) & \xi_{2,\mathbf{k}+\mathbf{q}} & & & & & & & & \\ \Delta_{12,\mathbf{k}}(\mathbf{q})^* & & \Delta_{2,\mathbf{k}}(\mathbf{q})^* & & & & & & & & \\ \dots & \dots & & & & & & & & & \\ & & \Delta_{n1,\mathbf{k}}(\mathbf{q}) & & & & & & & & \\ \Delta_{1n,\mathbf{k}}(\mathbf{q})^* & & & & & & & & & & \xi_{n,\mathbf{k}+\mathbf{q}} & \Delta_{n,\mathbf{k}}(\mathbf{q}) \\ & & & & & & & & & & \Delta_{n,\mathbf{k}}(\mathbf{q})^* & -\xi_{n,\mathbf{k}-\mathbf{q}} \end{pmatrix}, \quad (\text{D1})$$

where the empty entries are zeros. To aid in bookkeeping, in $H_{\mathbf{k}}(\mathbf{q})$ we have assigned the $(2l-1)$ th label to electrons, and the $2l$ th label to holes of the l th band.

Let $\Lambda_{\mathbf{k}}(\mathbf{q})$ be some generalized Bogoliubov transformation that exactly diagonalizes $H_{\mathbf{k}}(\mathbf{q})$,

$$\Lambda_{\mathbf{k}}(\mathbf{q})^\dagger H_{\mathbf{k}}(\mathbf{q}) \Lambda_{\mathbf{k}}(\mathbf{q}) = \hat{E}_{\mathbf{k}}(\mathbf{q}). \quad (\text{D2})$$

Typically $\Lambda_{\mathbf{k}}(\mathbf{q})$ can only be determined numerically, and

$$\hat{E}_{\mathbf{k}}(\mathbf{q}) = \text{diag}\{E_{1\mathbf{k}+}(\mathbf{q}), E_{1\mathbf{k}-}(\mathbf{q}), \dots\} \quad (\text{D3})$$

is a diagonal matrix consisting of eigenvalues of $H_{\mathbf{k}}(\mathbf{q})$ (a caret is used to distinguish from a number). The $2n$ eigenvalues correspond to the n fluctuated Bogoliubov quasiparticle bands (+) and n quasihole bands (-). At $\mathbf{q} = \mathbf{0}$ the spectrum is particle-hole symmetric (PHS), $E_{l\mathbf{k}\pm}(0) = \pm\sqrt{\xi_{l\mathbf{k}}^2 + \Delta^2}$ (we also use symbol $E_{l\mathbf{k}}$ for $\sqrt{\xi_{l\mathbf{k}}^2 + \Delta^2}$).

After the diagonalization, $\hat{H}_{\mathcal{C}}(\mathbf{q})$ of Eq. (7) reads

$$\hat{H}_{\mathcal{C}}(\mathbf{q}) = \sum_{\mathbf{k}} \left[\tilde{\mathcal{Y}}_{\mathbf{k},\mathbf{q}}^\dagger \hat{E}_{\mathbf{k}}(\mathbf{q}) \tilde{\mathcal{Y}}_{\mathbf{k},\mathbf{q}} + \sum_{l \in \mathcal{C}} \xi_{l,-\mathbf{k}+\mathbf{q}}^\downarrow \right] + N \sum_{\alpha=1}^s \frac{|\Delta_{\mathbf{q},\alpha}|^2}{U_\alpha}, \quad (\text{D4})$$

where $\tilde{\mathcal{Y}}_{\mathbf{k},\mathbf{q}}$ is the Bogoliubov band spinor that exactly diagonalizes $H_{\mathbf{k}}(\mathbf{q})$. The projected grand potential is

$$\begin{aligned} \Omega_{\mathcal{C}} &= -\frac{1}{\beta} \ln \text{Tr} \{ e^{-\beta \hat{H}_{\mathcal{C}}(\mathbf{q})} \} \\ &= -\frac{1}{\beta} \sum_{\mathbf{k}} \text{Tr} \ln (1 + e^{-\beta \hat{E}_{\mathbf{k}}(\mathbf{q})}) + \sum_{\mathbf{k}} \sum_{l \in \mathcal{C}} \xi_{l,-\mathbf{k}+\mathbf{q}}^\downarrow \\ &\quad + N \sum_{\alpha=1}^s \frac{|\Delta_{\mathbf{q},\alpha}|^2}{U_\alpha}. \end{aligned} \quad (\text{D5})$$

1. Nondegenerate perturbation

Starting from the mean-field Hamiltonian projected to the composite bands, Eq. (7), the first and third terms can be organized into the $2n$ -dim BdG form

In $D_{s,\mu\nu}^{(1)} = \partial_\mu \partial_\nu \Omega_{\mathcal{C}}|_{\mathbf{q}=\mathbf{0}}$, the derivative acts on explicit \mathbf{q} only and does not act on $\mu_{\mathbf{q}}$ or $\hat{\Delta}_{\mathbf{q}}$, giving [16]

$$D_{s,\mu\nu}^{(1)} = -\frac{1}{2} \sum_{\mathbf{k}} \text{Tr} \left\{ \frac{\partial^2 \hat{E}_{\mathbf{k}}(\mathbf{q})}{\partial q_\mu \partial q_\nu} \tanh \frac{\beta \hat{E}_{\mathbf{k}}(\mathbf{q})}{2} + \frac{\beta}{2} \frac{\partial \hat{E}_{\mathbf{k}}(\mathbf{q})}{\partial q_\mu} \frac{\partial \hat{E}_{\mathbf{k}}(\mathbf{q})}{\partial q_\nu} \text{sech}^2 \frac{\beta \hat{E}_{\mathbf{k}}(\mathbf{q})}{2} \right\} \Bigg|_{\mathbf{q}=\mathbf{0}}. \quad (\text{D6})$$

Equation (D6) involves the first and second derivative of $E_{l\mathbf{k}\pm}(\mathbf{q})$. If we treat \mathbf{q} as perturbation and find the eigenvalues of $H_{\mathbf{k}}(\mathbf{q})$ up to q^2 order, then $D_s^{(1)}$ can be determined. To proceed, we approximate $\Lambda_{\mathbf{k}}(\mathbf{q})$ as

$$\Lambda_{\mathbf{k}}(\mathbf{q}) \simeq U_{\mathbf{k}} = U_{1\mathbf{k}} \oplus \dots \oplus U_{n\mathbf{k}}, \quad (\text{D7})$$

where

$$U_{l\mathbf{k}} = \begin{pmatrix} w_{l\mathbf{k}} & -v_{l\mathbf{k}} \\ v_{l\mathbf{k}} & w_{l\mathbf{k}} \end{pmatrix} \quad (\text{D8})$$

is the Bogoliubov transformation for the l th band at $\mathbf{q} = \mathbf{0}$, with

$$w_{l\mathbf{k}} = \sqrt{\frac{1}{2} \left(1 + \frac{\xi_{l\mathbf{k}}}{E_{l\mathbf{k}}} \right)}, \quad v_{l\mathbf{k}} = \sqrt{\frac{1}{2} \left(1 - \frac{\xi_{l\mathbf{k}}}{E_{l\mathbf{k}}} \right)}. \quad (\text{D9})$$

Transformation $U_{\mathbf{k}}$ makes the off-diagonal elements of $H_{\mathbf{k}}(\mathbf{q})$ small, therefore it splits into two parts,

$$U_{\mathbf{k}}^\dagger H_{\mathbf{k}}(\mathbf{q}) U_{\mathbf{k}} = \hat{E}_{\mathbf{k}}(0) + H_{\mathbf{k}}^{(1)}(\mathbf{q}), \quad (\text{D10})$$

where $\hat{E}_{\mathbf{k}}(0) = \text{diag}\{E_{1\mathbf{k}}, -E_{1\mathbf{k}}, \dots, E_{n\mathbf{k}}, -E_{n\mathbf{k}}\}$ is the unperturbed PHS Bogoliubov spectrum, and $H_{\mathbf{k}}^{(1)}(\mathbf{q})$ is the perturbing matrix.

This is equivalent to expressing $\hat{H}_{\mathcal{C}}(\mathbf{q})$ in the Bogoliubov band basis defined by $|l\mathbf{k}\pm\rangle \equiv \gamma_{l\mathbf{k}\pm}^\dagger(\mathbf{q})|0\rangle$, where $\gamma_{l\mathbf{k}\pm}$ denote the Bogoliubov operators of the l th band. The $2n$ -component Bogoliubov band spinor $\mathcal{Y}_{\mathbf{k},\mathbf{q}} = (\gamma_{1\mathbf{k}+}(\mathbf{q}), \gamma_{1\mathbf{k}-}(\mathbf{q}), \dots)^T$ is related to the electronic band operator through

$$\mathcal{Y}_{\mathbf{k},\mathbf{q}} = U_{\mathbf{k}}^\dagger (c_{1,\mathbf{k}+\mathbf{q}\uparrow}, c_{1,-\mathbf{k}+\mathbf{q}\downarrow}^\dagger, \dots)^T. \quad (\text{D11})$$

As we see below, the separation Eq. (D10) results in an excitation Hamiltonian

$$\hat{H}_{\mathcal{C}}^{(1)}(\mathbf{q}) = \sum_{\mathbf{k}} \mathcal{Y}_{\mathbf{k},\mathbf{q}}^\dagger H_{\mathbf{k}}^{(1)}(\mathbf{q}) \mathcal{Y}_{\mathbf{k},\mathbf{q}}, \quad (\text{D12})$$

which separately accounts for the SW contributions from intra- and interband transitions.

We first assume that at any \mathbf{k} -point, no two bands of the composite are degenerate ($\xi_{l\mathbf{k}} = \xi_{l'\mathbf{k}}$), whether accidentally or enforced by symmetry; additionally, we assume no two bands

have opposite energies ($\xi_{l\mathbf{k}} = -\xi_{l'\mathbf{k}}$). These restrictions mean the $2n$ Bogoliubov bands at $\mathbf{q} = \mathbf{0}$ are disconnected throughout the Brillouin zone, so nondegenerate perturbation can be applied. We find that the energy eigenvalues of $H_{\mathbf{k}}(\mathbf{q})$ up to $O(q^2)$ terms give n quasiparticle bands and n quasihole bands,

$$\begin{aligned} E_{l\mathbf{k}+}(\mathbf{q}) &= E_{l\mathbf{k}} + H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l-1,2l-1} + \sum_{l' \in \mathcal{C}, l' \neq l} \frac{|H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l-1,2l'-1}|^2}{E_{l\mathbf{k}} - E_{l'\mathbf{k}}} + \sum_{l' \in \mathcal{C}} \frac{|H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l-1,2l'}|^2}{E_{l\mathbf{k}} + E_{l'\mathbf{k}}} + O(q^3), \\ E_{l\mathbf{k}-}(\mathbf{q}) &= -E_{l\mathbf{k}} + H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l,2l} + \sum_{l' \in \mathcal{C}} \frac{|H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l,2l'-1}|^2}{-E_{l\mathbf{k}} - E_{l'\mathbf{k}}} + \sum_{l' \in \mathcal{C}, l' \neq l} \frac{|H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l,2l'}|^2}{-E_{l\mathbf{k}} + E_{l'\mathbf{k}}} + O(q^3). \end{aligned} \quad (\text{D13})$$

Here $H_{\mathbf{k}}^{(1)}(\mathbf{q})_{ij}$ denotes the (i, j) th entry of matrix $H_{\mathbf{k}}^{(1)}(\mathbf{q})$. In terms of the Bogoliubov basis, they are

$$\begin{aligned} H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l-1,2l'-1} &\equiv \langle l\mathbf{k} + | H_{\mathbf{k}}^{(1)}(\mathbf{q}) | l'\mathbf{k} + \rangle, \\ H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l,2l'} &\equiv \langle l\mathbf{k} - | H_{\mathbf{k}}^{(1)}(\mathbf{q}) | l'\mathbf{k} - \rangle, \\ H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l-1,2l'} &\equiv \langle l\mathbf{k} + | H_{\mathbf{k}}^{(1)}(\mathbf{q}) | l'\mathbf{k} - \rangle, \end{aligned} \quad (\text{D14})$$

which can be explicitly computed from Eqs. (D1) and (D7).

After some algebra, we find that the derivatives of Eq. (D13) with respect to \mathbf{q} (which do not act on $\mu_{\mathbf{q}}$ or $\hat{\Delta}_{\mathbf{q}}$) give

$$\partial_{\mu} E_{l\mathbf{k}\pm}(\mathbf{q}) \Big|_{\mathbf{q}=\mathbf{0}} = \partial_{\mu} \xi_{l\mathbf{k}}, \quad (\text{D15})$$

$$\begin{aligned} \partial_{\mu} \partial_{\nu} E_{l\mathbf{k}\pm}(\mathbf{q}) \Big|_{\mathbf{q}=\mathbf{0}} &= \pm \left\{ \frac{\xi_{l\mathbf{k}}}{E_{l\mathbf{k}}} \partial_{\mu} \partial_{\nu} \xi_{l\mathbf{k}} - \frac{4\Delta^2}{E_{l\mathbf{k}}} g_{\mu\nu}^l(\mathbf{k}) \right. \\ &\quad \left. - \sum_{l' \in \mathcal{C}, l' \neq l} 8\Delta^2 \left[\frac{p_{ll'}^{(+)}(\mathbf{k})}{E_{l\mathbf{k}} + E_{l'\mathbf{k}}} + \frac{p_{ll'}^{(-)}(\mathbf{k})}{E_{l\mathbf{k}} - E_{l'\mathbf{k}}} \right] g_{\mu\nu}^{ll'}(\mathbf{k}) \right\}, \end{aligned} \quad (\text{D16})$$

where the coherence factors

$$\begin{aligned} p_{ll'}^{(+)}(\mathbf{k}) &= \frac{1}{2} \left(1 + \frac{\xi_{l\mathbf{k}} \xi_{l'\mathbf{k}} + \Delta^2}{E_{l\mathbf{k}} E_{l'\mathbf{k}}} \right) = (w_{l\mathbf{k}} w_{l'\mathbf{k}} + v_{l\mathbf{k}} v_{l'\mathbf{k}})^2, \\ p_{ll'}^{(-)}(\mathbf{k}) &= \frac{1}{2} \left(1 - \frac{\xi_{l\mathbf{k}} \xi_{l'\mathbf{k}} + \Delta^2}{E_{l\mathbf{k}} E_{l'\mathbf{k}}} \right) = (w_{l\mathbf{k}} v_{l'\mathbf{k}} - v_{l\mathbf{k}} w_{l'\mathbf{k}})^2 \end{aligned} \quad (\text{D17})$$

come from the second derivative $\partial_{\mu} \partial_{\nu} |H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l-1,2l'}|^2$, $\partial_{\mu} \partial_{\nu} |H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l,2l'-1}|^2$ and $\partial_{\mu} \partial_{\nu} |H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l-1,2l'-1}|^2$, $\partial_{\mu} \partial_{\nu} |H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l,2l'}|^2$, respectively. Physically, $p_{ll'}^{(+)}(\mathbf{k})$ accounts for the transitions between a quasiparticle and quasihole band, while $p_{ll'}^{(-)}(\mathbf{k})$ accounts for transitions between two quasiparticle bands or between two quasihole bands.

Also, one notices that the intra- and interband quantum metric comes from the expansion of intra- and interband gap functions. If the fluctuation of $\hat{\Delta}_{\mathbf{q}}$ is ignored, they are [see definition Eq. (8)]

$$\begin{aligned} \Delta_{l,\mathbf{k}}(\mathbf{q}) &= \Delta \{ 1 - 2 \langle u_{l\mathbf{k}} | \partial_{\mu} u_{l\mathbf{k}} \rangle q_{\mu} \\ &\quad - [\langle \partial_{\mu} u_{l\mathbf{k}} | \partial_{\nu} u_{l\mathbf{k}} \rangle + \text{c.c.}] q_{\mu} q_{\nu} \} + O(q^3), \end{aligned} \quad (\text{D18})$$

$$\Delta_{l'l',\mathbf{k}}(\mathbf{q}) = -2\Delta \langle u_{l\mathbf{k}} | \partial_{\mu} u_{l'\mathbf{k}} \rangle q_{\mu} + O(q^2), \quad l \neq l'. \quad (\text{D19})$$

Since all matrix elements $H_{\mathbf{k}}^{(1)}(\mathbf{q})_{ij} \sim O(q)$, the intraband quantum metric $g_{\mu\nu}^l$ in Eq. (D16) comes from the $O(q^2)$ term of $H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l-1,2l-1}$ combined with the $O(q)$ term of $H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l-1,2l}$ or the $O(q^2)$ term of $H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l,2l}$ combined with the $O(q)$ term of $H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l,2l-1}$. Whereas the interband quantum metric $g_{\mu\nu}^{ll'}$ only comes from the $O(q)$ term of $H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l-1,2l'-1}$, $H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l-1,2l'}$, $H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l,2l'-1}$, and $H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l,2l'}$ of $l \neq l'$. The transition processes they represent are illustrated in Fig. 1.

Inserting Eqs. (D15) and (D16) into Eq. (D6), one gets Eq. (9) in the main text.

2. Degenerate perturbation

To get Eq. (9), we assumed that there are no two Bogoliubov bands at $\mathbf{q} = \mathbf{0}$ being degenerate at any \mathbf{k} point, so nondegenerate perturbation was used. Otherwise, if a few quasiparticle bands are degenerate at some isolated \mathbf{k} points or completely degenerate throughout the momentum space (which requires the band energy $\xi_{l\mathbf{k}} = \pm \xi_{l'\mathbf{k}}$), then degenerate perturbation must be applied.

However, using standard degenerate perturbation, one can prove that Eq. (9) remains the same even in the presence of band degeneracy, which agrees with the general Kubo formula result. In calculating current responses using the Kubo formula, whenever two bands become degenerate, the only change is to make the substitution

$$\frac{n(E_1) - n(E_2)}{E_1 - E_2} \rightarrow \frac{dn(E)}{dE} \Big|_{E=E_1}. \quad (\text{D20})$$

Similarly, for Eq. (9), when $E_{l\mathbf{k}} = E_{l'\mathbf{k}}$, one only needs to replace

$$\frac{\tanh(\beta E_{l\mathbf{k}}/2) - \tanh(\beta E_{l'\mathbf{k}}/2)}{E_{l\mathbf{k}} - E_{l'\mathbf{k}}} \rightarrow \frac{\beta}{2} \text{sech}^2 \frac{\beta E_{l\mathbf{k}}}{2}. \quad (\text{D21})$$

Therefore, we conclude that band degeneracy poses no additional mathematical difficulty for expressing the SW $D_s^{(1)}$ as Eq. (9).

APPENDIX E: POSITIVE SEMIDEFINITENESS OF THE SUPERFLUID WEIGHT

The purpose of this Appendix is to show that the first term $D_s^{(1)}$, Eq. (9), is positive semidefinite. This proof will be independent of lattice geometry. Since the total SW $D_s = D_s^{(1)} + D_s^{(2)}$ is geometry-independent and $D_s^{(2)}$ can be made zero by choosing the MQM, it also shows that the total D_s is positive semidefinite for the uniform pairing channel, regardless of temperature and any composite bands.

$$D_{s,\mu\nu}^{(1)\text{geo}} = - \sum_{\mathbf{k}} \sum_{l \in \mathcal{C}, l' \notin \mathcal{C}} \frac{4\Delta^2}{E_{l\mathbf{k}}} \tanh \frac{\beta E_{l\mathbf{k}}}{2} g_{\mu\nu}^{l'}(\mathbf{k}) - \sum_{\mathbf{k}} \sum_{l, l' \in \mathcal{C}, l' > l} 4\Delta^2 \left\{ \tanh \frac{\beta E_{l\mathbf{k}}}{2} \left[\frac{1}{E_{l\mathbf{k}}} - \frac{2p_{l'}^{(+)}(\mathbf{k})}{E_{l\mathbf{k}} + E_{l'\mathbf{k}}} - \frac{2p_{l'}^{(-)}(\mathbf{k})}{E_{l\mathbf{k}} - E_{l'\mathbf{k}}} \right] + l \leftrightarrow l' \right\} g_{\mu\nu}^{l'}(\mathbf{k}). \quad (\text{E2})$$

Since each $g_{\mu\nu}^{l'} (l \neq l')$ is negative semidefinite, all we need to show is that each quantity

$$f(\xi_{l\mathbf{k}}, \xi_{l'\mathbf{k}}) = \tanh \frac{\beta E_{l\mathbf{k}}}{2} \left[\frac{1}{E_{l\mathbf{k}}} - \frac{2p_{l'}^{(+)}(\mathbf{k})}{E_{l\mathbf{k}} + E_{l'\mathbf{k}}} - \frac{2p_{l'}^{(-)}(\mathbf{k})}{E_{l\mathbf{k}} - E_{l'\mathbf{k}}} \right] + l \leftrightarrow l' \quad (\text{E3})$$

is positive. Using definition (D17), we find

$$f(\xi_{l\mathbf{k}}, \xi_{l'\mathbf{k}}) = - \left(\frac{1}{E_{l\mathbf{k}}} \tanh \frac{\beta E_{l\mathbf{k}}}{2} - \frac{1}{E_{l'\mathbf{k}}} \tanh \frac{\beta E_{l'\mathbf{k}}}{2} \right) \frac{\xi_{l\mathbf{k}} - \xi_{l'\mathbf{k}}}{\xi_{l\mathbf{k}} + \xi_{l'\mathbf{k}}}. \quad (\text{E4})$$

Note the factor $\frac{\xi_{l\mathbf{k}} - \xi_{l'\mathbf{k}}}{\xi_{l\mathbf{k}} + \xi_{l'\mathbf{k}}} = \frac{(\xi_{l\mathbf{k}} - \xi_{l'\mathbf{k}})^2}{(E_{l\mathbf{k}} + E_{l'\mathbf{k}})(E_{l\mathbf{k}} - E_{l'\mathbf{k}})}$, and the function $(1/x) \tanh x$ has a negative slope at $x > 0$ [same as Eq. (E1)], therefore $f(\xi_{l\mathbf{k}}, \xi_{l'\mathbf{k}}) > 0$ and the positive semidefiniteness is proved.

APPENDIX F: CALCULATION OF THE PAIRING AMPLITUDE

In this Appendix, we give details of using the perturbation method to calculate the pairing amplitude $\langle c_{l', -\mathbf{k}+\mathbf{q}} \downarrow c_{l, \mathbf{k}+\mathbf{q}} \uparrow \rangle_{\mathbf{q}}$. Recall that under transformation $U_{\mathbf{k}}$, the mean-field Hamiltonian can be expressed as

$$\hat{\mathcal{H}}_{\mathcal{C}}(\mathbf{q}) = \sum_{\mathbf{k}} \boldsymbol{\gamma}_{\mathbf{k}, \mathbf{q}}^\dagger [\hat{E}_{\mathbf{k}}(0) + H_{\mathbf{k}}^{(1)}(\mathbf{q})] \boldsymbol{\gamma}_{\mathbf{k}, \mathbf{q}}, \quad (\text{F1})$$

where the perturbation matrix $H_{\mathbf{k}}^{(1)}$ mixes Bogoliubov bands of different indices. Using the standard perturbation method, the annihilation operator of the band-resolved quasiparticles that exactly diagonalize $\hat{\mathcal{H}}_{\mathcal{C}}(\mathbf{q})$, $\tilde{\boldsymbol{\gamma}}$, can be expressed as a linear combination of $\boldsymbol{\gamma}$ operators:

$$\begin{aligned} \tilde{\boldsymbol{\gamma}}_{l\mathbf{k}+}(\mathbf{q}) &= \boldsymbol{\gamma}_{l\mathbf{k}+}(\mathbf{q}) + \sum_{l' \in \mathcal{C}, l' \neq l} \frac{H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l-1, 2l'-1}}{E_{l\mathbf{k}} - E_{l'\mathbf{k}}} \boldsymbol{\gamma}_{l'\mathbf{k}+}(\mathbf{q}) + \sum_{l' \in \mathcal{C}} \frac{H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l-1, 2l'}}{E_{l\mathbf{k}} + E_{l'\mathbf{k}}} \boldsymbol{\gamma}_{l'\mathbf{k}-}(\mathbf{q}) + O(q^2), \\ \tilde{\boldsymbol{\gamma}}_{l\mathbf{k}-}(\mathbf{q}) &= \boldsymbol{\gamma}_{l\mathbf{k}-}(\mathbf{q}) + \sum_{l' \in \mathcal{C}} \frac{H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l, 2l'-1}}{-E_{l\mathbf{k}} - E_{l'\mathbf{k}}} \boldsymbol{\gamma}_{l'\mathbf{k}+}(\mathbf{q}) + \sum_{l' \in \mathcal{C}, l' \neq l} \frac{H_{\mathbf{k}}^{(1)}(\mathbf{q})_{2l, 2l'}}{-E_{l\mathbf{k}} + E_{l'\mathbf{k}}} \boldsymbol{\gamma}_{l'\mathbf{k}-}(\mathbf{q}) + O(q^2). \end{aligned} \quad (\text{F2})$$

Here, to expand $H_{\mathbf{k}}^{(1)}(\mathbf{q})_{ij}$ in powers of \mathbf{q} , we must take into account the \mathbf{q} -dependence of $\hat{\Delta}_{\mathbf{q}}$, therefore we use

$$\begin{aligned} \Delta_{ll', \mathbf{k}}(\mathbf{q}) &= \Delta \delta_{ll'} + (-2\Delta \langle u_{l\mathbf{k}} | \partial_{\mu} u_{l'\mathbf{k}} \rangle \\ &+ \sum_{\alpha=1}^s u_{l\mathbf{k}\alpha}^* u_{l'\mathbf{k}\alpha} d_{\mu} \Delta_{\alpha}) q_{\mu} + O(q^2) \end{aligned} \quad (\text{F3})$$

instead of Eqs. (D18) and (D19). The normalization of $\tilde{\boldsymbol{\gamma}}$ operators is ignored as it leads to $O(q^2)$ corrections. Equation (F2) can be viewed as a linear transformation $\tilde{\boldsymbol{\gamma}} = A\boldsymbol{\gamma}$ between the

One first notices that the function

$$\tanh \frac{\beta E_{l\mathbf{k}}}{2} - \frac{\beta E_{l\mathbf{k}}}{2} \text{sech}^2 \frac{\beta E_{l\mathbf{k}}}{2} > 0, \quad (\text{E1})$$

so the conventional part of Eq. (9) is positive semidefinite. To analyze the geometric term, we break the intraband quantum metric $g_{\mu\nu}^l$ into interband ones $g_{\mu\nu}^{l'}$, and collect all the terms with the same $g_{\mu\nu}^{l'}$ (including the symmetric term $l \leftrightarrow l'$), to arrive at the following split expression:

spinors $\tilde{\boldsymbol{\gamma}}$ and $\boldsymbol{\gamma}$, where $A_{ij} = \delta_{ij} + a_{ij}$ is a matrix close to identity, with $a_{ij} \sim O(q)$. The inverse of A has an approximate form $(A^{-1})_{ij} = \delta_{ij} - a_{ij} + O(q^2)$, which enables us to write operators $\boldsymbol{\gamma}$ in terms of $\tilde{\boldsymbol{\gamma}}$. Since the electron operators c are related to $\boldsymbol{\gamma}$ through the transformation $U_{\mathbf{k}}$, we can finally write c in terms of $\tilde{\boldsymbol{\gamma}}$.

Since the $\tilde{\boldsymbol{\gamma}}$ operators exactly diagonalize the BdG Hamiltonian of composite bands, we have

$$\langle \tilde{\boldsymbol{\gamma}}_{l\mathbf{k}\pm}(\mathbf{q})^\dagger \tilde{\boldsymbol{\gamma}}_{l\mathbf{k}\pm}(\mathbf{q}) \rangle_{\mathbf{q}} \approx n_F(\pm E_{l\mathbf{k}}) \quad (\text{F4})$$

to the lowest order of \mathbf{q} , where n_F is the Fermi-Dirac function. Finally, one obtains the pairing amplitude

$$\langle c_{l', -\mathbf{k}+\mathbf{q}\downarrow} c_{l, \mathbf{k}+\mathbf{q}\uparrow} \rangle_{\mathbf{q}} = \begin{cases} -\frac{\tanh(\beta E_{l\mathbf{k}}/2)}{2E_{l\mathbf{k}}} \left[\Delta + (-2\Delta \langle u_{l\mathbf{k}} | \partial_\mu u_{l\mathbf{k}} \rangle + \sum_{\beta=1}^s |u_{l\mathbf{k}\beta}|^2 d_\mu \Delta_\beta) q_\mu \right] + O(q^2), & l = l', \\ \frac{1}{2} \left[\frac{P_{l'l'}^{(+)}(\mathbf{k})}{E_{l\mathbf{k}}+E_{l'\mathbf{k}}} \left(\tanh \frac{\beta E_{l\mathbf{k}}}{2} + \tanh \frac{\beta E_{l'\mathbf{k}}}{2} \right) + \frac{P_{l'l'}^{(-)}(\mathbf{k})}{E_{l\mathbf{k}}-E_{l'\mathbf{k}}} \left(\tanh \frac{\beta E_{l\mathbf{k}}}{2} - \tanh \frac{\beta E_{l'\mathbf{k}}}{2} \right) \right] \\ \times \left(2\Delta \langle u_{l\mathbf{k}} | \partial_\mu u_{l'\mathbf{k}} \rangle - \sum_{\beta=1}^s u_{l\mathbf{k}\beta}^* u_{l'\mathbf{k}\beta} d_\mu \Delta_\beta \right) q_\mu + O(q^2). & l \neq l'. \end{cases} \quad (\text{F5})$$

From this to get Eqs. (29) and (30), we have also used the $\mathbf{q} = \mathbf{0}$ gap equation

$$1 = \frac{U_\alpha}{N} \sum_{\mathbf{k}} \sum_{l \in \mathcal{C}} |u_{l\mathbf{k}\alpha}|^2 \frac{\tanh(\beta E_{l\mathbf{k}}/2)}{2E_{l\mathbf{k}}}, \quad \forall \alpha. \quad (\text{F6})$$

APPENDIX G: POSITIVE SEMIDEFINITENESS AND RANK OF THE HESSIAN MATRIX FOR UNIFORM PAIRING

This Appendix serves to prove the rank and positive semidefiniteness of the Hessian matrix $M_{\alpha\beta}$ in Eq. (29).

We consider a general class of s -dim real symmetric matrices $M_{\alpha\beta}$, which have a kernel eigenvector $\mathbf{v}_0 = (1, 1, \dots, 1)^T$. It implies $\sum_{\beta=1}^s M_{\alpha\beta} = \sum_{\alpha=1}^s M_{\alpha\beta} = 0$. With this property, we write $M_{\alpha\beta}$ as

$$M_{\alpha\beta} = \begin{cases} \sum_{\gamma=1, \gamma \neq \alpha}^s C_{\alpha\gamma}, & \alpha = \beta, \\ -C_{\alpha\beta}, & \alpha \neq \beta, \end{cases} \quad (\text{G1})$$

where $C_{\alpha\beta}$ ($\alpha \neq \beta$) are just the off-diagonal elements of M with a minus sign. We give three propositions below.

Proposition 1. If $C_{\alpha\beta} > 0$ for all $1 \leq \alpha, \beta \leq s$, $\alpha \neq \beta$, then $M_{\alpha\beta}$ is positive semidefinite and $\text{Rank}(M) = s - 1$.

We use the criterion that all its leading principal minors are non-negative to show the positive semidefiniteness. Let us denote the leading principal minor of M of order k ($1 \leq k \leq s$) by $D_k(M)$. We find

$$D_1(M) = M_{11} = \sum_{\alpha \neq 1}^s C_{1\alpha} \geq 0, \quad (\text{G2})$$

$$D_2(M) = \det \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = \sum_{\alpha_1 \neq 1, \alpha_2 \neq 2}^s C_{1\alpha_1} C_{2\alpha_2} - C_{12} C_{21}, \quad (\text{G3})$$

and

$$D_k(M) = \sum_{\alpha_1, \dots, \alpha_k}^s C_{1\alpha_1} C_{2\alpha_2} \cdots C_{k\alpha_k}. \quad (\text{G4})$$

Here, \sum' means the summation imposed by the single rule that there is not any subset $\{i_1, \dots, i_j\} \subseteq \{1, \dots, k\}$ such that $\{\alpha_{i_1}, \dots, \alpha_{i_j}\}$ is its permutation. This single rule leads to the following subrules: (i) no $C_{\alpha\alpha}$ appears in the sum [e.g., (G2)], since $\{\alpha\}$ is a permutation of $\{\alpha\}$; (ii) no squares of any C appear in the sum, i.e., for $\alpha \neq \beta$, $C_{\alpha\beta} C_{\beta\alpha}$ is not allowed since $\{\beta, \alpha\}$ is a permutation of $\{\alpha, \beta\}$ [e.g., Eq. (G3)]; (iii) in every term of $D_k(M)$, there is at least an α_j ($1 \leq j \leq k$) that is not in the set $\{1, \dots, k\}$. Subrule (iii) is a simple result of the general permutation rule.

Using (iii), it is easy to show that $\det M = D_s(M) = 0$, thus $\text{Rank}(M) \leq s - 1$. Moreover, since each leading principal minor $D_k(M) \geq 0$, $M_{\alpha\beta}$ is positive semidefinite.

Next, we prove $\text{Rank}(M) = s - 1$ by contradiction—if $\text{Rank}(M) \leq s - 2$, then any minor of order $s - 1$ should vanish. However,

$$D_{s-1}(M) = \sum_{\alpha_1, \dots, \alpha_{s-1}}^s C_{1\alpha_1} C_{2\alpha_2} \cdots C_{s-1, \alpha_{s-1}} > 0 \quad (\text{G5})$$

since it contains at least one term $C_{1s} C_{2s} \cdots C_{s-1, s}$, a contradiction (QED).

We want to emphasize that Proposition 1 together with Eq. (G1) is a statement about UPC. It can be equivalently stated as ‘‘UPC leads to a positive-semidefinite M and $\text{Rank}(M) = s - 1$.’’ We cannot prove the most general case, but we will prove two special cases below, which still contain enough information for understanding this general property.

Proposition 2. Under the UPC, if an isolated band m contains s orbitals, then the Hessian matrix M is positive semidefinite and $\text{Rank}(M) = s - 1$.

The condition above can be stated as ‘‘for each $1 \leq \alpha \leq s$ there exists a neighborhood of some \mathbf{k} -point in Brillouin zone such that $|u_{m\mathbf{k}\alpha}| \neq 0$.’’ Based on Proposition 1, we only need to show $C_{\alpha\beta} > 0$. From Eq. (29) we find for a single isolated band m ,

$$C_{\alpha\beta} = \sum_{\mathbf{k}} \frac{\tanh(\beta E_{m\mathbf{k}}/2)}{2E_{m\mathbf{k}}} |u_{m\mathbf{k}\alpha}|^2 |u_{m\mathbf{k}\beta}|^2, \quad \alpha \neq \beta, \quad (\text{G6})$$

which is positive. Therefore, the proposition is proved.

By induction, we know that whenever an orbital is removed from the band, one positive eigenvalue of M will approach 0, lowering the rank by 1. It can be easily seen that $|u_{m\mathbf{k}r}| \rightarrow 0$ if the r th orbital is removed. Then M will have an additional kernel eigenvector $\mathbf{e}_r = (\dots, 0, 1, 0, \dots)^T$ (with its r th component nonzero).

Proposition 3. Under the UPC, for a composite of n bands formed from s orbitals, if (i) the composite is incomplete ($n < s$), (ii) the n bands are energetically close to each other compared to the interaction scale Δ , and (iii) the composite contains all the s orbitals, then the Hessian matrix M is positive semidefinite and $\text{Rank}(M) = s - 1$.

This proposition is based on three conditions, but the first two can be relaxed. Similarly, the third condition can be stated as ‘‘for each $1 \leq \alpha \leq s$ there exists some band $l \in \mathcal{C}$ and a neighborhood of some \mathbf{k} -point in Brillouin zone such that $|u_{l\mathbf{k}\alpha}| \neq 0$.’’ The second condition states that the n bands form an ICFB. With this condition one can omit the band index in $E_{l\mathbf{k}}, E_{l'\mathbf{k}} \rightarrow E_{\mathbf{k}}$. From Eq. (29), $C_{\alpha\beta}$ of the composite bands

can be expressed as

$$\begin{aligned} C_{\alpha\beta} &\approx \sum_{\mathbf{k}} \frac{\tanh(\beta E_{\mathbf{k}}/2)}{2E_{\mathbf{k}}} \sum_{l,l' \in \mathcal{C}} u_{l\mathbf{k}\alpha}^* u_{l\mathbf{k}\alpha} u_{l\mathbf{k}\beta}^* u_{l'\mathbf{k}\beta} \\ &= \sum_{\mathbf{k}} \frac{\tanh(\beta E_{\mathbf{k}}/2)}{2E_{\mathbf{k}}} |b_{\mathbf{k},\alpha\beta}|^2, \end{aligned} \quad (\text{G7})$$

where we have defined

$$b_{\mathbf{k},\alpha\beta} = \sum_{l \in \mathcal{C}} u_{l\mathbf{k}\alpha}^* u_{l\mathbf{k}\beta}. \quad (\text{G8})$$

Equation (G7) is the leading term of $C_{\alpha\beta}$ if it is expanded in powers of $\xi_{l\mathbf{k}} - \xi_{l'\mathbf{k}}$. Since it is required that the composite is incomplete ($n < s$), we have $|b_{\mathbf{k},\alpha\beta}|$ strictly greater than 0. Then $C_{\alpha\beta} > 0$, and the proposition is proved. If instead $n = s$, then $b_{\mathbf{k},\alpha\beta} = \delta_{\alpha\beta}$, making the leading term of $C_{\alpha\beta}$ vanish.

For cases other than those stated in Proposition 3, one should be able to numerically check that $C_{\alpha\beta} > 0$ always holds under UPC. Analogous to the single isolated band case,

$$\begin{aligned} \delta g_{\mu\nu}^I(\mathbf{k}) &= \langle \delta x_{\mu} \delta x_{\nu} \rangle_{l\mathbf{k}}^0 - \langle \delta x_{\mu} \rangle_{l\mathbf{k}}^0 \langle \delta x_{\nu} \rangle_{l\mathbf{k}}^0 + \left[\left(\frac{i}{2} \sum_{\alpha} \delta x_{\alpha,\mu} u_{l\mathbf{k}\alpha}^{0*} \partial_{\nu} u_{l\mathbf{k}\alpha}^0 + \text{c.c.} - i \langle \delta x_{\mu} \rangle_{l\mathbf{k}}^0 \langle u_{l\mathbf{k}}^0 | \partial_{\nu} u_{l\mathbf{k}}^0 \right) + \mu \leftrightarrow \nu \right], \\ \delta g_{\mu\nu}^{II}(\mathbf{k}) &= \left[-\frac{1}{2} \langle \delta x_{\mu} \rangle_{l'l\mathbf{k}}^0 \langle \delta x_{\nu} \rangle_{l'l\mathbf{k}}^0 - \frac{i}{2} \left(\langle \delta x_{\mu} \rangle_{l'l\mathbf{k}}^0 \langle u_{l\mathbf{k}}^0 | \partial_{\nu} u_{l\mathbf{k}}^0 \rangle + \langle \delta x_{\nu} \rangle_{l'l\mathbf{k}}^0 \langle u_{l\mathbf{k}}^0 | \partial_{\mu} u_{l\mathbf{k}}^0 \rangle \right) \right] + \mu \leftrightarrow \nu. \end{aligned} \quad (\text{H2})$$

Here $\langle \rangle_{l\mathbf{k}}^0$ represents the average over different orbitals in the initial state $u_{l\mathbf{k}}^0$, while $\langle \rangle_{l'l\mathbf{k}}^0$ represents the overlap between different bands, i.e.,

$$\begin{aligned} \langle \delta x_{\mu} \rangle_{l\mathbf{k}}^0 &= \sum_{\alpha=1}^s \delta x_{\alpha,\mu} |u_{l\mathbf{k}\alpha}^0|^2, \\ \langle \delta x_{\mu} \delta x_{\nu} \rangle_{l\mathbf{k}}^0 &= \sum_{\alpha=1}^s \delta x_{\alpha,\mu} \delta x_{\alpha,\nu} |u_{l\mathbf{k}\alpha}^0|^2, \\ \langle \delta x_{\mu} \rangle_{l'l\mathbf{k}}^0 &= \sum_{\alpha=1}^s \delta x_{\mu,\alpha} u_{l\mathbf{k}\alpha}^{0*} u_{l'\mathbf{k}\alpha}^0. \end{aligned} \quad (\text{H3})$$

With these established, let us vary the functional I in Eq. (20) around some fixed positions $\{\mathbf{x}_{\alpha}^0\}$. One can readily show the following identity:

$$\left. \frac{\partial I}{\partial x_{\alpha,\mu}} \right|_{\{\mathbf{x}_{\alpha}^0\}} = \left(\frac{2i}{\Delta} \right) V_{\alpha,\mu}^0, \quad (\text{H4})$$

where $V_{\alpha,\mu}^0$ is Eq. (30) evaluated at $\{\mathbf{x}_{\alpha}^0\}$. Based on Definition 2, if $\{\mathbf{x}_{\alpha}^0\}$ extremize I , then $V_{\alpha,\mu}^0 = M_{\alpha\beta} d_{\mu} \Delta_{\beta}^0 = 0$, implying $D_s^{(2)} = 0$ in Eq. (6). Therefore, we have proved that Definition 2 leads to Definition 1.

To show the other way requires the rank of the Hessian matrix $\partial^2 \Omega / \partial_{\mu} \Delta_{\alpha} \partial_{\nu} \Delta_{\beta}$ to be $s - 1$. The uniform pairing case has been proved in Appendix G. Assuming $\text{Rank}(M) = s - 1$, then the vanishing of $D_s^{(2)}$ in Eq. (6) has two solutions: either (i) $d_{\mu} \Delta_{\alpha} = 0$ or (ii) $d_{\mu} \Delta_1 = d_{\mu} \Delta_2 = \dots = d_{\mu} \Delta_s = i\lambda_{\mu}$, $\mu = x, y$. These two solutions are identical up to a $U(1)$ gauge transformation [30,31]. To see this, we write the second

whenever an r th orbital is removed from the composite, \mathbf{e}_r becomes an additional kernel eigenvector and $\text{Rank}(M)$ is lowered by 1.

APPENDIX H: EQUIVALENCE OF THE TWO DEFINITIONS OF MINIMAL QUANTUM METRIC

In this Appendix, we show how the two definitions of MQM given in Sec. IV are equivalent to each other based on the rank information of matrix $\partial^2 \Omega / \partial \Delta_{\alpha}^I \partial \Delta_{\beta}^I$.

Consider the geometric transformation that each orbital's position transforms as $\mathbf{x}_{\alpha} = \mathbf{x}_{\alpha}^0 + \delta \mathbf{x}_{\alpha}$. During this transformation, hopping integrals $t_{ij,\alpha\beta}^{\sigma}$ are fixed, while the Bloch components $u_{l\mathbf{k}\alpha}$ undergo the change

$$u_{l\mathbf{k}\alpha} = e^{-i\mathbf{k} \cdot \delta \mathbf{x}_{\alpha}} u_{l\mathbf{k}\alpha}^0. \quad (\text{H1})$$

The intra- and interband quantum metric transform accordingly, $g_{\mu\nu}^I = g_{\mu\nu}^{I,0} + \delta g_{\mu\nu}^I$, $g_{\mu\nu}^{II} = g_{\mu\nu}^{II,0} + \delta g_{\mu\nu}^{II}$, with

solution as

$$\Delta_{\mathbf{q},\alpha} = \Delta [1 + i\boldsymbol{\lambda} \cdot \mathbf{q} + S_{\alpha}(q^2)], \quad (\text{H5})$$

where $\boldsymbol{\lambda} = (\lambda_x, \lambda_y)$ is a real vector and $S_{\alpha}(q^2)$ is a complex function of q^2 order. A new order parameter that has an overall phase difference can be defined,

$$\tilde{\Delta}_{\mathbf{q},\alpha} = e^{-i\boldsymbol{\lambda} \cdot \mathbf{q}} \Delta_{\mathbf{q},\alpha}, \quad (\text{H6})$$

which satisfies $d_{\mu} \tilde{\Delta}_{\alpha} = 0$ and recovers the first solution. Both solutions above lead to the vanishing of extremization Eq. (H4), since $V_{\alpha,\mu} = M_{\alpha\beta} d_{\mu} \Delta_{\alpha}$. We have shown that Definition 1 implies Definition 2. Therefore, the two definitions are equivalent.

With the knowledge that $\text{Rank}(M) = s - 1$, one can further show that the minimal positions exist and are unique, up to fixing the position of one orbital [31].

Starting from some general positions $\{\mathbf{x}_{\alpha}^0\}$, let us consider the transformation $\mathbf{x}_{\alpha} = \mathbf{x}_{\alpha}^0 + \delta \mathbf{x}_{\alpha}$ again, under which $d_{\mu} \Delta_{\alpha} = d_{\mu} \Delta_{\alpha}^0 + \delta d_{\mu} \Delta_{\alpha}$ and $V_{\alpha,\mu} = V_{\alpha,\mu}^0 + \delta V_{\alpha,\mu}$. Using Eqs. (30) and (H1), the change of $V_{\alpha,\mu}$ is found to be

$$\delta V_{\alpha,\mu} = -2i \Delta M_{\alpha\beta} \delta x_{\beta,\mu}. \quad (\text{H7})$$

By the invertibility of $M_{\alpha\beta}$ in the $(s - 1)$ -dim subspace, we obtain

$$\delta d_{\mu} \Delta_{\alpha} = -2i \Delta \delta x_{\alpha,\mu}. \quad (\text{H8})$$

Imposing $d_{\mu} \Delta_{\alpha}^0 + \delta d_{\mu} \Delta_{\alpha} = 0$, the minimal positions are thus located at

$$\delta x_{\alpha,\mu} = -\frac{i}{2\Delta} d_{\mu} \Delta_{\alpha}^0, \quad (\text{H9})$$

from the initial positions $\{\mathbf{x}_{\alpha}^0\}$.

As discussed at the end of Sec. IV, when some orbitals are removed from the composite bands, their positions become irrelevant to the geometric functional I . Thus, the MQM orbital positions are hyperlines or hyperplanes in the geometric space. We use two-orbital models as an example to illustrate this in Appendix I.

APPENDIX I: TWO-ORBITAL MODELS

Inserting Eq. (H2) into Eq. (9), and inserting Eq. (H8) into Eq. (32), we find both $\delta D_s^{(1)}$ and $\delta D_s^{(2)}$ have a quadratic form of the orbital coordinate change $\delta x_{\alpha,\mu}$, therefore they take a parabolic shape in the $3(s-1)$ -dim geometric space. The eigenvalues of Hessian matrix $M_{\alpha\beta}$ show the steepness of the parabola, while the eigenvectors tell the directions where the MQM functional undergoes the steepest change. Whenever an orbital is removed from the composite, one eigenvalue of $M_{\alpha\beta}$ reaches zero, and its position becomes irrelevant to the functional I . In this Appendix, we illustrate this using two-orbital models.

For two-orbital models, one can define the composite to contain either one (valence or conduction) band or both bands, depending on the Fermi energy and interaction scale. Since the position of one orbital can permanently be fixed, we write I as a function $I(\mathbf{r})$, where $\mathbf{r} = (x, y) \equiv \mathbf{x}_2 - \mathbf{x}_1$ is orbital 2's position relative to orbital 1. To calculate $I(\mathbf{r})$, one can use the method of the Bloch function, i.e., using Eq. (H1) to get (H2). Here, instead, we use the Bloch Hamiltonian method.

We choose the lattice geometry where the two orbitals sit on the same site as the reference geometry, $\mathbf{r} = \mathbf{0}$. This defines the Bloch Hamiltonian of a two-orbital model,

$$h(\mathbf{k}) = d_0(\mathbf{k})\sigma_0 + \sum_{j=x,y,z} d_j(\mathbf{k})\sigma_j \quad (I1)$$

[we omitted the spin index, so $h(\mathbf{k})$ is for spin- \uparrow only and the spin- \downarrow sector is its time-reversal counterpart] where σ_j are Pauli matrices in the orbital space. Then, the quantum metric is

$$g_{\mu\nu} \equiv g_{\mu\nu}^v = g_{\mu\nu}^c = -g_{\mu\nu}^{vc} = \frac{1}{4} \partial_\mu \hat{\mathbf{d}} \cdot \partial_\nu \hat{\mathbf{d}}, \quad (I2)$$

where $\hat{\mathbf{d}} = (d_x, d_y, d_z)$ and $\hat{\mathbf{d}} = \hat{\mathbf{d}}/|\hat{\mathbf{d}}|$ is a unit vector.

Under the geometric transformation, $h(\mathbf{k})$ is transformed by the unitary matrix $\mathcal{U}(\mathbf{k}) = \text{diag}\{1, e^{i\mathbf{k}\cdot\mathbf{r}}\}$:

$$\tilde{h}(\mathbf{k}) = \mathcal{U}(\mathbf{k})^\dagger h(\mathbf{k}) \mathcal{U}(\mathbf{k}), \quad (I3)$$

therefore vector $\hat{\mathbf{d}}$ is rotated as

$$\begin{aligned} \tilde{d}_x &= d_x \cos(\mathbf{k} \cdot \mathbf{r}) + d_y \sin(\mathbf{k} \cdot \mathbf{r}), \\ \tilde{d}_y &= -d_x \sin(\mathbf{k} \cdot \mathbf{r}) + d_y \cos(\mathbf{k} \cdot \mathbf{r}), \\ \tilde{d}_z &= d_z, \end{aligned} \quad (I4)$$

which gives the quantum metric change

$$\begin{aligned} \tilde{g}_{\mu\nu} &= g_{\mu\nu} + \frac{1}{4} [(-\hat{d}_x \partial_\mu \hat{d}_y + \hat{d}_y \partial_\mu \hat{d}_x) r_\nu \\ &+ (-\hat{d}_x \partial_\nu \hat{d}_y + \hat{d}_y \partial_\nu \hat{d}_x) r_\mu + (\hat{d}_x^2 + \hat{d}_y^2) r_\mu r_\nu], \end{aligned} \quad (I5)$$

where μ or $r_\mu = x$ or y . Then $I(\mathbf{r})$ of Eq. (20) is

$$I(\mathbf{r}) = I_0 + I_{1x}x + I_{1y}y + I_2(x^2 + y^2), \quad (I6)$$

with

$$\begin{aligned} I_0 &= \sum_{\mathbf{k}} f(\mathbf{k}) \text{Tr}g(\mathbf{k}), \\ I_{1\mu} &= \frac{1}{2} \sum_{\mathbf{k}} f(\mathbf{k}) (-\hat{d}_x \partial_\mu \hat{d}_y + \hat{d}_y \partial_\mu \hat{d}_x), \\ I_2 &= \frac{1}{4} \sum_{\mathbf{k}} f(\mathbf{k}) (\hat{d}_x^2 + \hat{d}_y^2). \end{aligned} \quad (I7)$$

Here, the form of $f(\mathbf{k})$ depends on whether the composite contains only one or both bands. For the former, $f(\mathbf{k}) = f_{v(c)}(\mathbf{k}) = \tanh(\beta E_{v(c)\mathbf{k}}/2)/E_{v(c)\mathbf{k}}$; for the latter,

$$\begin{aligned} f(\mathbf{k}) &= \frac{1}{E_{v\mathbf{k}}} \tanh \frac{\beta E_{v\mathbf{k}}}{2} + \frac{1}{E_{c\mathbf{k}}} \tanh \frac{\beta E_{c\mathbf{k}}}{2} \\ &- \tanh \frac{\beta E_{v\mathbf{k}}}{2} \left[\frac{2p_{vc}^{(+)}(\mathbf{k})}{E_{v\mathbf{k}} + E_{c\mathbf{k}}} + \frac{2p_{vc}^{(-)}(\mathbf{k})}{E_{v\mathbf{k}} - E_{c\mathbf{k}}} \right] \\ &- \tanh \frac{\beta E_{c\mathbf{k}}}{2} \left[\frac{2p_{vc}^{(+)}(\mathbf{k})}{E_{v\mathbf{k}} + E_{c\mathbf{k}}} + \frac{2p_{vc}^{(-)}(\mathbf{k})}{E_{c\mathbf{k}} - E_{v\mathbf{k}}} \right]. \end{aligned} \quad (I8)$$

Notice that $I_0, I_{1\mu}, I_2$ are all geometry-independent quantities. Completing the squares in Eq. (I6), one gets

$$I(\mathbf{r}) = I_0 - \frac{I_{1x}^2 + I_{1y}^2}{4I_2} + I_2 \left[\left(x + \frac{I_{1x}}{2I_2} \right)^2 + \left(y + \frac{I_{1y}}{2I_2} \right)^2 \right], \quad (I9)$$

indicating that the extremal position is located at $\mathbf{r}_{\min} = -(I_{1x}, I_{1y})/(2I_2)$. The sign of the parabola is determined by $\text{sgn}(I_2) = \text{sgn}(f(\mathbf{k}))$. It turns out that Eq. (I8) is the same as Eq. (E3), which we have proved to be positive. Therefore, for two-orbital models, no matter whether the composite contains one band or both the valence and conduction band, $I_2 > 0$, and the function is minimized at the point \mathbf{r}_{\min} . This is another example showing that the Hessian matrix M for a composite of two bands of a two-orbital model is positive semidefinite and $\text{Rank}(M) = 1$, with the first two conditions stated in Proposition 3 relaxed.

Next, we consider two prototype models, the Bravais-lattice BHZ model [80,81] and the non-Bravais-lattice Haldane model [82], to show how the parabola evolves under topological phase transitions.

The BHZ model [80,81] is defined on a square lattice. Choosing the geometric gauge where both orbitals sit on the same site, the Hamiltonian has

$$\mathbf{d}(\mathbf{k}) = (t \sin k_x, t \sin k_y, m + t \cos k_x + t \cos k_y). \quad (I10)$$

Inserting this into Eq. (I7), one gets $\mathbf{r}_{\min} = (0, 0)$, regardless of the composite, temperature, and value of m/t . This is enforced by the C_4 symmetry of the model hopping graph.

Similarly, the Bloch Hamiltonian of the Haldane model has

$$\begin{aligned} d_0(\mathbf{k}) &= 2t_2 \cos \phi \sum_{i=1}^3 \cos(\mathbf{k} \cdot \mathbf{a}_i), \\ d_x(\mathbf{k}) &= t_1 [1 + \cos(\mathbf{k} \cdot \mathbf{a}_2) + \cos(\mathbf{k} \cdot \mathbf{a}_3)], \\ d_y(\mathbf{k}) &= t_1 [\sin(\mathbf{k} \cdot \mathbf{a}_2) - \sin(\mathbf{k} \cdot \mathbf{a}_3)], \\ d_z(\mathbf{k}) &= m - 2t_2 \sin \phi \sum_{i=1}^3 \sin(\mathbf{k} \cdot \mathbf{a}_i). \end{aligned} \quad (I11)$$

Inserting this into Eq. (17), we find $\mathbf{r}_{\min} = (0, \sqrt{3})$, regardless of the composite, temperature, t_1 , t_2 , and m values. This is enforced by the C_6 symmetry of the hopping graph.

As $m/t \rightarrow \infty$, both the BHZ and Haldane model transit to the topologically trivial phase, in which $\hat{d}_x^2 + \hat{d}_y^2 \propto t^2/m^2 \rightarrow 0$ (during the transition, we assume t, t_1, t_2 are fixed but m is varied). Suppose the composite contains the isolated valence or conduction band only ($\Delta \sim t \ll m$). In that case, we find $f(\mathbf{k}) \sim 1/\Delta$, which has no dependence on m , therefore $I_2 \propto f(\mathbf{k})(\hat{d}_x^2 + \hat{d}_y^2) \rightarrow 0$, implying that the parabola in Eq. (19) becomes flat. This means the functional $I(\mathbf{r})$ becomes a constant in the geometric space as one orbital is removed from the band.

Conversely, if the composite contains both the valence and conduction band ($\Delta \sim m \gg t$), it always contains two orbitals, even in the topologically trivial phase. In the atomic limit, from Eq. (18), one can show

$$f(\mathbf{k}) \sim \frac{m^2}{\Delta^3}. \quad (I12)$$

Therefore, $I_2 \sim t^2/\Delta^3$ remains finite, and the rank of the Hessian matrix does not decrease. This means $I(\mathbf{r})$ of Eq. (19) remains parabolic in the atomic limit.

APPENDIX J: HESSIAN MATRIX OF NONUNIFORM PAIRING

This Appendix studies the properties of the matrix of the second derivative of the grand potential with order parameters beyond the uniform pairing. In particular, we show that this matrix may not be positive semidefinite.

We restrict the interaction to be an on-site intraorbital density-density interaction. We also assume a time-reversal invariant channel $\hat{\Delta}$ in orbital space, i.e., under TRS, the matrix $\hat{\Delta}$ is mapped to itself up to a $U(1)$ phase. Then for our interaction type, the pairing matrix at $\mathbf{q} = \mathbf{0}$ takes the diagonal form $\hat{\Delta} = \text{diag}\{\Delta_1, \Delta_2, \dots, \Delta_s\}$, whose entries are taken to be real but may be nonuniform.

For simplicity, we consider the case of a single isolated band at $T = 0$, with the gap equation given by Eq. (27). The

$\mathbf{q} = \mathbf{0}$ gap equation reads

$$\Delta_\alpha = \frac{U_\alpha}{N} \sum_{\mathbf{k}} |u_{m\mathbf{k}\alpha}|^2 \frac{\Delta_{m,\mathbf{k}}(0)}{2E_{m\mathbf{k}}}, \quad 1 \leq \alpha \leq s. \quad (J1)$$

Here $\Delta_{m,\mathbf{k}}(0) = \langle u_{m\mathbf{k}} | \hat{\Delta} | u_{m\mathbf{k}} \rangle$ is the band-projected gap at $\mathbf{q} = \mathbf{0}$, and $E_{m\mathbf{k}} = \sqrt{\xi_{m\mathbf{k}}^2 + \Delta_{m,\mathbf{k}}(0)^2}$ is the quasiparticle energy.

Following the discussions at the end of Appendix C and computing the derivative of Eq. (27), we find

$$M_{\alpha\beta} = \frac{\delta_{\alpha\beta}}{\Delta_\alpha} \sum_{\mathbf{k}} \frac{\Delta_{m,\mathbf{k}}(0)}{2E_{m\mathbf{k}}} |u_{m\mathbf{k}\alpha}|^2 - \sum_{\mathbf{k}} \frac{1}{2E_{m\mathbf{k}}} |u_{m\mathbf{k}\alpha}|^2 |u_{m\mathbf{k}\beta}|^2 \quad (J2)$$

and

$$V_{\alpha,\mu} = \sum_{\mathbf{k}} \frac{1}{2E_{m\mathbf{k}}} [(u_{m\mathbf{k}\alpha}^* \partial_\mu u_{m\mathbf{k}\alpha} - \partial_\mu u_{m\mathbf{k}\alpha}^* u_{m\mathbf{k}\alpha}) \Delta_{m,\mathbf{k}}(0) - 2|u_{m\mathbf{k}\alpha}|^2 \text{Im}\langle u_{m\mathbf{k}} | \hat{\Delta} | \partial_\mu u_{m\mathbf{k}} \rangle]. \quad (J3)$$

Now $U(1)$ symmetry imposes $\sum_{\beta=1}^s M_{\alpha\beta} \Delta_\beta = 0$ and $\sum_{\beta=1}^s V_{\alpha,\mu} \Delta_\beta = 0$, so the kernel vector is instead $\mathbf{v}_0 = (\Delta_1, \Delta_2, \dots, \Delta_s)^T$.

For the most general case, $\text{Rank}(M) = s - 1$. To study the semidefiniteness, we take two-orbital models as an example. Note that the off-diagonal elements of $M_{\alpha\beta}$ are all negative, so we write

$$M_{\alpha\beta} = \begin{pmatrix} a & -b \\ -b & c \end{pmatrix}, \quad (J4)$$

with $b > 0$. Kernel eigenvector \mathbf{v}_0 leads to $a = (\Delta_2/\Delta_1)b$ and $c = (\Delta_1/\Delta_2)b$. Since a, c are the diagonal entries of M , we conclude that for the two-orbital case, the Hessian matrix is positive semidefinite if and only if $\text{sgn}(\Delta_1 \Delta_2) = 1$. This result coincides largely but not completely with the pair density-wave transition discovered in Ref. [58] when one Hubbard interaction turns repulsive, $U_1 U_2 < 0$. However, as a reminder, there it was also found that a solution channel with $\text{sgn}(\Delta_1 \Delta_2) = -1$ exists when both interactions are attractive, $U_1, U_2 > 0$.

For models with more than two orbitals, similar but more complicated conditions will be required for a nonpositive-definite Hessian matrix.

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