Törmä, Päivi; Liang, Long; Peotta, Sebastiano

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Quantum metric and effective mass of a two-body bound state in a flat band

P. Törmä,* L. Liang,† and S. Peotta
Department of Applied Physics, Aalto University, FI-00076 Aalto, Finland

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We consider two-body bound states in a flat band of a multiband system. The existence of pair dispersion predicts the possibility of breaking the degeneracy of the band and creating order, such as superconductivity. Within a separable interaction potential approximation, we find that the finiteness of the effective mass of a bound pair is determined by a band-structure invariant, which in the uniform case becomes the quantum metric. The results offer a simple foundation to understand and predict flat-band superconductivity. We propose an experiment to test the interaction-induced pair motion.

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The concept of a flat band refers to Bloch bands of periodic systems, which are either perfectly dispersionless or where the bandwidth is negligible compared to other energy scales. The effects of interactions and disorder are enhanced in such systems. This may lead to magnetic order [1–3] and fractional Chern insulators [4]. Also, a high critical temperature for Cooper pairing has been predicted [5–7] in the case of attractive (effective) interactions. The group velocity of a single particle is zero and its effective mass \( m_{\text{eff}} \) infinite in a flat band. The conventional single-band prediction for supercurrent, \( n/m_{\text{eff}} \), where \( n \) is the superfluid density, would thus suggest the absence of superfluidity. However, it has been predicted that, in a multiband system, interaction-induced movement of pairs is possible [8–11] while single particles remain localized [12]. In recent experiments on bilayer graphene [13,14], superconductivity was found to coincide with the formation of flat bands at certain angles of the bilayer twist [15,16]. The large number of differing theoretical descriptions for these observations demonstrates the importance of understanding the origin of flat-band superconductivity in as simple terms as possible. Here, we show that the two-body problem can be used to predict the possibility of superfluidity in a flat band. We find that the pair effective mass is characterized by band invariant quantities proportional to derivatives of the Bloch functions, in particular, the quantum metric.

In the Cooper problem [17], the bound state energy of two fermions of opposite spins was solved while restricting the available phase space to a thin shell around the Fermi sea. This revealed that the Fermi sea is unstable towards the formation of Cooper pairs for arbitrarily small attractive interactions, while without the Fermi sea, bound states require a finite interaction. Since flat-band states are degenerate, a Fermi level cannot be defined for noninteracting particles. To form a many-body state with some symmetry broken order, such as superconductivity, the degeneracy has to be lifted. We now ask whether the tendency for breaking the degeneracy can be predicted from the two-body problem. In contrast to the Cooper problem and conventional superconductivity, we are interested in the instability of the degeneracy instead of instability of the Fermi sea. In the flat-band case, showing that a bound state exists is not as such sufficient: If the bound pair energy remains degenerate, then condensation to a certain pair momentum state—the basic mechanism of superconductivity—is not likely. We argue that the existence of a dispersion and finite effective mass for the pairs points to breaking the degeneracy and the formation of superfluid/superconducting order in the many-body case. We now proceed to find under which general conditions the flat-band two-body problem in a multiband system may feature bound states with a dispersion. Our goal and results are different from the calculation of scattering states in a flat band [18], and from the Cooper problem in a single dispersive band [19].

We consider two interacting particles in a periodic potential and interacting via an interaction potential \( \lambda V(1, 2) \). The two-body Schrödinger equation is \( (T_1 + T_2 + \lambda V(1, 2))|\psi(1, 2)\rangle = E|\psi(1, 2)\rangle \), where \( T_1 + T_2 \) contains the kinetic energies and the periodic potential. The two particles can be either fermions or bosons. The solution for \( \lambda = 0 \) is the two-particle state given by \( (T_1 + T_2)|\phi_n\rangle = E_n|\psi_n\rangle \), where \( n \) contains all quantum numbers (band index, lattice momentum, spin) of the two-particle state. Let \( |\phi(1, 2)\rangle \) denote the state of the particles in the absence of interactions and \( E_0 \) the corresponding energy. We consider a flat band where \( E_n = E_0 \) (or \( E_n \approx E_0 \)). We denote by \( n \) the states in this flat band and by \( n' \) those in other dispersive or flat bands. The solution that fulfills the Schrödinger equation is given by

\[
|\psi(1, 2)\rangle = |\phi(1, 2)\rangle + \sum_{n \neq 0} \frac{|\phi_n\rangle}{E - E_0} \psi_n\lambda V|\psi(1, 2)\rangle
\]

\[
+ \sum_{n'} \frac{|\phi_{n'}\rangle}{E - E_{n'}} \psi_{n'}\lambda V|\psi(1, 2)\rangle,
\]

\[
E - E_0 = \langle \phi_0|\lambda V|\psi(1, 2)\rangle.
\]

We then assume the isolated flat-band limit: The lowest/highest energies \( E'_{\min/\max} \) of the bands above/below the flat band are separated from it by a band gap that is larger than the
interactions, \(|E_0 - E'_{\text{min}/\max}| \geq |\lambda|\). If we further assume that \(E\) is close to \(E_0\) (weak interactions), then \(|E - E'_{\text{min}/\max}| \geq |\lambda|\) and the last term of Eq. (1) becomes negligible. We proceed with

\[|\psi(1, 2)| = |\varphi_0(1, 2)| + \frac{1}{E - E_0} \sum_{n \neq 0} |\varphi_n| |\lambda V| |\psi(1, 2)|,\]

where \(n\) refers to quantum numbers in the isolated flat band, and we introduced the notation \(E_0\) for the pairing binding energy. We use units where \(\hbar\) and the system volume are set to one.

We use the Bloch functions \(e^{i k \cdot x} m_k(x)\) of the flat band where \(k\) is the lattice momentum and the band and spin indices are not marked explicitly. Then, \(\varphi_0(x_1, x_2) = e^{i k_1 \cdot x_1} m_{k_1}(x_1) e^{i k_2 \cdot x_2} m_{k_2}(x_2) = e^{i q \cdot \mathbf{R}} e^{i k \cdot x} m_{k + \frac{1}{2}}(x_1) m_{k - \frac{1}{2}}(x_2)\), where \(q = k_1 + k_2\), \(k = (k_1 - k_2)/2\), \(\mathbf{R} = (x_1 + x_2)/2\), \(r = x_1 - x_2\) are the center-of-mass (c.m.) and relative momenta and coordinates, respectively. We consider interaction potentials \(V\), whose dependence on the c.m. coordinate has the same periodicity as the lattice, then the c.m. momentum \(q\) of the two particles is conserved. Even when we consider the two-body problem in the isolated flat band, the multiband nature of the system is inherent in the spatial dependence of the periodic part of the Bloch function, \(m_k(x)\). In the language of lattice models, it contains the orbital dependence of the Bloch function. We consider a general interaction potential \(V = V(x_1, x_2)\) instead of \(V = V(r)\) to incorporate the possible effects arising from the spatial (orbital) dependence of the interaction and the Bloch functions.

We now make our second approximation: Consider a separable potential \([20]\) \(V(x_1, x_2) \rightarrow u(x_1, x_2) u(x_1, x_2)\), and assume \(u\) real. Until Eq. (5), we adapt to the flat-band case the calculations of Sec. 36 of Ref. [20], and the intermediate steps are given in the Supplemental Material [21] (where we also show that an alternative approach using a variational ansatz produces the same results). The result becomes

\[E_b = \lambda \sum_k |\bar{u}(q, k)|^2,\]

\(\bar{u}(q, k) = \int d x_1 d x_2 e^{-i k \cdot x} m^*_{k + \frac{1}{2}}(x_1) m^*_{k - \frac{1}{2}}(x_2) u(x_1, x_2)\), and the momentum summation is over the first Brillouin zone. This shows that, for attractive (effective) interactions \((\lambda < 0)\), a bound state \((E_b < 0)\) exists whenever \(\bar{u}(k_1, k_2)\) is nonzero for a sufficiently large number of momenta so that the sum in (4) is nonvanishing in the thermodynamical limit. Importantly, the bound state energy is linearly proportional to the coupling constant \(\lambda\). Bardeen-Cooper-Schrieffer (BCS) mean-field theory for a flat-band system predicts a linear dependence of the order parameter (pairing gap) \([6, 22]\) and the superfluid weight \([11]\) on the coupling constant. Our result shows that this dependence is predicted already at the two-body level. The linear dependence is in striking contrast to the exponential suppression by \(\lambda\) of the order parameter (pairing gap) in the BCS theory and two-body Cooper problem in a dispersive system. The bound state energy in dispersive systems is, for small \(\lambda\), proportional to \(\lambda^2\) in one dimension and exponentially suppressed by \(\lambda\) in two dimensions \([23]\), similarly to the BCS result. The linear dependence of \(E_b\) in Eq. (4) is different from these and independent of dimension.

To find out whether the bound pair has a dispersion, we study \(|\bar{u}(k_1, k_2)|^2\) further. We bring back the original interaction potential using \(u(x_1, x_2) u(x_1', x_2') \rightarrow V(x_1, x_2) \delta(x_1 - x_1') \delta(x_2 - x_2')\). Furthermore, we assume a contact interaction \(V(x_1, x_2) = V(x_1) \delta(x_1 - x_2)\), consider interacting particles that have opposite spins, and use the relation (consequence of time-reversal symmetry) \(m^*_{k_1} = m^*_{k_2} \equiv m_k\). The potential \(V(x_1)\) has the periodicity of the lattice but may be different at each site of the unit cell (orbital). We obtain

\[E_b = \lambda \sum_k \int d x V(x) |m_{k + \frac{1}{2}}(x) m_{k - \frac{1}{2}}(x)|^2.\]

The result is intuitive: In a flat band, kinetic energy effects are absent, thus the pairing energy is given solely by the probability of the particles to overlap in space and the local interaction potential.

We now expand the result (5) with respect to small pair momentum, \(m_{k + \frac{1}{2}} = m_k + \frac{1}{2} \partial_i m_k + \frac{3}{2} q_i q_j \partial_i \partial_j m_k + O(q^3)\). Summation is assumed over repeated indices and \(\partial_i \equiv \partial/\partial k_i\). This gives

\[E_b \simeq \lambda \sum_k \int d x V(x) \left( P_k(x)^2 - \frac{q_i q_j}{4} \left[ \partial_i P_k(x) \partial_j P_k(x) - P_k(x) \partial_i \partial_j P_k(x) \right] \right) - \frac{q_i q_j}{2} \partial_i P_k(x) \partial_j P_k(x),\]

where \(P_k(x) = m_k^* m_k(x) = \langle x | m_k^* | m_k(x) \rangle\) is the diagonal element of the Bloch state projector \(P_k = |m_k^* m_k\rangle \langle m_k^* m_k|\). The effective mass tensor is therefore

\[\begin{bmatrix} \frac{1}{m^*} \end{bmatrix}_{ij} = -\lambda \sum_k \int d x V(x) [\partial_i P_k(x) \partial_j P_k(x)].\]

This means that the existence of a finite, positive effective mass, and thus the possibility of breaking the degeneracy towards an ordered state, depends on the derivatives of the flat-band projector in a simple way. The result is gauge invariant and independent of the basis. In the case of a trivial flat band, such as a single-band lattice model with vanishing hopping, the periodic part of the Bloch function is independent of momentum and the pair mass remains infinite, preventing superfluidity. In a multiband lattice model, the derivatives can be finite. Bear in mind that the separable potential approximation leads to only one bound state, which is the sum of the exact bound states. However, we show in the following that, for several interesting lattice models, only one (significantly) dispersive bound state exists and therefore the result (8) is actually an excellent estimate for the pair effective mass, although the energy (7) has an offset from the exact value.

The superfluid weight \(D_{ij}\) defined as the change in energy density \(\delta E = D_{ij} q_i q_j / 2\) due to supercurrent \(\mathbf{q}\) has been shown to be proportional to the quantum metric by multi-band mean-field theory \([11, 24]\), dynamical mean-field theory, density-matrix renormalization-group calculations and exact diagonalization \([12, 25–27]\), as well as by semiclassical \([28]\)
and perturbative [29] approaches. The quantum metric [30] (Fubini-Study metric) $g_{ij}(\mathbf{k})$ can be defined via the infinitesimal Bures distance between two quantum states $D^2_{\text{Bures}} = 1 - |\langle \psi(\mathbf{k}) | \psi(\mathbf{k} + d\mathbf{k}) \rangle|^2 \simeq \sum_i g_{ij}(\mathbf{k}) dk_i dk_j$ when a parameter $\mathbf{k}$ is varied. The quantum metric is the real part of the quantum geometric tensor whose imaginary part is the Berry curvature. This connection allows us to determine the finite Chern number and Berry curvature as the lower bounds for superfluid weight using multiband BCS theory [11,26]. Remarkably, the essentials of such lower bounds can already be obtained from the two-body problem in a flat band, as we will show below.

To make a connection to previous many-body results, let us first note that the continuum results (5)–(8) can be mapped to a tight-binding description (see Supplemental Material [21]), with the only consequence being that in (8) the integration of the position coordinate becomes a summation over the orbital coordinate within one unit cell (u.c.), and we write the system volume, namely, the number of unit cells $N_c$, explicitly. We consider now an interaction potential that does not depend on position (orbital-independent potential), $V(\mathbf{x}) = 1$. The inverse effective mass (8) then becomes $-\lambda/N_c \sum_{\mathbf{x} \in \text{u.c.}} |\mathbf{x} \rangle \langle \mathbf{x}| \partial_i P_\mathbf{k} \partial_j P_\mathbf{k} |\mathbf{x} \rangle \langle \mathbf{x}|$. We approximate this by $-\lambda/(N_c N_{\text{orb}}) \sum_{\mathbf{x} \in \text{u.c.}} |\mathbf{x} \rangle \langle \mathbf{x}| \partial_i P_\mathbf{k} \partial_j P_\mathbf{k} |\mathbf{x} \rangle \langle \mathbf{x}|$, where $N_{\text{orb}}$ is the number of orbitals in the unit cell, which is valid when $|\mathbf{x} \rangle \langle \mathbf{x}| \sim |\mathbf{x} \rangle \langle \mathbf{x}|$. The approximation is further motivated by its similarity to the BCS mean-field approach (see Supplemental Material [21]). Using $\sum_{\mathbf{x} \in \text{u.c.}} |\mathbf{x} \rangle \langle \mathbf{x}| = 1$ we obtain

$$\left[ \frac{1}{m^*} \right]_{ij} = -\frac{\lambda}{N_c N_{\text{orb}}} \sum_\mathbf{k} \text{Tr} [\partial_i P_\mathbf{k} \partial_j P_\mathbf{k}] = -\frac{\lambda}{N_c N_{\text{orb}}} \sum_\mathbf{k} g_{ij}(\mathbf{k}),$$

(9)

where $g_{ij}(\mathbf{k})$ is the quantum metric. In Refs. [11,26,29], the superfluid weight $D_{ij}$ was derived in the isolated flat-band approximation and assuming uniform pairing (precisely, the orbital-independent interaction and $\int d\mathbf{k} |m_\mathbf{k}(\mathbf{x})|^2$ being the same for all $\mathbf{x}$). The relation between the superfluid weight and the effective mass in a flat band (see Supplemental Material [21]) is $D_{ij} \simeq n(1/m^*)_{ij}$ when the Cooper pair density $n$ is small. Using this, the reference effective mass given by Ref. [11] becomes $(1/m^*)_{ij} = -\lambda/(N_c N_{\text{orb}}) \sum_\mathbf{k} g_{ij}(\mathbf{k})$, which is the same as the result (9) obtained by the two-body calculation.

The result (6) inspires us to introduce and calculate the infinitesimal difference in local (orbital-specific) wave-function overlaps as follows,

$$D_{\text{overlap}} = |m_\mathbf{k}(\mathbf{x}) m_\mathbf{k}(\mathbf{x})|^2 - |m_{\mathbf{k} + d\mathbf{k}}(\mathbf{x}) m_{\mathbf{k} - d\mathbf{k}}(\mathbf{x})|^2$$

$$\simeq \sum_{ij} [\partial_i P_\mathbf{k} \partial_j P_\mathbf{k} (\mathbf{x}) - P_\mathbf{k}(\mathbf{x}) \partial_i \partial_j P_\mathbf{k}(\mathbf{x})] dk_idk_j$$

$$\equiv \sum_{ij} g_{ij}^{\text{local}}(\mathbf{k}, \mathbf{x}) dk_idk_j,$$

(10)

where we have defined the “local quantum metric” $g_{ij}^{\text{local}}(\mathbf{k}, \mathbf{x})$, which is of the same form as the usual quantum metric but with the projector $P_\mathbf{k} = |m_\mathbf{k}|^2/m_\mathbf{k}$ replaced by its local matrix element $P_\mathbf{k}(\mathbf{x}) = |m_\mathbf{k}(\mathbf{x})|^2/m_\mathbf{k}(\mathbf{x})^2$.

The local quantum metric is both basis and gauge independent, unlike the conventional quantum metric and Berry curvature that are gauge invariant but depend on the basis [31,32], but on the other hand, it is not positive semidefinite and thus not a Riemannian metric. We have shown in (6) that the local quantum metric determines the flat-band bound pair effective mass, and can be connected to the usual (global) quantum metric when assuming uniform pairing. Whether a physically meaningful “local Berry connection (curvature)” exists is a topic of future research.

We test the analytical results against exact numerical solutions of the two-body Schrödinger equation in selected lattice models that feature flat bands. The contact interaction is used. For the one-dimensional (1D) sawtooth ladder, which has one flat band [Fig. 1(a)], we solve the two-body problem numerically by taking into account all the bands. We find two bands formed by the bound states, and the dispersion of the bound state energy obtained from the separable potential approximation (7) agrees (with an offset) with that of the exact lower band [see Fig. 1(a)]. For the two-dimensional (2D) Lieb lattice, the middle band is flat and can be made gapped from the lower and upper bands by staggered hopping. We solve the Lieb lattice two-body problem within the
have been studied in experiments (see, e.g., Ref. [34]) where gas experiments [33]. The propagation speeds of particles interaction strength and is essentially determined by Eq. (8). should propagate with a speed that increases linearly with the particles for motion. In a flat band, noninteracting atoms the lattice potential is initially combined with a harmonic interaction gives

\[ v_{\text{exp}} = \frac{\pi n}{\sqrt{\lambda^2 t}} \]

form obtained by calculating the ground state of a trapping potential of the body bound state in the sawtooth ladder. The initial wave-packet is released and expands as shown in the inset for the specific case \( V_0 = -2t \) and \( \lambda = -3t \). There, \( i \) is the unit cell label and \( \rho(i) \) the density distribution (identical for the two particles) summed over all orbitals in unit cell \( i \), at times \( 100/t, 250/t, \) and \( 350/t \). In the main plot the expansion velocity \( v_{\text{exp}} \) is shown as a function of the interaction strength \( |\lambda| \) for two different values of \( V_0 \). Red lines show fits to \( |\lambda|^r \); for details, see the text.

isolated band approximation by considering only the middle band. Again, we find that the lower bound state band dispersion agrees with the result from the separable potential approximation (7). For results on the Harper model (Landau levels forming a flat band), see the Supplemental Material [21].

Our results can be directly tested in ultracold quantum gas experiments [33]. The propagation speeds of particles have been studied in experiments (see, e.g., Ref. [34]) where the lattice potential is initially combined with a harmonic trapping potential that is later switched off, releasing the particles for motion. In a flat band, noninteracting atoms are expected to stay localized, while with interactions, pairs should propagate with a speed that increases linearly with the interaction strength and is essentially determined by Eq. (8). This is strikingly different from the dispersive band case when the single-particle band structure alone is complex, and for \( \lambda > 0 \), so-called repulsively bound pairs could be observed [35].

In summary, we show that the energy of a two-body bound state in a flat band is linearly proportional to the interaction constant and depends on the overlap of the periodic part of the Bloch functions and the orbital structure of the interaction potential in a simple way. The pair momentum dependence of the bound state energy can be used to determine the effective mass. Within the separable potential approximation, we find that it is essentially defined by a gauge- and basis-independent quantity that we call the local quantum metric. With further approximations on the uniformity of the interactions and Bloch functions, we recover the dependence of the effective mass on geometric quantities, such as the (global) quantum metric and Berry curvature predicted earlier by many-body approaches. We demonstrate the adequacy of our approximate analytical results by comparison to exact solutions of the two-particle problem in the sawtooth ladder, Lieb lattice, and Harper models; these and other flat-band models can be realized, for instance, with ultracold gases [36–40] or designer materials [41,42], and the Brillouin zone integrated quantum metric can be measured [43]. We propose a direct signature of the predictions via an ultracold gas expansion experiment.

Our results show that the two-particle problem already gives the salient features of the corresponding BCS mean-field (and other many-body) theory predictions. This suggests that in understanding and predicting superconductivity in flat bands of multiband systems, knowledge of the orbital dependence of the interaction and the noninteracting band structure can already be quite powerful. This may be advantageous when the single-particle band structure alone is complex, for instance, involving a large unit cell as in twisted bilayer 2D materials, and therefore formulating a suitable many-particle lattice model is a challenge. Our approach can be easily extended to different pairing symmetries. The two-body approach may also be, due to its computational lightness, well suited for materials discovery and optimization to find new flat-band superconducting materials. The two-body effective mass also gives the first-order estimate of the Berezinskii-Kosterlitz-Thouless (BKT) temperature via the relation [44–46] \( T_{\text{BKT}} = \pi/2\sqrt{\det[D^2(T_{\text{BKT}})]} \leq \pi/2\sqrt{\det[D^2(T = 0)]} \sim \pi n/2\sqrt{\det[I/m^2]} \).

Furthermore, it gives a benchmark for full many-body descriptions to distinguish strong correlation effects. Our results highlight the role of the local and global quantum metric in a flat band and provide intuitive insight to the connection between superfluidity and quantum geometry. While all flat bands have a high density of states, the distances between the Bloch functions may differ in ways that are decisive for superconductivity.

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