

Real space decay of flat band projectors from compact localized states

Yeongjun Kim^{1,2,*} Sergej Flach^{1,2,3,†} and Alexei Andreanov^{1,2,‡}

¹Center for Theoretical Physics of Complex Systems, Institute for Basic Science (IBS), Daejeon, Korea, 34126

²Basic Science Program, Korea University of Science and Technology (UST), Daejeon 34113, Republic of Korea

³Centre for Theoretical Chemistry and Physics, The New Zealand Institute for Advanced Study (NZIAS), Massey University Albany, Auckland 0745, New Zealand

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Flatbands (FB) with compact localized eigenstates (CLS) fall into three main categories, controlled by the algebraic properties of the CLS set: orthogonal, linearly independent, linearly dependent (singular). A CLS parametrization allows us to continuously tune a linearly independent FB into a limiting orthogonal or a linearly dependent (singular) one. We derive the asymptotic real space decay of the flat band projectors for each category. The linearly independent FB is characterized by an exponentially decaying projector and a corresponding localization length ξ , all dressed by an algebraic prefactor. In the orthogonal limit, the localization length is $\xi = 0$, and the projector is compact. The singular FB limit corresponds to $\xi \rightarrow \infty$ with an emerging power law decay of the projector. We obtain analytical estimates for the localization length and the algebraic power law exponents depending on the dimension of the lattice and the number of bands involved. Numerical results are in excellent agreement with the analytics. Our results are of relevance for the understanding of the details of the FB quantum metric discussed in the context of FB superconductivity, the impact of disorder, and the response to local driving.

Introduction — Flat bands (FB) emerge in certain lattice models as bands with zero dispersion, leading to complete suppression of transport [1–4]. FB Hamiltonians with finite-range hopping support compact localized eigenstates (CLS) [5], eigenstates that turn strictly zero outside a finite volume due to destructive interference. The recent surge of interest in FBs is due to their non-trivial response to external perturbations such as unconventional superconductivity [6] and robust fractional quantum Hall effects in twisted bilayer graphene [7] due to nearly flat band/narrow dispersion, ferromagnetism [1, 8–11], anomalous Landau levels [12], disorder [13–18], many-body FB localization [19–23], and compact discrete breathers [24–26]. Flat bands have been realized in multiple experimental settings [27–43].

FB Hamiltonians can be obtained from the knowledge of the exact CLS using FB generators which assume a CLS and find the Hamiltonian supporting this CLS as an eigenstate [44–48]. We classify flat band models according to their CLS set properties. The set is obtained from translated copies of an irreducible CLS and can be (a) orthonormal (orthogonal), (b) linearly independent (but not orthogonal), and (c) linearly dependent [4]. Flat bands from class (c) are also coined *singular*. The simplest orthogonal FBs are obtained with a CLS residing in just one unit cell [49]. Linearly independent FBs are typically gapped away from a relevant dispersive part of the band structure [42, 44, 50]. Singular FBs exist only in lattice dimension $d \geq 2$ and necessarily band touches at least one dispersive band in at least one point in k -space [3, 47, 51, 52]. One dispersive band results in dou-

ble degeneracy and quadratic dispersion close to the degeneracy point (quadratic touching), while two dispersive bands can result in triple degeneracy, be (at least locally) symmetry related and have linear dispersion close to the degeneracy point (linear touching).

The algebraic features of the CLS set determine the real space properties of the FB projectors. Weakly perturbed FBs are effectively described by projecting a perturbation onto the flat band eigenspace [15–17, 42, 53]. The FB projector is also an experimentally relevant quantity: in experiments, prepared artificial lattices are often driven locally. The response to such a driving at the FB energy is controlled by the FB projector [42, 43, 50].

Main results — We obtain the asymptotic real space decay of FB projectors for the above three FB classes [2–4]:

- *Orthogonal FBs* result in compact (strictly finite support) FB projectors, very similar to their CLSs.
- *Linearly independent FBs* are gapped and characterized by exponentially decaying projectors dressed by algebraic prefactors, due to the nonzero overlap of neighboring CLSs. The exponent is related to a localization length scale ξ and the algebraic prefactor is given by $r^{-(d-1)/2}$. We obtain analytical estimates for ξ for small band gaps (Fig. 1 and text below).
- *Singular FBs* ($d \geq 2$): Linear dependence of the CLS set enforces n -fold degeneracy of the FB Hamiltonian at a singular location in k space, typically with $n = 2, 3$. The flat band touches one (or more) dispersive bands. The projector decay is entirely defined by the Taylor expansion of the FB Bloch eigenstates around the degeneracy point. The algebraic decay is r^{-d} , unless anisotropic corrections apply (Fig. 2 and text below).

* yeongjun.kim.04@gmail.com

† sflach@ibs.re.kr

‡ aalexei@ibs.re.kr

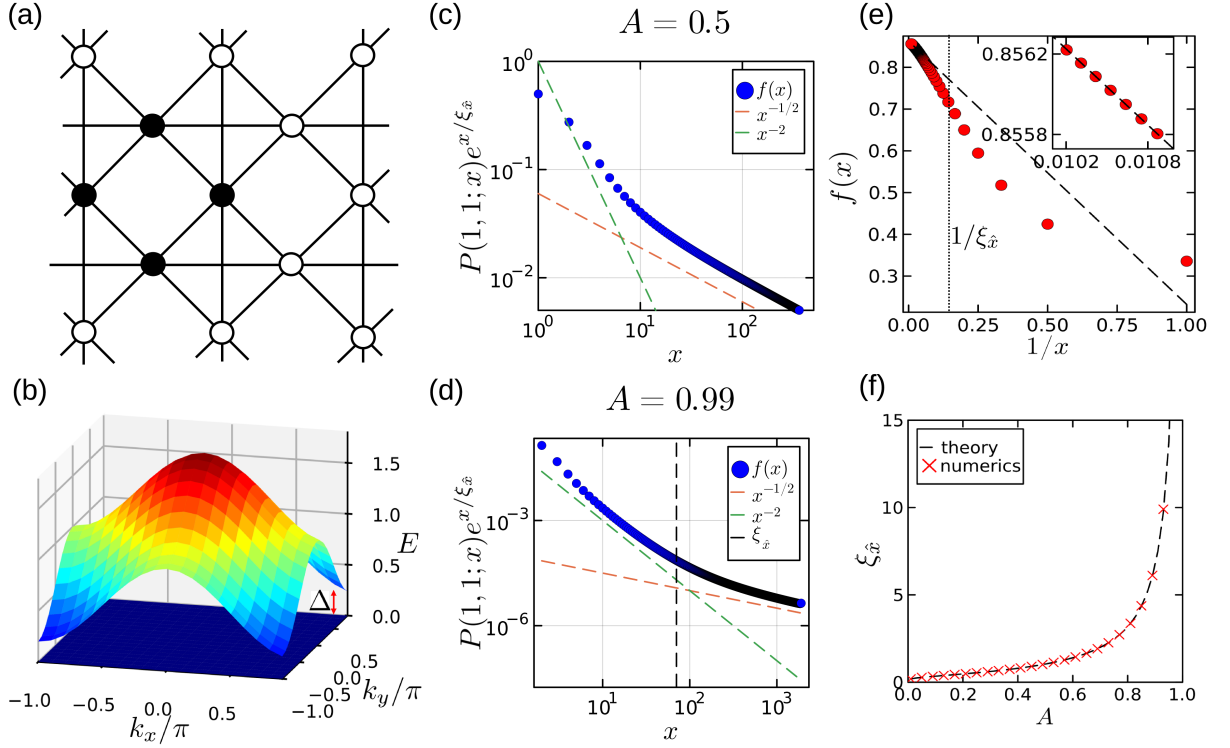


FIG. 1: The generalized 2D checkerboard lattice. Note that the black lines represent hoppings with tunable values. (a): The lattice structure. Black circles represent a CLS [See Eq. (5)]. For the values of hoppings and CLS amplitudes, see SM [54]. (b): The band structure. The two bands are $E_{\text{FB}} = 0$, and $E_{\text{DB}}(k) = \alpha^2(k)$. Here, $A = 0.5$. Δ is the band gap. (c) Algebraic part of the projector $P(x)e^{x/\xi}$ shown in log-log plot. The red and green dashed lines guide the eye for $x^{-1/2}$ and x^{-2} respectively. The parameter $A = 0.5$ places the FB model half way between orthogonal ($A = 0$) and singular ($A = 1$) limits. (d) Same as (c) but $A = 0.99$. This places the FB model in close proximity to the singular limit. The vertical black dashed line indicates the value of the localization length $\xi_{\hat{x}} = 70$ (e): ratio $f(x) = P(1, 1; x + 1)/P(1, 1; x)$ vs. $1/x$. Here $A = 0.9$. The straight black dashed line is obtained from a linear fit of the smallest $1/x$ data (see inset). Its intercept value with the y-axis is 0.86 and results in a numerical estimate of $\xi = 6.7$ in excellent agreement with our analytics. The slope of the dashed line is -0.54 (after dividing by y-intercept) in excellent agreement with the analytical prediction $-e^{-1/\xi}/2$ (the value gets close to -0.5 as larger system size increases). The departure of the data from the dashed line are observed precisely at $1/x = 1/\xi$ as predicted by analytics and indicated by the vertical dotted line. (f): Localization length $\xi_{\hat{x}}$ versus A . Symbols - numerical results from the above intercept fitting. Dashed line - analytics.

We demonstrate a smooth tuning of an orthogonal to linearly independent to singular flat band and its associated localization length. We further reveal the subtle emergence of the crossover from the $1/r^{(d-1)/2}$ decay component of a linearly independent FB projector to the $1/r^d$ projector decay of a singular FB at a distance of the order of ξ . We obtain analytical estimates for ξ in this regime, including its anisotropic directional dependence (Fig. 1). We then demonstrate the anisotropic algebraic decay of singular FB models in dimensions $d = 2, 3$ using several examples (Fig. 2).

Basic setup— We consider a finite-range hopping tight-binding Hamiltonian H on a d -dimensional lattice Λ with a number u of sublattices. In the momentum basis $|\mu, \mathbf{k}\rangle$, H is block-diagonalized into a $u \times u$ Hamiltonian matrix for each $\mathbf{k}$, $\mathcal{H}(\mu, \nu; \mathbf{k}) = \langle \mu, \mathbf{k} | H | \nu, \mathbf{k} \rangle$ with μ, ν the row and column orbital indices. Diagonalizing $\mathcal{H}(\mathbf{k})$ yields the band structure. We assume

a single perfectly flat band of energy E_{FB} with Bloch eigenvector $\psi_{\text{FB}}(\mu, \mathbf{k})$ in the band structure. For any FB with normalized Bloch eigenvector $\psi_{\text{FB}}(\mu, \mathbf{k})$ there exists a scalar gauge factor $\alpha(\mathbf{k})$ such that the Bloch-CLS (BCLS) $\phi_{\text{BCLS}}(\mu, \mathbf{k}) \equiv \alpha(\mathbf{k}) \psi_{\text{FB}}(\mu, \mathbf{k})$ is a finite Laurent polynomial in $z_j = e^{ik_j}$ [5]. We then observe that the CLS centered at the origin with amplitudes $\phi_{\text{CLS}}(\mu, \mathbf{r}) \equiv \langle \mu, \mathbf{r} | \text{CLS}^0 \rangle$ is the inverse lattice Fourier transform of $\phi_{\text{BCLS}}(\mu, \mathbf{k})$. We repeat that $\phi_{\text{CLS}}(\mu, \mathbf{r})$ is compact and has finite support. The gauge $\alpha(\mathbf{k})$ is chosen such that the resulting ϕ_{CLS} has minimal real-space support (irreducible CLS [44]). Equivalently, any common Laurent factor of the components of BCLS has been absorbed into $\alpha(\mathbf{k})$. Without loss of generality we can as-

sume $\alpha(\mathbf{k}) \geq 0$ and obtain (see SM [54])

$$\alpha^2(\mathbf{k}) = \sum_{\mathbf{r} \in \Lambda} \langle \text{CLS}^0 | \text{CLS}^{\mathbf{r}} \rangle e^{i\mathbf{k} \cdot \mathbf{r}} = \phi_{\text{BCLS}}^\dagger(\mathbf{k}) \phi_{\text{BCLS}}(\mathbf{k}). \quad (1)$$

$\alpha(\mathbf{k})$ is a signature for the threefold classes introduced above: (i) *orthogonal* FBs: $\alpha(\mathbf{k})$ is constant; (ii) *linearly independent* FBs: $\alpha(\mathbf{k})$ varies with $\mathbf{k}$ but is gapped away from zero for all $\mathbf{k}$; (iii) *singular* FBs: $\alpha(\mathbf{k})$ varies with $\mathbf{k}$ with no gap from zero such that $\alpha(\mathbf{k}_0) = 0$ for some $\mathbf{k}_0$ (see SM for the details [54]).

Real space behavior of flat band projectors — The real space and momentum space representation of projection onto the FB are given by:

$$P(\mu, \nu; \mathbf{r}) = \frac{1}{(2\pi)^d} \int_{\text{BZ}} \mathcal{P}(\mu, \nu; \mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}} d^d \mathbf{k} \quad (2)$$

$$\mathcal{P}(\mu, \nu; \mathbf{k}) = \frac{\phi_{\text{BCLS}}^*(\mu, \mathbf{k}) \phi_{\text{BCLS}}(\nu, \mathbf{k})}{\alpha^2(\mathbf{k})} \quad (3)$$

where BZ refers to Brillouin zone, and μ, ν are sublattice indices. Such projectors are localized in real space, since assuming $|\mathcal{P}(\mu, \nu; \mathbf{k})| < \infty$ results in $P(\mu, \nu; \mathbf{r}) \rightarrow 0$ when $\mathbf{r} \rightarrow \infty$ due to Riemann-Lebesgue lemma [55]. The asymptotic decay of $P(\mu, \nu; \mathbf{r})$ for large $\mathbf{r}$ depends of the FB class. For orthogonal flat bands the integrand in Eq. (2) is given as a finite Fourier series of the harmonics in Brillouin zone, since $\alpha(\mathbf{k}) = 1$. The projector in real space is therefore compact (see [54] for details, and earlier results for $d = 1$ in Ref. 56).

In the linearly independent case the long-distance behavior of the integral in Eq. (2) can be understood by interpreting $\mathcal{P}(\mu, \nu; \mathbf{k})$ in Eq. (3) as a lattice Green function at $E = 0$. The asymptotics of the projector is therefore similar to that of the Green's function evaluated outside the band. Using the saddle point analysis [57, 58], we obtain the Ornstein-Zernike (OZ) form for the generic case

$$P(\mu, \nu; \mathbf{r}) \sim r^{-\frac{d-1}{2}} \exp(-r/\xi_{\mathbf{r}}) \quad (4)$$

with a direction dependent localization length $\xi_{\mathbf{r}}$ (see Fig. 1, SM, and cf. Ref. [59]). Using Eq. (1), the relevant saddle (and thus $\xi_{\mathbf{r}}$) is determined by the pattern of overlaps between shifted CLSs. In the 1D case, the localization length ξ is an explicit function of the overlap σ , $\langle \text{CLS}_j | \text{CLS}_i \rangle = \delta_{i,j} + \sigma \delta_{i,\pm 1}$ derived in Refs. 42 and 60.

It is instructive to consider two limiting cases of linearly independent flat bands when tuned into singular and orthogonal FBs. We remind that such a tuning can be easily obtained by smoothly varying the amplitudes of the CLS accordingly. For the linearly independent FB close to becoming a singular one, the FB energy gap Δ is approaching zero. The flat band projector decays as r^{-d} for $r \ll \xi$, and follows the OZ decay for $r \gg \xi$, with an analytical expression for direction-dependence of $\xi_{\mathbf{r}}$, see SM [54]. The localization length scales as $\xi_{\mathbf{r}} \propto 1/\Delta^\gamma$,

with $\gamma = 1/2$ for quadratic touchings and $\gamma = 1$ for linear touchings. For the case of a linearly independent FB tuned into an orthogonal one, the overlap between CLS tends to zero, with localization length ξ consequently also going to zero. The bulk part of the projector is dominated by the compact projector in the orthogonal limit.

The case of a generic singular flat band is recovered as a limit of a linearly independent flat band when tuned into a singular one as discussed above: sending $\xi \rightarrow \infty$, the asymptotic exponential decay and Ornstein-Zernike power law decay are pushed to infinity. We recover the algebraic decay, r^{-d} , that has been observed in several settings: spin models defined on pyrochlore lattices and checkerboard lattices [13, 61, 62]. We provide the details in the SM [54].

Numerical simulations — We now confirm numerically the validity of the above statements. As an example we consider a ($d = 2$) FB model with 2 sublattices, ($u = 2$), based on a modified checkerboard lattice and with a CLS parametrized by parameter A , $0 \leq A \leq 1$, encompassing all the three classes: orthogonal ($A = 0$), linearly independent ($0 < A < 1$), singular ($A = 1$) (Fig. 1(b)). The CLS reads as follows:

$$|\text{CLS}^{\mathbf{r}}\rangle = A(|1, \mathbf{r}\rangle - |2, \mathbf{r}\rangle) + |1, \mathbf{r} + \hat{\mathbf{x}}\rangle - |2, \mathbf{r} - \hat{\mathbf{y}}\rangle \quad (5)$$

where we have omitted the normalization factor $\frac{1}{\sqrt{2A^2+2}}$. From this expression it is straightforward to obtain the BCLS $\phi_{\text{BCLS}}(\mathbf{k})$, and the projector (2) in real space. For $A = 0$ the CLS set is orthogonal, while for $A = 1$ the flat band is singular, with the touching at $k_x = k_y = \pi$. The above CLS alone is enough to construct the projector and analyze its properties. One of the many possible Hamiltonians is given by the spectral decomposition [47, 48]: $\mathcal{H}(\mathbf{k}) = \alpha^2(\mathbf{k})I - \phi_{\text{BCLS}}(\mathbf{k})\phi_{\text{BCLS}}^\dagger(\mathbf{k})$. Its lattice structure and the band structure are shown in Fig. 1(a)-(b). The two bands are given as $E_{\text{FB}} = 0$ and $E_{\text{DB}} = \alpha^2(\mathbf{k})$.

Next we compute numerically the real space projector in x -direction $P(1, 1; x)$ obtained from the CLS (5) using Eq. (2). To verify the asymptotic decay of the projector, we assume the OZ-like ansatz: $P(x) \sim x^a e^{-x/\xi_{\hat{x}}}$, where $\xi_{\hat{x}}$ is the localization length in the x -direction, and check its validity [Fig. 1(e-f)]. To extract parameters $\xi_{\hat{x}}$ and a , we devised a ratio-test type analysis [63] using the ratio $f(x) = \frac{P(1, 1; x+1)}{P(1, 1; x)}$ (Fig. 1(c)). With the OZ ansatz for the projector, the asymptotic behavior of $f(x)$ for large x is given by: $f(x) \sim \exp(-\xi_{\hat{x}}^{-1})(1 + ax^{-1})$. Since the algebraic part is linear in x^{-1} , we used a linear fit with respect to x^{-1} for large x . The slope and the y -intercept of the fit is then used to extract the parameters a and $\xi_{\hat{x}}$.

The OZ ansatz is confirmed by the linear behavior of $f(x)$ for large x (small x^{-1}) as shown in the inset of panel (e) of Fig. 1. The extracted length $\xi_{\hat{x}}$ is shown in panel (f), and agrees well with theory, see SM [54]. The panels (c) and (d) show the behavior of the algebraic prefactor, $P(x)e^{-x/\xi_{\hat{x}}}$. For large x , we observe the expected OZ decay, $x^{-1/2}$. Upon approaching the singular limit $A =$

0.9, panel (d), we observe a crossover around $x \approx \xi$ from an emergent algebraic decay of the singular case, x^{-2} for $x < \xi$, to the OZ decay, $x^{-1/2}$ for $x > \xi$, confirming our analytical predictions, see SM [54].

Anisotropic $d = 2$ singular flat bands — Anisotropies of the underlying lattice can result in singular FBs with a modified anisotropic algebraic decay. Indeed, for singular FBs the directional anisotropy of the BCLS $\phi_{\text{BCLS}}(\nu, \mathbf{k})$ near the touching at $\mathbf{k}_0$ alters the projector's asymptotic decay. To explain this, we consider the Taylor expansion of the BCLS around the touching point. Let us write $\mathbf{q} = \mathbf{k} - \mathbf{k}_0$, and expand the BCLS as $\phi_{\text{BCLS}}(\mathbf{k}_0 + \mathbf{q}) = i b \mathbf{q} + O(|\mathbf{q}|^2)$ with a $u \times d$ real matrix b for a real valued CLS. Then one obtains a quadratic form for $\alpha^2(\mathbf{k}_0 + \mathbf{q}) = \mathbf{q}^T B \mathbf{q} + \dots$, where $B = b^\dagger b$ is a $d \times d$ positive semi-definite Hermitian matrix. The previously derived r^{-d} decay corresponds to a nonsingular matrix B . However, if B is singular, its null space directions $\mathbf{q}_\parallel$ are responsible for a different, anisotropic decay in real space: the band touching is anisotropic, and is higher order than quadratic along $\mathbf{q}_\parallel$, as compared to a non-singular B . The decay is controlled by a nontrivial scaling between the $\mathbf{q}_\perp$ (generic directions) and $\mathbf{q}_\parallel$, see SM [54] for further details.

We illustrate the anisotropic decay with the following example of a modified 2D Lieb lattice Fig. 2(a). The anisotropy is due to additional longer range hoppings in the y -direction, and the anisotropic CLS is shown with filled circles. Since the chiral symmetry is not violated, the chiral flat band resides at energy $E = 0$ [64] and experiences a linear band touching with two dispersive bands (Fig. 2(b)). Note that we only need the BCLS to analyze the properties of a projector, since the full Hamiltonians can be constructed using the methods of Refs. 46–48. We consider first a 2D singular FB, where the BCLS is given as

$$\phi_{\text{BCLS}} = \begin{bmatrix} -e^{ik_x} - 1 \\ e^{ik_y} + e^{-ik_y} + 2 \end{bmatrix} \quad (6)$$

Near the touching point, $\mathbf{k} = (\pi, \pi)$ and $q_i = k_i + \pi$, $B = \text{diag}(1, 0)$ and we have $P(1, 1; \mathbf{k}) \sim q_x^2 / (q_x^2 + q_y^4)$ that is invariant under rescaling $(q_x, q_y) \rightarrow (\lambda q_x, \lambda^{1/2} q_y)$. Consequently, in real space, $P(\mu, \nu; \mathbf{r}) \sim |\mathbf{r}|^{-3/2}$, except for the y -direction, where $P(\mu, \nu; \mathbf{y}) \sim |\mathbf{y}|^{-3}$. This is verified numerically as shown in Fig. 2(c). We construct the Lieb-type lattice Hamiltonian $\mathcal{H}(\mathbf{k})$ that hosts the BCLS in Eq. (6), following the construction method of Ref. 47; see Fig. 2(a). The corresponding band structure is shown in Fig. 2(b). The real-space projector is obtained via a straightforward Fourier transform of the projector in the momentum space, and the result appears in Fig. 2(c). All calculations use system size $L = 3000$. A power law fit (linear fit in log-log) indicates that along the x direction the projector decays as $|\mathbf{x}|^{-3/2}$ (red), whereas along the y direction it decays as $|\mathbf{y}|^{-3}$ (blue).

It follows that for $d > 2$, the constraint to real CLS amplitudes and a number of sublattices $u < d$, the

above band touching anisotropy is enforced. Indeed, consider a BCLS with two sublattices ($u = 2$ in $d = 3$: $\phi_{\text{BCLS}} = (e^{ik_x} + e^{ik_y} - 2, e^{ik_z} - 1)^T$). At the touching point $\mathbf{k} = 0$, the matrix $B = b^\dagger b$ has to be singular since it is rank deficient: b is a 2×3 matrix. Here the real space decay is $|\mathbf{r}|^{-5/2}$ along generic directions, and $|\mathbf{r}|^{-5}$ along the nullspace directions of B . If we allow for complex valued CLS, we can evade the singularity of B even when $u < d$. For $\phi_{\text{BCLS}} = [(e^{ik_x} - 1) + i(e^{ik_y} - 1), e^{ik_z} - 1]^T$ the correct rank of b is three for real variables, restoring homogeneous decay r^{-d} along all directions [54].

The above results on the decay of FB projectors apply to the slowest asymptotic decay only, allowing for special directions with faster decay. A simple example is the Lieb lattice: the chiral symmetry enforces zero BCLS amplitude on minor sublattices, so if either μ or ν is chosen as those, the projector is identically zero. Directional dependence can be modified by symmetry: it might force the denominator of $\mathcal{P}(\mu, \nu; \mathbf{k})$ to cancel out with the numerator for some direction(s) $\mathbf{k}$, making the projector compact along that specific direction [54].

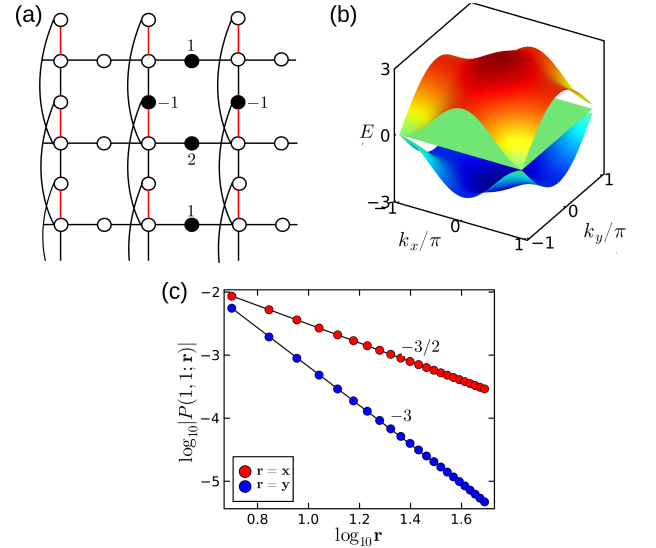


FIG. 2: A generalized anisotropic Lieb lattice which hosts an anisotropic singular flat band. (a) Lattice, the black lines are hoppings with strength 1, and the red lines are hoppings with strength 2. The CLS corresponds to the black colored circles [See Eq. (6) and SM [54]]. (b) Band structure of the lattice (a). (c) Decay of the projector $|P(1, 1; \mathbf{r})|$ vs. $\mathbf{r}$ in log-log scale. Red: x direction, linear fitting shows exponent $-3/2$, Blue: y direction, linear fitting shows exponent -3 .

Conclusion — We showed how the algebra of compact localized states (CLS) is directly related the qualitatively different long distance behavior of the flat band (FB) projector in real space. Orthogonal flat bands yield strictly compact projectors, while linearly independent flat bands exhibit Ornstein-Zernike decay with a direction-dependent localization length. Singular flat bands display algebraic decay r^{-d} in general, but strongly

anisotropic power law decay with different powers is possible for anisotropic cases. We have demonstrated a crossover: as a linearly independent FB approaches a singular one, the projector shows a crossover from emergent algebraic behavior at short distances, to the standard OZ power law decay, followed by exponential decay. We also identify an anisotropic singular FB class in which anisotropy of the band touching combined with higher order touching controls the decay: for generic spatial di-

rections the projector follows a slower algebraic decay, than the generic singular FBs with r^{-d} , while along special axes it shows a faster algebraic decay than the generic case. We believe that this new nongeneric class can be relevant to perturbed FBs, e.g. superconductivity, optical and transport response, and disordered systems. Local excitations of such lattices which resonate with the FB energy will generate a spatial response which follows the decay of the above real space projectors.

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Supplementary material for “Real space decay of flat band projectors from compact localized states”

Yeongjun Kim ^{1,2,*} Sergej Flach ^{1,2,3,†} and Alexei Andreanov ^{1,2,‡}

¹*Center for Theoretical Physics of Complex Systems, Institute for Basic Science (IBS), Daejeon, Korea, 34126*

²*Basic Science Program, Korea University of Science and Technology (UST), Daejeon 34113, Republic of Korea*

³*Centre for Theoretical Chemistry and Physics, The New Zealand Institute for Advanced Study (NZIAS), Massey University Albany, Auckland 0745, New Zealand*

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I. CLS CLASSIFICATION

A. Compact localized states (CLS) and the Bloch-CLS

Let us consider a flat band (FB) tight-binding Hamiltonian H defined on a lattice Λ , with u sublattices (u -orbitals), and its $u \times u$ momentum-space block $\mathcal{H}(\mathbf{k})$ discussed in the main text. The BCLS is defined as the non-normalized FB eigenstates with a proper gauge, $\phi_{\text{BCLS}}(\mu, \mathbf{k}) = \alpha(\mathbf{k})\psi_{\text{FB}}(\mu, \mathbf{k})$, such that we can write $\phi_{\text{BCLS}}(\mu, \mathbf{k})$ as a finite Fourier series:

$$\phi_{\text{BCLS}}(\mu, \mathbf{k}) = \sum_{\mathbf{r}} \phi_{\text{CLS}}(\mu, \mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}}, \quad (1)$$

where $\phi_{\text{CLS}}(\mu, \mathbf{r}) = 0$ for $|\mathbf{r}| > r_0$. Thus, for the CLS located at the unit cell $\mathbf{r}_0$, the amplitude is given by

$$\phi_{\text{CLS}}(\mu, \mathbf{r}; \mathbf{r}_0) = \phi_{\text{CLS}}(\mu, \mathbf{r} - \mathbf{r}_0) = \int \phi_{\text{BCLS}}(\mu, \mathbf{k}) e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}_0)} d^d \mathbf{k}. \quad (2)$$

The CLS is an eigenstate because it is a linear combination of BCLS.

* yeongjun.kim.04@gmail.com

† sflach@ibs.re.kr

‡ aalexei@ibs.re.kr

B. Irreducible CLS

The irreducibility of the CLS is important for the classification. To obtain the irreducible CLS, one ensures a BCLS $\phi_{\text{BCLS}}(\mathbf{k})$ does not contain a common finite Fourier series factor other than 1. To see why this results in irreducible CLS, let us suppose we have a suboptimal (reducible) BCLS as $\phi'_{\text{BCLS}}(\mathbf{k}) = (1 + e^{ik_1})\phi_{\text{BCLS}}(\mathbf{k})$, where the $\phi_{\text{BCLS}}(\mu, \mathbf{k})$ on the right-hand side is the irreducible BCLS. For this suboptimal (reducible) choice, we obtain

$$\phi'_{\text{CLS}}(\mu, \mathbf{r}; \mathbf{r}_0) = \int (1 + e^{ik_1}) e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}_0)} \phi_{\text{BCLS}}(\mu, \mathbf{k}) d^d \mathbf{k} \quad (3)$$

$$= \phi_{\text{CLS}}(\mu, \mathbf{r}; \mathbf{r}_0) + \phi_{\text{CLS}}(\mu, \mathbf{r}; \mathbf{r}_0 - \hat{\mathbf{x}}), \quad (4)$$

resulting in a linear combination of the irreducible CLSs located at $\mathbf{r}_0$ and $\mathbf{r}_0 - \hat{\mathbf{x}}$.

From this irreducibility condition one can map the projector properties and algebraic properties of the CLS one-to-one.

C. Overlap between CLS and the norm square of BCLS

The norm square of BCLS, $\alpha^2(\mathbf{k}) = \phi_{\text{BCLS}}^\dagger(\mathbf{k})\phi_{\text{BCLS}}(\mathbf{k})$, is a finite Fourier series, and the Fourier coefficients are the overlaps between CLS. We have

$$\begin{aligned} \alpha^2(\mathbf{k}) &= \sum_{\mathbf{r}, \mathbf{r}'} \phi_{\text{CLS}}^*(\mu, \mathbf{r}) \phi_{\text{CLS}}(\mu, \mathbf{r}') e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} \\ &= \sum_{\Delta} \left[\sum_{\mathbf{r}} \phi_{\text{CLS}}^*(\mu, \mathbf{r}) \phi_{\text{CLS}}(\mu, \mathbf{r} - \Delta) \right] e^{i\mathbf{k} \cdot \Delta} \\ &= \sum_{\Delta} \langle \text{CLS}_0 | \text{CLS}_\Delta \rangle e^{i\mathbf{k} \cdot \Delta}. \end{aligned} \quad (5)$$

It follows that if $\alpha^2(\mathbf{k}) = \text{const.}$, the CLS are orthogonal.

II. ORTHOGONAL FLAT BANDS

The projector used in the main text is given by

$$P(\mu, \nu; \mathbf{r}) = \frac{1}{(2\pi)^d} \int_{\text{BZ}} \mathcal{P}(\mu, \nu; \mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}} d^d \mathbf{k}, \quad (6)$$

where

$$\mathcal{P}(\mu, \nu; \mathbf{k}) = \frac{\phi_{\text{BCLS}}^*(\mu, \mathbf{k}) \phi_{\text{BCLS}}(\nu, \mathbf{k})}{\alpha^2(\mathbf{k})}. \quad (7)$$

For an orthogonal flat band we have $\alpha^2(\mathbf{k}) = 1$, so the projector in real space is

$$P(\mu, \nu; \mathbf{r}) = \frac{1}{(2\pi)^d} \int_{\text{BZ}} \phi_{\text{BCLS}}^*(\mu, \mathbf{k}) \phi_{\text{BCLS}}(\nu, \mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}} d^d \mathbf{k}. \quad (8)$$

The Fourier transform results in

$$P(\mu, \nu; \mathbf{r}) = \sum_{\mathbf{r}'} \phi_{\text{CLS}}^*(\mu, \mathbf{r}') \phi_{\text{CLS}}(\nu, \mathbf{r}' - \mathbf{r}), \quad (9)$$

which is compact.

We now prove that a compact projector implies orthogonality of CLS. Assume a compact projector $P(\mu, \nu; \mathbf{r})$ for all sublattices (μ, ν) . Then $\mathcal{P}(\mu, \nu; \mathbf{k})$ is a finite Fourier series (finite Laurent polynomial). If we assume linearly independent (but not orthogonal) CLS, $\alpha^2(\mathbf{k})$ must be cancelled by the denominators in $\phi_{\text{BCLS}}^*(\mu, \mathbf{k})\phi_{\text{BCLS}}(\nu, \mathbf{k})$. Note that $\alpha^2(\mathbf{k})$ is a finite Laurent polynomial. Therefore $\phi_{\text{BCLS}}^*(\mu, \mathbf{k})$ or $\phi_{\text{BCLS}}(\nu, \mathbf{k})$ should contain a common finite Laurent polynomial factor with $\alpha^2(\mathbf{k})$ other than 1 for every choice (μ, ν) . It is then straightforward to show that the BCLS is reducible, contradicting our initial assumption on BCLS.

III. NON-ORTHOGONAL FLAT BANDS

We provide here the details of the derivation of the Ornstein–Zernike decay for the projectors of exponential flat bands. The asymptotics of the projector (6) can be formally derived using the Schwinger parameterization for $\alpha^2(\mathbf{k})$ and the saddle-point approximation. Let us define $N(\mathbf{k}) = \phi^*(\mu, \mathbf{k}) \phi(\nu, \mathbf{k})$ and $P(\mu, \nu; \mathbf{r})$, so that the projector (6) reads

$$P(\mu, \nu; \mathbf{r}) = \int \frac{N(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}}}{\alpha^2(\mathbf{k})} d^d \mathbf{k}, \quad (10)$$

with $\mathbf{r} = r\hat{\mathbf{r}}$, where $|\hat{\mathbf{r}}| = 1$ is a unit vector and r is the distance. Using the Schwinger parameterization

$$\alpha^{-2}(\mathbf{k}) = \int_0^\infty e^{-s\alpha^2(\mathbf{k})} ds, \quad (11)$$

and defining a new integration variable $s = rt$, we obtain

$$P(\mu, \nu; \mathbf{r}) = r \int_0^\infty dt \int d^d \mathbf{k} \left(N(\mathbf{k}) e^{rf(t, \mathbf{k})} \right), \quad (12)$$

$$f(t, \mathbf{k}) = -t\alpha^2(\mathbf{k}) + i\mathbf{k} \cdot \hat{\mathbf{r}}.$$

This representation is suitable for the saddle-point approximation as $r \rightarrow \infty$, which controls the asymptotic decay of the projector. The saddle point in $(t, \mathbf{k})$ satisfies

$$\begin{aligned} \partial_t f(t, \mathbf{k}) &= -\alpha^2(\mathbf{k}) = 0, \\ \nabla_{\mathbf{k}} f(t, \mathbf{k}) &= -t\nabla_{\mathbf{k}} \alpha^2(\mathbf{k}) + i\hat{\mathbf{r}} = 0. \end{aligned} \quad (13)$$

We note that $|\alpha(\mathbf{k})| = 0$ cannot occur for real $\mathbf{k}$ for nonsingular flat bands, and we must shift the integration contour so that it crosses the zero. Solving Eq. (13) gives the saddle point $(t_0(\hat{\mathbf{r}}), \mathbf{k}_0(\hat{\mathbf{r}}))$ (in case of multiple solutions, the relevant one has the smallest $|\text{Im } \mathbf{k}_0|$). Let us write $\mathbf{k}_0(\hat{\mathbf{r}}) = \mathbf{k}_0$ and $t_0(\hat{\mathbf{r}}) = t_0$. After locating the saddle, expand the exponent to quadratic order in $(t, \mathbf{k})$. Let $t' = t - t_0$. We have

$$f(t, \mathbf{k}) = it'(\mathbf{q} \cdot \vec{v}) + \mathbf{q}^T B \mathbf{q} + O(|\mathbf{q}|^3), \quad (14)$$

where $\mathbf{q} = \mathbf{k} - \mathbf{k}_0$, $\vec{v} = \hat{\mathbf{r}}/t_0$, and $B_{ij}(\mathbf{k}_0) = \frac{t_0}{2} \partial_{k_i} \partial_{k_j} \alpha^2(\mathbf{k})|_{\mathbf{k}=\mathbf{k}_0}$. Importantly, we assume $B = B(\mathbf{k}_0)$ to be nonsingular at the saddle. We also consider the case $N(\mathbf{k}) \approx N_0$. Completing the square, we have

$$f(t, \mathbf{k}) \approx \mathbf{q}^T B \mathbf{q}' - t'^2 \vec{v}^T B^{-1} \vec{v}. \quad (15)$$

The integrand is now a product of two independent Gaussians. The $\mathbf{q}'$ integration gives $(2\pi)^{d/2} [\det B]^{-1/2} (rt_0)^{-d/2}$. The t' integration contributes $(2\pi r^{-1} t_0^2 / c_{\hat{\mathbf{r}}})^{1/2}$, where $c_{\hat{\mathbf{r}}} = \hat{\mathbf{r}}^T B^{-1} \hat{\mathbf{r}}$. Multiplying the two factors gives $r^{-d/2-1/2}$ decay. Combining with the outside r prefactor, we obtain

$$P(\mu, \nu; \mathbf{r}) \sim \frac{e^{-r/\xi_{\hat{\mathbf{r}}}}}{r^{(d-1)/2}}, \quad (16)$$

which is the OZ decay [1, 2].

We have assumed a non-vanishing zeroth order of $N(\mathbf{k})$ near the saddle $\mathbf{k}_0(\hat{\mathbf{r}})$. If this is not the case, one can apply Feynman's trick: if $N(\mathbf{k})$ starts from first order near the saddle, the $\mathbf{k}$ -prefactor becomes derivatives in real space. Therefore, the algebraic prefactor becomes $r^{-(d+1)/2}$. However, it is more common that symmetry forces $N(\mathbf{k}_0(\hat{\mathbf{r}})) = 0$, i.e., the integral vanishes. In this case the projector is compact in that particular $\hat{\mathbf{r}}$ direction.

IV. SINGULAR FLAT BANDS

A. Generic case

Here we consider the limit of the nonsingular flat band becoming a singular one, i.e., the band gap between a flat and dispersive band vanishes, $\Delta \rightarrow 0$. For any $\Delta > 0$ the $r \rightarrow \infty$ results of Section III still apply for

$$P(\mu, \nu; \mathbf{r}) = \int \frac{N(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}}}{\alpha^2(\mathbf{k})} d^d \mathbf{k}. \quad (17)$$

As $\Delta \rightarrow 0$, the relevant zero of $\alpha^2(\mathbf{k})$ approaches the real axis, and simultaneously so does the zero of $N(\mathbf{k})$. Exactly at $\Delta = 0$, the situation depends on the dimension of space. In 1D, this leads to the cancellation of the zeros, producing an orthogonal flat band. However, in $d > 1$, while the zeros also cancel out, there might be a residual direction dependence in approaching the zero, which is not possible in 1D. For small enough, but nonzero Δ , this leads to the emergence of the singular flat band projector decay, r^{-d} , followed by the Ornstein–Zernike decay. This intermediate asymptotics is not captured by the saddle-point derivation of Section III. However, for small Δ , we can directly evaluate the saddle-point integral (17) by using an approximation of the denominator $\alpha^2(\mathbf{k})$. In the nearly singular case, the following expression becomes valid:

$$\alpha^2(\mathbf{k}) = \Delta + (\mathbf{k} - \mathbf{k}_1)^T B (\mathbf{k} - \mathbf{k}_1). \quad (18)$$

One can obtain a *real* $\mathbf{k}_1$ directly from the Taylor expansion of $\alpha^2(\mathbf{k})$. Here, B is a positive semidefinite matrix due to positivity of $\alpha^2(\mathbf{k})$, but for now we will assume that B is nonsingular (positive definite). To find a saddle, write $\mathbf{k}_0 = \mathbf{k}_1 + \vec{\chi} + i\vec{\eta}$ and solve the saddle-point equations. Then, we obtain

$$\mathbf{k}_0 = \mathbf{k}_1 + i \frac{\sqrt{\Delta}}{\sqrt{\hat{\mathbf{r}}^T B^{-1} \hat{\mathbf{r}}}} B^{-1} \hat{\mathbf{r}}, \quad (19)$$

$$t_0 = \frac{1}{2\Delta} \sqrt{\hat{\mathbf{r}}^T B^{-1} \hat{\mathbf{r}}}. \quad (20)$$

This gives us the analytical form of the localization length.

For small Δ one can expand the numerator $N(\mathbf{k})$ as

$$N(\mathbf{k}) \approx a_0 + \vec{a} \cdot \mathbf{q} + \mathbf{q}^T A \mathbf{q}. \quad (21)$$

To obtain the intermediate decay, we integrate $\mathcal{P}(\mu, \nu; \mathbf{k})$ without the Schwinger parameterization:

$$\mathcal{P}(\mu, \nu; \mathbf{k}) = \frac{a_0 + \vec{a} \cdot \mathbf{q} + \mathbf{q}^T A \mathbf{q}}{\Delta + \mathbf{q}^T B \mathbf{q}} + O(q^3) = P_{\text{IR}}(\mu, \nu; \mathbf{k}) + O(q^3). \quad (22)$$

The band gap Δ and matrix B control the anisotropic length scale ξ [3, 4]. The decay of the real-space projector is given by the Fourier transform of the above expression and is controlled by its small- $\mathbf{q}$ behavior:

$$P(\mathbf{r}) \sim \int_{\mathbb{R}^d} P_{\text{IR}}(\mathbf{q}) e^{i\mathbf{q} \cdot \mathbf{r}} d^d \mathbf{q}. \quad (23)$$

Since we have assumed a nonsingular B , consider the transformation $U^T B U = \Lambda = \text{diag}(\{\lambda_i\})$ and define $\mathbf{q}' = \Lambda^{1/2} U^T \mathbf{q}$, so that $\mathbf{q}^T B \mathbf{q} = q'^2$. We then have

$$P(\mu, \nu; \mathbf{r}) \sim \det(B)^{-1/2} \int \frac{a_0 + \vec{a}' \cdot \mathbf{q}' + \mathbf{q}'^T A' \mathbf{q}'}{q'^2 + \xi^{-2}} e^{i\mathbf{q}' \cdot \mathbf{r}'} d^d \mathbf{q}', \quad (24)$$

where

$$\begin{aligned} \vec{a}' &= \Lambda^{-1/2} U^T \vec{a}, & A' &= \Lambda^{-1/2} U^T A U \Lambda^{-1/2}, \\ \Delta &= \xi^{-2}, & \mathbf{r}' &= B^{-1/2} \mathbf{r}. \end{aligned} \quad (25)$$

The expression in the denominator is well known and appears in various settings (screened/Yukawa potential [5], correlation length near T_c [6]); Δ is often referred to as the “mass gap”. The Fourier transform of the denominator alone is given by $\rho(r'/\xi) = K_{(d-2)/2}(r'/\xi)/r'^{(d-2)/2}$, where $K_{(d-2)/2}$ is the modified Bessel function of the second kind, while the numerator produces derivatives in real space. Overall,

$$\begin{aligned} P(\mu, \nu; \mathbf{r}) \sim a_0 \rho\left(\frac{r'}{\xi}\right) &+ \sum_i a'_i \partial_{r'_i} \rho\left(\frac{r'}{\xi}\right) + \\ &\sum_{ij} A'_{ij} \partial_{r'_i} \partial_{r'_j} \rho\left(\frac{r'}{\xi}\right). \end{aligned} \quad (26)$$

This directional dependence of projector decay is confirmed for a two-band square-lattice flat band (see the main text), as shown in Fig. 2(b).

Excluding the asymptotic exponential decay, for $r' \ll \xi$ we have

$$\rho\left(\frac{r'}{\xi}\right) \sim \frac{1}{r'^{d-2}}. \quad (27)$$

For a nearly singular flat band, $a'_0, \bar{a}' \rightarrow 0$, and the second-derivative term in Eq. (26) gives the dominant contribution, yielding the decay r^{-d} . For $r' \gg \xi$ the first term gives the OZ decay, since a_0 is finite.

For a quadratic band touching, the divergence of the length upon approaching the singular limit is $\xi_{\tilde{\mathbf{r}}} \propto \Delta^{-1/2}$, while for a linear band touching with chiral symmetry (e.g., Lieb lattice), the exponent is $\gamma = -1$. A simple way to see this is the following: Squaring the chiral Hamiltonian block diagonalizes it, and one of the blocks includes a flat band with quadratic band touching with a gap $\Delta' = \Delta^2$, so that $\xi \propto \Delta'^{-1/2} = \Delta^{-1}$.

1. Example: generalized checkerboard lattice

Starting from Eq. (5) of the main text, we write the BCLS as

$$\phi_{\text{BCLS}}(\mathbf{k}) = \begin{bmatrix} A + e^{ik_x} \\ -(A + e^{-ik_y}) \end{bmatrix}, \quad (28)$$

and the dual (dispersive-band) vector as

$$\phi_{\text{DB}}(\mathbf{k}) = \begin{bmatrix} A + e^{-ik_y} \\ A + e^{ik_x} \end{bmatrix}. \quad (29)$$

One readily checks orthogonality and equal norms

$$\phi_{\text{BCLS}}^\dagger(\mathbf{k}) \phi_{\text{DB}}(\mathbf{k}) = 0, \quad (30)$$

$$\|\phi_{\text{BCLS}}(\mathbf{k})\|^2 = \|\phi_{\text{DB}}(\mathbf{k})\|^2 \equiv \alpha^2(\mathbf{k}), \quad (31)$$

with

$$\begin{aligned} \alpha^2(\mathbf{k}) &= |A + e^{ik_x}|^2 + |A + e^{-ik_y}|^2 \\ &= 2(A^2 + 1) + 2A(\cos k_x + \cos k_y). \end{aligned} \quad (32)$$

The Hamiltonian that hosts the CLS in Eq. (28) can then be constructed as a rank-one projector onto ϕ_{DB} ,

$$\mathcal{H}(\mathbf{k}) = \phi_{\text{DB}}(\mathbf{k}) \phi_{\text{DB}}^\dagger(\mathbf{k}) = \alpha^2(\mathbf{k}) \mathbb{I} - \phi_{\text{BCLS}}(\mathbf{k}) \phi_{\text{BCLS}}^\dagger(\mathbf{k}), \quad (33)$$

i.e., explicitly

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} |A + e^{-ik_y}|^2 & (A + e^{-ik_y})(A + e^{-ik_x}) \\ (A + e^{ik_y})(A + e^{ik_x}) & |A + e^{ik_x}|^2 \end{pmatrix}. \quad (34)$$

By construction,

$$\mathcal{H}(\mathbf{k}) \phi_{\text{BCLS}}(\mathbf{k}) = 0, \quad \mathcal{H}(\mathbf{k}) \phi_{\text{DB}}(\mathbf{k}) = \alpha^2(\mathbf{k}) \phi_{\text{DB}}(\mathbf{k}), \quad (35)$$

so the spectrum consists of a perfectly flat band at $E_{\text{FB}}(\mathbf{k}) = 0$ spanned by ϕ_{BCLS} , and a generally dispersive band $E_{\text{DB}}(\mathbf{k}) = \alpha^2(\mathbf{k})$ spanned by ϕ_{DB} .

The band gap is therefore

$$\Delta = \min_{\mathbf{k}} \alpha^2(\mathbf{k}) = 2(|A| - 1)^2, \quad (36)$$

attained at $\mathbf{k} = (\pi, \pi)$ for $A > 0$ and at $\mathbf{k} = (0, 0)$ for $A < 0$. Hence the gap closes at $A = \pm 1$ and opens quadratically in $|A| - 1$, providing a single-parameter tunable gap.

We denote by $t_{\mathbf{R},\alpha\beta}$ the hopping amplitude from sublattice β in the reference cell to sublattice α in the cell displaced by $\mathbf{R}$. The nonzero amplitudes are

$$\begin{aligned} t_{\mathbf{0},11} &= A^2 + 1, & t_{\pm\hat{\mathbf{y}},11} &= A, \\ t_{\mathbf{0},22} &= A^2 + 1, & t_{\pm\hat{\mathbf{x}},22} &= A, \\ t_{\mathbf{0},12} &= A^2, & t_{-\hat{\mathbf{x}},12} &= A, & t_{-\hat{\mathbf{y}},12} &= A, & t_{-(\hat{\mathbf{x}}+\hat{\mathbf{y}}),12} &= 1. \end{aligned} \quad (37)$$

All other $t_{\mathbf{R},\alpha\beta} = 0$. Hopping amplitudes in opposite directions are identical, $t_{-\mathbf{R},\alpha\beta} = t_{\mathbf{R},\alpha\beta}$. These hoppings define the checkerboard-like lattice shown in Fig. 1.

We now consider normalized CLS (CLS normalized to 1) by multiplying a normalization constant $1/\sqrt{2A^2 + 2}$. The zeroth-order term of $\alpha^2(\mathbf{k})$ becomes 1. The overlaps of the CLS in the x and y directions are given by $A/(2A^2 + 2)$. Defining

$$A' \equiv \frac{2A}{2A^2 + 2} = \frac{A}{A^2 + 1}, \quad (38)$$

we have

$$\alpha^2(\mathbf{k}) = 1 + A'(\cos k_x + \cos k_y). \quad (39)$$

The direct gap occurs at $\mathbf{k} = (\pi, \pi)$ and is

$$\Delta = 1 - 2A'. \quad (40)$$

We expand near $\mathbf{k} = (\pi, \pi)$. Write

$$k_i = \pi + q_i \quad (i = x, y), \quad |q_i| \ll 1, \quad (41)$$

so that $\cos k_i = \cos(\pi + q_i) = -\cos q_i \simeq -(1 - \frac{q_i^2}{2})$. Then

$$\alpha^2(\mathbf{k}) \simeq 1 + A' \left[-2 + \frac{q_x^2 + q_y^2}{2} \right] = (1 - 2A') + \frac{A'}{2}(q_x^2 + q_y^2). \quad (42)$$

With the BCLS choice $\phi_{\text{BCLS}}(\mathbf{k}) = (A + e^{ik_x}, -[A + e^{-ik_y}])^T$, the projector matrix elements (normalized by $2(A^2 + 1)$) expand as

$$\begin{aligned} \frac{|\phi_{\text{BCLS}}(1, \mathbf{k})|^2}{2(A^2 + 1)} &\simeq \left(\frac{1}{2} - A' \right) + \frac{A'}{2} q_x^2, \\ \frac{|\phi_{\text{BCLS}}(2, \mathbf{k})|^2}{2(A^2 + 1)} &\simeq \left(\frac{1}{2} - A' \right) + \frac{A'}{2} q_y^2, \\ \frac{\phi_{\text{BCLS}}^*(1, \mathbf{k}) \phi_{\text{BCLS}}(2, \mathbf{k})}{2(A^2 + 1)} &\simeq \frac{1}{2A^2 + 2} \left[-(A - 1)^2 - i(A - 1)(q_x + q_y) - \frac{A - 1}{2}(q_x^2 + q_y^2) + q_x q_y \right]. \end{aligned} \quad (43)$$

(Here we used $e^{ik_x} = -e^{iq_x}$ and $e^{-ik_y} = -e^{-iq_y}$ near (π, π) .)

Note that as $A \rightarrow 1$ the constant and linear terms in (43) vanish while the quadratic terms remain. For any sublattice choice, this yields the correlation length $\xi \propto (1 - 2A')^{-1/2} = \Delta^{-1/2}$ for small A' , as expected. The scaling and the directional dependence of ξ are shown in Fig. 2.

B. Examples of nongeneric case

We provide here some comments and examples for the case of a singular B in Eq. (22). Let us first discuss how the matrix B is related to the flat band BCLS for the singular flat band. For simplicity, let us consider real CLS. In this case we have BCLS $\vec{\phi}_{\text{BCLS}}(\mathbf{k}_0) = 0$ for real $\mathbf{k}_0$, and around this point we expand the BCLS as

$$\vec{\phi}_{\text{BCLS}}(\mathbf{k}_0 + \mathbf{q}) = i b \mathbf{q} + O(|\mathbf{q}|^2), \quad (44)$$

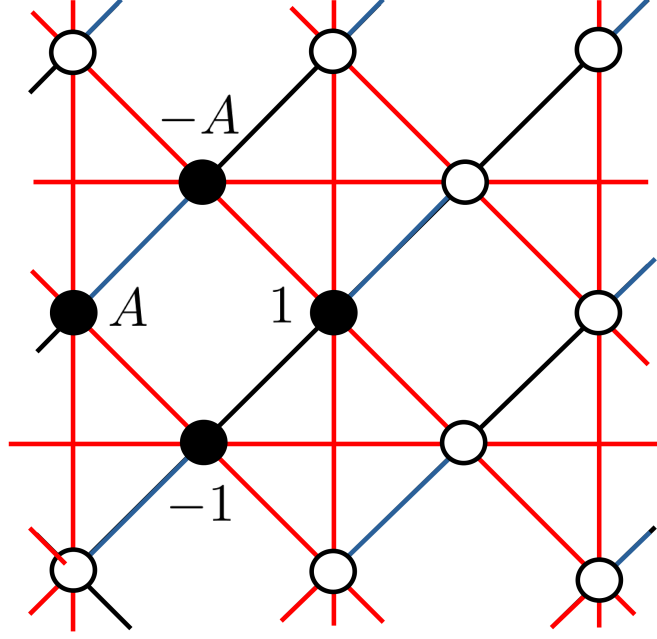


FIG. 1: Generalized checkerboard lattice. The CLS are black circles. Hoppings: black lines = 1, red lines = A , blue lines = A^2 .

where b is a $u \times d$ real matrix (with u the number of bands/orbitals), and $\mathbf{q} = \mathbf{k} - \mathbf{k}_0$. The matrix b encodes the directional dependence of the normalized Bloch flat band eigenstate [7]: approaching $\mathbf{k}_0$ along direction q_i gives the vector proportional to the i th column of b . From Eq. (44) we find $\alpha^2(\mathbf{k}) = \vec{\phi}_{\text{BCLS}}^\dagger \vec{\phi}_{\text{BCLS}}$, so that

$$\alpha^2(\mathbf{k}_0 + \mathbf{q}) = \mathbf{q}^T (b^\dagger b) \mathbf{q} + O(|\mathbf{q}|^4). \quad (45)$$

We identify $B = b^\dagger b$, a positive semidefinite matrix, ensuring $\alpha^2(\mathbf{k}) \geq 0$.

In the main text we assumed positive-definiteness of B . For a singular B we have $B\mathbf{q}_{\text{null}} = 0$ for at least one $\mathbf{q}_{\text{null}}$. There are several possibilities: (i) $[\vec{\phi}(\mathbf{k})]_\mu$ are independent of $\{\mathbf{q}_{\text{null}}\}$ and so is $\alpha(\mathbf{k})^2$, and the band touching is not point-like. Then the integral in Eq. (6) is separable in $\mathbf{q}_{\text{null}}$ and the flat band projector is compact in the directions corresponding to the nullspace of B . If the dimension of the null space of B is m , then the exponent of the power-law spatial decay in the orthogonal directions is $d - m$ and not d , as in the generic case. (ii) $\mathbf{q}_{\text{null}}$ -related terms appear in higher orders of the expansion of $\alpha(\mathbf{k})$, corresponding to flat bands with anisotropic touchings (e.g., mixed quadratic and quartic). Handling this case requires a change of basis into $\mathbf{q}_{\text{null}}$ and the rest $\{\mathbf{q}_\perp\}$.

We consider a simple 2D example falling under (ii), with a singular B :

$$\vec{\phi}_{\text{BCLS}}(\mathbf{k}) = \begin{bmatrix} e^{ik_x} - 1 \\ (e^{ik_y} - 1)^2 \end{bmatrix}. \quad (46)$$

Near the singularity $\mathbf{k} = 0$, we have

$$\vec{\phi}_{\text{BCLS}}(\mathbf{k}) \sim i \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} k_x \\ k_y \end{bmatrix} - \begin{bmatrix} -\frac{1}{2}k_x^2 \\ -k_y^2 \end{bmatrix}, \quad (47)$$

and

$$B = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}. \quad (48)$$

The asymptotic decay of the projector integral (6) is governed by the Taylor expansion near the singularity:

$$P(\mathbf{r}) \sim \int_{\mathbb{R}^2} \mathcal{P}_{\text{IR}}(k_x, k_y) e^{i(k_x x + k_y y)} dk_x dk_y, \quad (49)$$

$$\mathcal{P}_{\text{IR}}(k_x, k_y) = \frac{k_x^2}{k_x^2 + k_y^4}.$$

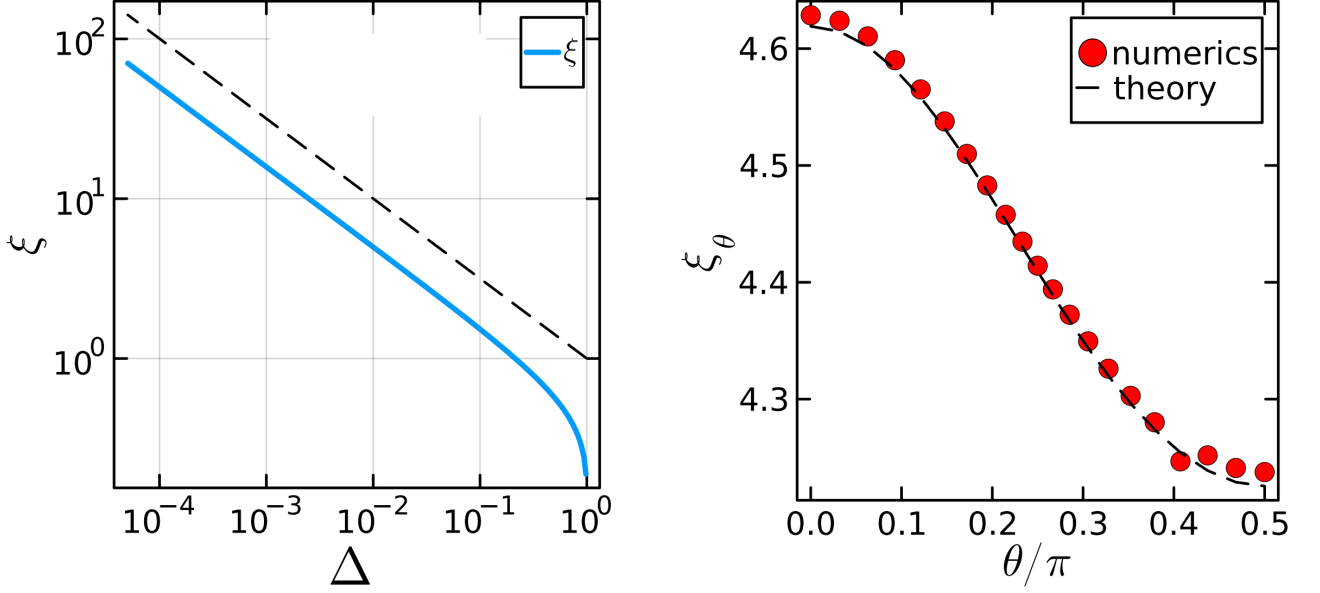


FIG. 2: Dependence of the localization length ξ of the square-lattice flat band projector on parameters. (a) Scaling of ξ with decreasing band gap Δ . The dashed line shows the $\Delta^{-1/2}$ trend. (b) Directional dependence of ξ versus the slice direction $\theta = \arctan(y/x)$ in the 2D projector, where (x, y) labels a lattice site.

The integrand is a homogeneous function:

$$\mathcal{P}_{\text{IR}}(k_x, k_y) = \mathcal{P}_{\text{IR}}(\lambda k_x, \lambda^{1/2} k_y). \quad (50)$$

This implies the following scaling in real space:

$$P(x, y) = \lambda^{-3/2} P(\lambda x, \lambda^{1/2} y). \quad (51)$$

Hence $P(0, y) \sim y^{-3}$ and $P(x, 0) \sim x^{-3/2}$, or in combined form

$$P(x, y) \sim \frac{1}{y^3 + x^{3/2}}. \quad (52)$$

We also note that $B = b^\dagger b$ is always singular if the number of bands $u < d$ ($d > 2$) in the time-reversal case, because b is $u \times d$ and B is rank deficient. The flat band projector then has an anisotropic decay. As an example, consider a 3D BCLS with two orbitals

$$\vec{\phi}_{\text{BCLS}}(\mathbf{k}) = \begin{bmatrix} e^{ik_x} + e^{ik_y} - 2 \\ e^{ik_z} - 1 \end{bmatrix}. \quad (53)$$

The singular band touching is at $\mathbf{k} = 0$. Near this singularity, the BCLS is

$$\vec{\phi}_{\text{BCLS}}(\mathbf{k}) \sim i \begin{bmatrix} 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} k_x \\ k_y \\ k_z \end{bmatrix} = b \begin{bmatrix} k_x \\ k_y \\ k_z \end{bmatrix}. \quad (54)$$

We have

$$B = b^\dagger b = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad (55)$$

which is singular, with $\mathbf{q}_{\text{null}} = [-1, 1, 0]^T$. Repeating the homogeneous-function argument, the decay is $|\mathbf{r}|^{-5/2}$ in all directions except along $\mathbf{r} = [-1, 1, 0]$, where we have $|\mathbf{r}|^{-5}$.

Now let us allow CLS amplitudes to take imaginary values. The matrix b may be complex, and the null space of b may then be spanned only by complex vectors, which are not relevant for real momenta $\mathbf{k} \in \mathbb{R}^d$. A more accurate rank counting can be done by separating the real and imaginary parts of $\vec{\phi}$. If the number of bands is u , the matrix b should be treated as $2u \times d$ (over $\mathbb{R}$) instead of $u \times d$ (over $\mathbb{C}$). In other words, even if $u < d$, it can happen that the decay is homogeneous. A simple example is a slightly tweaked variant of Eq. (53) which breaks time-reversal symmetry:

$$\vec{\phi}_{\text{BCLS}}(\mathbf{k}) = \begin{bmatrix} (e^{ik_x} - 1) + i(e^{ik_y} - 1) \\ e^{ik_z} - 1 \end{bmatrix}. \quad (56)$$

For this model, near $\mathbf{k} = 0$ we have

$$\vec{\phi}_{\text{BCLS}}(\mathbf{k}) \sim i \begin{bmatrix} 1 & i & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} k_x \\ k_y \\ k_z \end{bmatrix}. \quad (57)$$

Here, the first-order term vanishes along the $(i, -1, 0)$ direction, but for $\mathbf{k} \in \mathbb{R}^d$ the first-order term never vanishes. Instead, one may consider the realified form

$$\begin{bmatrix} \text{Re}[\phi_{\text{BCLS}}(\mathbf{k})]_a \\ \text{Im}[\phi_{\text{BCLS}}(\mathbf{k})]_a \\ \text{Re}[\phi_{\text{BCLS}}(\mathbf{k})]_b \\ \text{Im}[\phi_{\text{BCLS}}(\mathbf{k})]_b \end{bmatrix} \sim \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} k_x \\ k_y \\ k_z \end{bmatrix}, \quad (58)$$

which correctly counts the rank as 3, equal to the dimension $d = 3$.

C. Anisotropic Lieb lattice

We start with the BCLS

$$\phi_{\text{BCLS}}(\mathbf{k}) = \begin{bmatrix} -1 - e^{ik_x} \\ 2 + e^{ik_y} + e^{-ik_y} \end{bmatrix}. \quad (59)$$

To construct the chiral flat band with the BCLS given in Eq. (59), first one considers the vector v which satisfies $v^\dagger \phi = 0$. Then the chiral flat band is

$$\mathcal{H}(\mathbf{k}) = \begin{bmatrix} 0 & v^\dagger \\ v & 0 \end{bmatrix} = \begin{bmatrix} 0 & 2 + e^{ik_y} + e^{-ik_y} & 1 + e^{ik_x} \\ 1 + e^{ik_x} & 0 & 0 \\ 2 + e^{ik_y} + e^{-ik_y} & 0 & 0 \end{bmatrix}. \quad (60)$$

This model possesses the BCLS with an additional entry of zero amplitude:

$$\phi_{\text{BCLS}}(\mathbf{k}) = \begin{bmatrix} 0 \\ -1 - e^{ik_x} \\ 2 + e^{ik_y} + e^{-ik_y} \end{bmatrix}. \quad (61)$$

One can easily check that $\mathcal{H}(\mathbf{k}) \phi_{\text{BCLS}}(\mathbf{k}) = 0$, confirming this is a BCLS eigenstate of the central flat band at $E = 0$. The lattice structure and the band structure are illustrated in Fig. 2(a) and (b).

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