Effective tight-binding models in optical moiré potentials

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A twist between two periodic systems offers the possibility to drastically control quantum transport properties. At discrete sets of commensurate twisting angles, a moiré periodic pattern is formed, and the low-energy singleparticle spectrum forms distinct bands and gaps. Here, we consider twisted systems at a commensurate angle made of two continuous-space periodic potentials. We devise a general approach, based on a hierarchy of energy scales, to derive effective tight-binding models that capture the energy spectrum, focusing on the case of square lattices. Localized states in the moiré unit cell are coupled by strong intracell and weak intercell tunnelings, generating a series of energy bands and subbands that correspond to distinct, periodic lattices. For sufficiently deep potentials, we find excellent agreement between the spectrum of the continuous-space system and the tight-binding approximation thus constructed. Our approach allows for the interpretation of moiré band structures and the extraction of parameters for the effective tight-binding models. Applications to the physics of many-body systems and extensions to other twisted models are also discussed.

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I. INTRODUCTION

In condensed matter physics, twistronics has emerged as an exciting field where novel electronic phenomena are observed [1,2]. By stacking layers of twisted two-dimensional (2D) materials, exotic properties can emerge from the complex interplay of quantum interference, interparticle interactions, and structural properties, ranging from moiré superlattices [3–6] or excitons [7–9] to quantum Hall effects [10–13]. A key component to the realization of these properties relates to the underlying single-particle band structure. For instance, in twisted bilayer graphene, the appearance of flat momentum bands at magic twisting angles significantly enhances quantum correlations [14-18], which leads to the appearance of unconventional superconductivity [19-22] and highly correlated insulators [23–25]. In addition, twisted systems allow one to interpolate between periodic and quasiperiodic structures by adjusting the twist angle. In some materials, however, interlayer couplings favor periodic structures, which obscures quasiperiodic effects [3,26,27].

Over recent years, ultracold atomic gases have been proposed as highly versatile platforms to quantum simulate a variety of problems [28–33], including nonstandard lattice models [34] and twisted systems [35–37]. Bilayer models can be emulated, in which different internal atomic states represent the different layers, which are Raman coupled and subjected to optical lattices twisted one to the other [35]. Alternatively, a single-layer model can be realized when both twisted optical lattices apply to the same internal state [38]. The latter case also models bilayers in the strong interlayer coupling limit [37]. In all cases, the twist angle can be freely tuned in experiments by adjusting the angular alignment of optical lattices.

Generally speaking, arbitrary twist angles result in quasiperiodic, or quasicrystalline, optical potentials. An interesting set of quasiperiodic potentials are those which possess a rotational symmetry incompatible with crystalline order, i.e., superimposed optical lattices that are aligned along forbidden rotational symmetries [39–41]. In recent years, the exotic properties of these quasiperiodic systems have been extensively studied in both single-particle [42–44] and many-body [45–49] scenarios. Alternatively, for a countable set of twist angles, the same devices realize superlattice moiré patterns with rich internal structure. Such potentials likewise exhibit novel properties which are distinct from that of ordinary periodic systems [38,50–53].

For both quasiperiodic and moiré lattices, the gapped-band structure plays a central role in determining the physical behavior of single particles, as well as the many-body properties. Importantly, bands and subbands can be mapped onto effective tight-binding models, which describe a lattice of sites associated to localized Wannier states coupled by tunneling processes. In the incommensurate case, the strong inhomogeneities of the potential induces a complex set of nonuniform Wannier states, from which such models can be built [54]. In the commensurate case, one can take advantage of periodicity. For simple optical potentials, such as a square lattice, each site is associated to a potential minimum and the structure of the lattice simply reproduces the Bravais lattice of elementary cells. In contrast, for moiré potentials, each elementary cell has several potential minima that are not equivalent and effective tight-binding models need to be constructed with care.

An approach to constructing effective tight-binding models for optical moiré potentials has been outlined in Ref. [38]. The primary objective of the present paper is to discuss this construction in more detail and extract effective tight-binding parameters by fitting them to the native continuous-space model.

Within a moiré potential, each unit cell is composed of unique sets of potential minima, forming distinct structures. In general, resonant intracell couplings dominate and induce separated subbands, while subdominant intercell couplings



FIG. 1. Illustration of twisted moiré potentials. Here, we take (a) two optical lattices V_A and V_B with a twist angle θ between them. By superimposing the two lattices, we generate a (b) twisted moiré potential. Examples of moiré potentials are plotted for commensurate angles (c1) $\theta_{2,1} \approx 36.87^\circ$, (c2) $\theta_{3,5} \approx 28.07^\circ$, (c3) $\theta_{2,3} \approx 22.37^\circ$, and (c4) $\theta_{2,5} \approx 43.60^\circ$, with black squares showing the unit cells.

generate dispersion relations associated to different effective tight-binding models, some of which possess a structure that differs from the initial Bravais lattice. For some cases, however, intercell couplings dominate over intracell couplings, and the construction of effective tight-binding models requires the definition of bipartite lattices. By comparing the energy spectra of the tight-binding and continuous-space models, we are able to determine the validity of the former and extract relevant physical parameters, including tunneling rates. In this work, we focus our discussion to the simplest case of square moiré lattices. However, our approach is general and may be extended to other forms of twisted potentials that have moiré unit cells with unique sets of potential minima.

The layout of our results is as follows. First, we introduce, in Sec. II, twisted optical moiré potentials as constructed from the sum of two identical squares lattices making a commensurate angle between each other, alongside a discussion of the spectral properties as obtained from exact numerical diagonalization for the continuous-space model in Sec. III. Comparison with a harmonic approximation of the moiré potential in the vicinity of the various minima allows us to classify the main band structures. We then discuss, in Sec. IV, the construction of effective tight-binding models in each band, taking advantage of energy-scale separation between intracell and intercell couplings. Accurate fitting between the spectra obtained for tight-binding and continuous-space models can then be performed, which we outline in Sec. V. This allows us to characterize the behavior and validity of the tightbinding models. We finally discuss extensions to other moiré potentials in Sec. VI, before ending with our conclusions in Sec. VII.

II. TWISTED MOIRÉ POTENTIALS

We consider single particles trapped in a twisted optical potential $V(\mathbf{r})$, with Hamiltonian

$$\hat{H} = -\frac{\hbar^2 \nabla^2}{2M} + V(\mathbf{r}), \tag{1}$$

where *M* is the particle mass and $\mathbf{r} = (x, y)$ is the position. The twisted optical lattice is defined by

$$V(\mathbf{r}) = V \times [v(R^{+}\mathbf{r}) + v(R^{-}\mathbf{r})], \qquad (2)$$

where V is the potential depth, R^{\pm} is the rotation matrix with angle $\pm \theta/2$, and, for concreteness, we consider squares lattices such that

$$v(\mathbf{r}) = \cos^2(\pi x/a) + \cos^2(\pi y/a),$$
 (3)

where $a = \lambda/2$ is the lattice constant and λ is the optical wavelength. All energies will be expressed in terms of the recoil energy $E_r = \pi^2 \hbar^2/(2Ma^2)$. A visualization of the potential is given in Figs. 1(a) and 1(b). For a specific set of commensurate twist angles θ , it is possible to form periodic, moiré patterns in real space. Here we only outline their properties, with further details and proofs presented in Appendix A. The commensurate angles can be directly written as

$$\theta_{m,n} = \cos^{-1}\left(\frac{2mn}{m^2 + n^2}\right),\tag{4}$$

where m and n are coprime integers [35]. Since the underlying structure is periodic and shows fourfold rotation symmetry, the system possesses a well-defined square unit cell with dimensionless size

$$\ell_{m,n}/a = \begin{cases} \sqrt{(m^2 + n^2)/2} & \text{if } m + n \text{ even,} \\ \sqrt{m^2 + n^2} & \text{if } m + n \text{ odd.} \end{cases}$$
(5)

This set of moiré angles can be deduced by considering the coincidence of two lattice vectors tilted by $\theta_{m,n}$, where *m* and *n* define an intersection point at $\mathbf{r}/a = (m, n)$. To determine the true period, it is important to note that geometrically equivalent moiré angles can exist for different *m* and *n*, and hence for distinct m + n either even or odd; see details and proof in Appendix A. In Figs. 1(c1)–1(c4), some examples of the moiré potentials are plotted, with their corresponding moiré cell is enlarged, with richer inhomogeneous structure. As will be shown later in our discussions, a very important quantity that characterizes the band structure is the total number of

distinct, local minima or maxima of the potential, which is given by

$$\mathcal{M}_{m,n} = \begin{cases} (\ell_{m,n}^2/a^2 - 1)/4 & \text{if } m + n \text{ even,} \\ (\ell_{m,n}^2/a^2 - 1)/4 + 1 & \text{if } m + n \text{ odd.} \end{cases}$$
(6)

Note that in this align, $\mathcal{M}_{m,n}$ is always an integer, a formal proof of which is provided in Appendix A.

III. SPECTRAL PROPERTIES

A. Dispersion relations

For a periodic potential $V(\mathbf{r})$, the Hamiltonian \hat{H} can be solved using a standard Bloch transformation [55]. We write the wave function as $\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u(\mathbf{r})$, where $u(\mathbf{r})$ is a Bloch function, which is periodic with period equal to the moiré unit length $\ell_{m,n}$, and $\mathbf{k} = (k_x, k_y)$ is the quasimomentum, which can be restricted to the first Brillouin zone, $k_{x/y}\ell_{m,n} \in$ $[-\pi \dots \pi]$. Inserting the Bloch transformed wave function into the Schrödinger align, $\hat{H}\psi(\mathbf{r}) = E\psi(\mathbf{r})$ with \hat{H} given in Eq. (1), we obtain the reduced align

$$\varepsilon(\mathbf{k})u(\mathbf{r}) = \left[\frac{\hbar^2}{2M}(\mathbf{k}^2 - 2i\mathbf{k}\cdot\nabla - \nabla^2) + V(\mathbf{r})\right]u(\mathbf{r}), \quad (7)$$

where $\varepsilon(\mathbf{k})$ spans the set of energies *E* that fulfill the periodic boundary conditions for each quasimomentum \mathbf{k} . We then solve for the Bloch functions $u(\mathbf{r})$ and eigenenergies (dispersion relations) $\varepsilon(\mathbf{k})$ via exact diagonalization, using discretization with a grid spacing of at least h/a = 0.05. Since $u(\mathbf{r})$ is a periodic function in the moiré unit cell, we can diagonalize in an $\ell_{m,n} \times \ell_{m,n}$ box with periodic boundary conditions without loss of generality. Throughout this work, we refer to continuous-space calculations as those in which Eq. (7) is diagonalized with some very small discretization h/a, in contrast to discrete tight-binding models.

In Fig. 2, we plot an example of the dispersion relations $\varepsilon(\mathbf{k})$ obtained in the first Brillouin zone for the moiré potential with twist angle $\theta_{3,5} \approx 28.07^{\circ}$ and amplitude $V = 6E_{\rm r}$. As expected for a sufficiently deep potential, we observe the formation of wide spectral gaps, separating almost flat dispersive bands; see Fig. 2(a). The different bands are labeled with an index β , which ranges from 1 to 5 for the considered energy range. Each band (except $\beta = 1$) splits into a set of narrower subbands (with index α). A magnification of band $\beta = 5$, plotted in Fig. 2(b), shows that each subband displays a cosinelike dispersion, which is to be expected for a deep optical lattice. Note that the subbands $\alpha = 2$ and $\alpha = 3$ are quasidegenerate, with each one corresponding to one branch of the observed cross structure.

For the remainder of this work, we will discuss how these results may be understood using tight-binding models. Generally speaking, tight-binding theories can be built using the framework outlined in Appendix B. In brief, the main bands (β) are explained by a simple harmonic approximation around the local minima of the moiré potential, as discussed in Sec. III B. In contrast, the subbands (α) and their dispersion relations are explained by tight-binding models,



FIG. 2. Exact energy spectrum $(E - E_g)/E_r$, with E_g the singleparticle ground-state energy, obtained from the continuous model for amplitude $V = 6E_r$ and twist angle $\theta_{3,5} \approx 28.07^\circ$. Colored lines denote different bands of states with index β , with colors representing distinct minima over which a state is distributed; see Fig. 3(a). In (a), we plot the dispersion relations across high-symmetry points of the first Brillouin zone, with a zoom in (b) given of subbands with index α in band $\beta = 5$. For $E - E_g \gtrsim 5E_r$, well-separated bands can no longer be identified (gray lines).

the structure of which depends on the band, as discussed in Sec. IV.

B. Harmonic approximation

If V/E_r is sufficiently large, the eigenstates are distributed around the local minima of the potential. Neglecting tunneling between degenerate local minima, which are sufficiently far apart, each local minimum may accommodate a set of welllocalized Wannier functions, corresponding to the ground and excited states in a given well. Figures 3(a) and 3(b) show such local minima in a unit cell for the moiré potentials with twist angles $\theta_{3,5} \approx 28.07^{\circ}$ and $\theta_{2,1} \approx 36.87^{\circ}$, respectively. The lowest minimum (red, labeled by u = 1) is unique, while the higher ones (green, u = 2; blue, u = 3; purple, u = 4) are fourfold degenerate. Note that in agreement with Eqs. (5)



FIG. 3. Zoom of two twisted moiré unit cells for angles (a) $\theta_{3,5} \approx 28.07^{\circ}$, where $\mathcal{M}_{3,5} = 4$, and (b) $\theta_{2,1} \approx 36.87^{\circ}$, where $\mathcal{M}_{2,1} = 2$, using the same color scale as in Fig. 1. Colored points denote distinct sets of potential minima with index *u* (white numbers), ordered from lowest to highest energy. Note that minima located on the unit cell edges or corners are marked by their geometrically identical local maxima within the unit cell (sets 1 and 4), for clarity (see text).



FIG. 4. Comparison of continuous (gray lines) and harmonic (colored lines) energy spectra $(E - E_g)/E_r$, where E_g is the continuous ground-state energy. The lowest gray lines thus correspond to $E_g = 0$. (a1)–(a4) The twist angle $\theta_{3,5} \approx 28.07^\circ$. (b1)–(b4) The twist angle $\theta_{2,1} \approx 36.87^\circ$. From the left to right columns, we consider decreasing potential depths of (a1), (b1) $V = 1000E_r$, (a2), (b2) $V = 100E_r$, (a3), (b3) $V = 10E_r$, and (a4), (b4) $V = 6E_r$. The colors of the harmonic energies denote the *u*th distinct set of potential minima, as in Fig. 3, with some arrows at lower V/E_r indicating bands in which continuous-space eigenstates match or look similar to a harmonic eigenstate.

and (6), we find, respectively, $\mathcal{M}_{3,5} = 4$ and $\mathcal{M}_{2,1} = 2$ distinct local minima in each unit cell. By shifting $V(\mathbf{r})$ such that the global minimum is enclosed in the unit cell center, i.e., a positional shift of $(+\ell/2, +\ell/2)$, and setting +V to -V, we have the same potentials as depicted in Fig. 3. In other words, twisted square moiré potentials will exhibit the same physics for both blue- or red-detuned systems (i.e., localization of atoms to minima or maxima), and hence we write the minima with u = 1 (red) and u = 4 (purple) at the equivalent sets of local maxima in Fig. 3 for compactness.

Expanding the potential around a local minimum centered at \mathbf{R} , we write

$$V(\mathbf{R} + \mathbf{r}) = V(\mathbf{R}) + \frac{1}{2}(\Omega_{xx}x^2 + 2\Omega_{xy}xy + \Omega_{yy}y^2) + \mathcal{O}(\dots), \qquad (8)$$

where $\Omega_{uv} = \partial^2 V / \partial u \partial v$ and $\mathcal{O}(...)$ accounts for anharmonic corrections. Diagonalizing the Hessian matrix Ω , we then find

$$V(\mathbf{R} + \mathbf{r}) \approx V(\mathbf{R}) + \frac{M}{2}(\omega_{+}^{2}x'^{2} + \omega_{-}^{2}y'^{2}),$$
 (9)

with

$$\omega_{\pm}^{2} = \frac{\Omega_{xx} + \Omega_{yy} \pm \sqrt{(\Omega_{xx} - \Omega_{yy})^{2} + 4\Omega_{xy}^{2}}}{2M}, \quad (10)$$

and x'-y' coordinates in a rotated orthogonal frame. The eigenvalues of the 2D harmonic oscillator in Eq. (9) are given by

$$E_{n_+/n_-} = V(\mathbf{R}) + \hbar\omega_+(n_+ + 1/2) + \hbar\omega_-(n_- + 1/2), \quad (11)$$

where $n_{\pm} \in \mathbb{N}$. If $\omega_{+} = \omega_{-}$, the *n*th excited state of the spectrum will be (n + 1)-fold degenerate. However, in general,

we have $\omega_+ \neq \omega_-$, i.e., all degeneracies are split, except for some accidental matchings. The final spectrum is then the combination of all energies from Eq. (11) for each potential minimum labeled by its position **R**. Each minimum forms a ladder set, which are degenerate within a given family of minima *u*. Depending on the relative strength of V/E_r , different sets for different minima may be located between one another, or potentially overlap, leading to an intricate spectrum.

In Figs. 4(a1)-4(a4), we compare the exact spectra of Eq. (7) (gray lines) at midband $\mathbf{k}\ell_{m,n} = (\pi/2, \pi/2)$ to that of Eq. (11), using the moiré angle $\theta_{3,5}$ and for decreasing values of V/E_r . Colored lines show the harmonic energies of Eq. (11), with different colors, corresponding to each unique type of potential minimum shown in Fig. 3 and labeled by u = 1, 2, 3, and 4. Starting with the larger values of $V/E_r = 1000$ and $V/E_r = 100$ in Figs. 4(a1) and (a2), we find good agreement between the exact and harmonic spectra. Each minimum forms a series of distinct bands, where each state in a harmonic band matches a state in the continuous-space bands (including degeneracies). Prominent gaps can also form, depending on the relative separation between eigenenergies of the local minima. Discrepancies and degeneracy splitting between exact and harmonic eigenenergies becomes more apparent at higher energy. This is expected since the higher-energy eigenstates contain larger components further away from a local minima, and anharmonic corrections become more important. For smaller lattice amplitudes, for instance $V/E_r = 10$ and $V/E_r = 6$ in Figs. 4(a3) and 4(a4), we still find some qualitative agreement between the exact and harmonic results for some of the lowest-energy states. Some colored arrows for the lowest-energy states are also

plotted, indicating which continuous-space bands match with the harmonic bands in terms of similar looking eigenstates. Discrepancies between energy levels are again seen due to the fact that smaller V/E_r will enhance anharmonic terms. Overall, we find that the low-energy bands and gap structure of the twisted moiré potential remains reminiscent of that of the harmonic spectrum, with quantitative accuracy for large potential depths.

Equivalent properties are also observed at different moiré angles, e.g., $\theta_{2,1}$ as shown in Figs. 4(b1)–4(b4). For this angle, we generally find larger gaps compared to that of $\theta_{3,5}$, which can be explained as follows. Each $\theta_{m,n}$ corresponds to $\mathcal{M}_{m,n}$ distinct local minima. If $\mathcal{M}_{m,n}$ is small (which implies that the moiré cell is small due to the dependence on $\ell_{m,n}$), the relative energy between different minima will be large, therefore producing wide spectral gaps. On the contrary, if $\mathcal{M}_{m,n}$ is large (which implies that the moiré cell is also large), the underlying gaps are less significant due to the smaller energy differences between minima.

IV. TIGHT-BINDING MODELS

As discussed in the previous sections, the single-particle spectrum of twisted optical potentials separates into distinct energy bands. The energy range of the latter can be approximately understood via harmonic energies associated to different sets of local minima. In order to describe the dispersion relation of the various bands, we now introduce finite tunneling rates between these minima. Tunneling processes are dominated by the resonant ones, i.e., those that couple minima with equal energies. This leads to tight-binding models with different structures in different bands, as we discuss now. Throughout this section, we focus on the case of amplitude $V = 6E_r$ and twist angle $\theta = \theta_{3,5}$ from Fig. 2. However, as we will show, the approaches and classifications here can be applied to any commensurate angle and sufficiently large potential amplitude. To ease on notation, we omit the commensurate twist angle indices and write the moiré unit length $\ell = \ell_{m,n}$.

A. Band $\beta = 1$

We start with the simplest case of band $\beta = 1$, which describes the ground state, the density distribution of which is shown in Fig. 5(a1). The approach we use is standard and we briefly outline it for reference. Since there is a single minimum in each unit cell, we can model the band with a simple square lattice, where sites are located at those minima, as in Fig. 5(a2). In such bands, the Hamiltonian is

$$\hat{H} = \epsilon^{\beta} \sum_{i} \hat{a}_{i}^{\dagger} \hat{a}_{i} - J^{\beta} \sum_{\langle i,j \rangle} \hat{a}_{i}^{\dagger} \hat{a}_{j}, \qquad (12)$$

where *i*, *j* are site indices, ϵ^{β} is the on-site energy, J^{β} is the corresponding tunneling between sites, and $\langle i, j \rangle$ denotes summation over nearest-neighboring sites. The dispersion relation is readily found by introducing the Fourier-transformed operators,

$$\hat{a}_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_i},\tag{13}$$



FIG. 5. Plot of (a1) the ground-state density profile for band 1 and (a2) the corresponding tight-binding model, taking density spots as lattice sites (purple disks) with nearest-neighbor coupling J^1 . This produces a square lattice with period ℓ , where the white and black squares in (a1) and (a2) denote the moiré unit cell.

where *N* is the total number of sites and **k** spans a discrete set of step $2\pi/N$ in each direction *x* and *y* within the first Brillouin zone, $k_{x/y}\ell \in [-\pi \dots \pi]$. Using

$$\sum_{i} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_{i}} = N\delta_{\mathbf{k},\mathbf{k}'}$$
(14)

and \mathbf{r}_i spanning the lattice sites, Hamiltonian (12) may be written as

$$\hat{H} = \sum_{\mathbf{k}} \varepsilon(\mathbf{k}) \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}}, \qquad (15)$$

where the dispersion relation $\varepsilon(\mathbf{k})$ is given by

$$\varepsilon(\mathbf{k}) = \epsilon^{\beta} - 2J^{\beta}(\cos k_x \ell + \cos k_y \ell). \tag{16}$$

This generates a standard band dispersion relation with cosine dependence in both the *x* and *y* directions. The unknown quantities ϵ^{β} and J^{β} can then be readily extracted by fitting Eq. (16) to the exact dispersion relation found from continuous-space calculations, as done in Sec. III A. The result is discussed in Sec. V.

B. Bands $\beta = 3, 4, 5$

For all other bands, we have a different situation, where there are now four potential minima within each moiré cell, with different geometries in different bands; see Fig. 6 for bands $\beta = 3$, 4, and 5. For now, we forgo the discussion of band 2, which is more complicated, and focus on bands 3–5. In order to model one of these bands, we separate the tunneling rates into two distinct energy scales: intracell tunnelings (\mathcal{I}^{β} and \mathcal{I}'^{β} for band β) and intercell tunneling (J^{β}_{α} for subband α in band β). Owing to the exponential decay of tunneling rates with site separation, the intracell couplings generally exceed the intercell couplings, i.e., $\mathcal{I}^{\beta}, \mathcal{I}'^{\beta} \gg J^{\beta}_{\alpha}$. We may then treat the intercell couplings as perturbations of the intracell ones.

We begin by writing the Hamiltonian describing the intracell tunnelings within one unit moiré cell, corresponding to one of the green squares in Figs. 6(a2), 6(b2), and 6(c2). Note that in Figs. 6(b2) and 6(c2), we have shifted the green unit cell across the diagonal in order to enclose four sites in the vicinity of the cell center and have a description similar to that of band 3 in Fig. 6(a2). Each unit cell contains four sites located at the spots of the



FIG. 6. Plots of the (a1), (b1), and (c1) density profiles for a state in bands 3, 4, and 5, respectively, and (a2), (b2), and (c2) the corresponding tight-binding models, taking density spots (maxima) as lattice sites (purple disks). The green squares in (a2), (b2), and (c2) are unit cells of length ℓ , which contain four sites with nearest-neighbor coupling \mathcal{I}^{β} (blue) and next-nearest-neighbor coupling \mathcal{I}^{β} (red).

considered band. In matrix form, the Hamiltonian can be written as

$$\hat{H}_{\text{cell}} = \begin{pmatrix} \epsilon^{\beta} & -\mathcal{I}^{\beta} & -\mathcal{I}'^{\beta} & -\mathcal{I}^{\beta} \\ -\mathcal{I}^{\beta} & \epsilon^{\beta} & -\mathcal{I}^{\beta} & -\mathcal{I}'^{\beta} \\ -\mathcal{I}'^{\beta} & -\mathcal{I}^{\beta} & \epsilon^{\beta} & -\mathcal{I}^{\beta} \\ -\mathcal{I}^{\beta} & -\mathcal{I}'^{\beta} & -\mathcal{I}^{\beta} & \epsilon^{\beta} \end{pmatrix}, \qquad (17)$$

where \mathcal{I}^{β} denotes nearest-neighbor tunneling, \mathcal{I}'^{β} is nextnearest-neighbour tunneling, and ϵ^{β} is the on-site energy of the band. Since all sites lie in equivalent potential minima and the system has fourfold rotational symmetry, ϵ^{β} is the same for each site. Moreover, each set of intracell tunnelings is equal. The matrix in Eq. (17) can thus be diagonalized, with



FIG. 7. Intercell couplings between the intracell eigenstates from Eq. (18) and nearest-neighbor green unit cells as in Figs. 6(a2), 6(b2), and 6(c2). Black lines denote the states of each subband α , with corresponding energy E_{α}^{β} , where $E_{B}^{\beta} = E_{C}^{\beta}$. The energy spacing between states is shown outside the right-hand green cell.

normalized eigenstates given by

$$|a\rangle = \frac{1}{2} \begin{pmatrix} 1\\1\\1\\1 \end{pmatrix}, \quad |B\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\0\\-1\\0 \end{pmatrix},$$
$$|C\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0\\1\\0\\-1 \end{pmatrix}, \quad |d\rangle = \frac{1}{2} \begin{pmatrix} 1\\-1\\1\\-1 \end{pmatrix}, \quad (18)$$

and eigenvalues

$$E_{a}^{\beta} = \epsilon^{\beta} + 2\mathcal{I}^{\beta} - \mathcal{I}^{\prime\beta}, \quad E_{B,C}^{\beta} = \epsilon^{\beta} + \mathcal{I}^{\prime\beta},$$
$$E_{d}^{\beta} = \epsilon^{\beta} - 2\mathcal{I}^{\beta} - \mathcal{I}^{\prime\beta}, \tag{19}$$

where the degeneracy $E_B^{\beta} = E_C^{\beta}$ is also due to the fourfold rotational symmetry. Each isolated moiré cell of Fig. 6 can thus be described as a four-level system, with each level corresponding to each eigenstate of Hamiltonian (17). Two of them (*a* and *d*) are isolated in energy, while two others (*B* and *C*) are exactly degenerate due to fourfold rotational symmetry of the system. It implies that the state $|C\rangle$, which is obtained by a $\pi/2$ rotation of the state $|B\rangle$, has exactly the same energy as the latter. We adopt a convention where uppercase and lowercase letters denote degenerate and nondegenerate states, respectively.

To capture tunneling between nearest-neighbor moiré cells, we then couple the four-level systems by different intercell tunnelings, as depicted in Fig. 7. This forms an effective square lattice with period ℓ , where each site has four internal states. Restricting ourselves to the dominant (resonant) intercell tunnelings between equal energy eigenstates, we find the effective tight-binding Hamiltonian,

$$\begin{aligned} \hat{H} &= E_a^\beta \sum_i \hat{a}_i^\dagger \hat{a}_i - J_a^\beta \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + E_B^\beta \sum_i (\hat{B}_i^\dagger \hat{B}_i + \hat{C}_i^\dagger \hat{C}_i) \\ &- J_B^\beta \sum_{\langle i,j \rangle} (\hat{B}_i^\dagger \hat{B}_j + \hat{C}_i^\dagger \hat{C}_j) - \sum_{\langle i,j \rangle} W_{B;i,j}^\beta (\hat{B}_i^\dagger \hat{C}_j + \hat{C}_i^\dagger \hat{B}_j) \\ &+ E_d^\beta \sum_i \hat{d}_i^\dagger \hat{d}_i - J_d^\beta \sum_{\langle i,j \rangle} \hat{d}_i^\dagger \hat{d}_j, \end{aligned}$$
(20)

where \hat{a}_i , \hat{B}_i , \hat{C}_i , and \hat{d}_i are the annihilation operators of a particle in site *i* for the corresponding eigenstate in Eq. (18). Note that a directional dependence in the coupling $W_{B;i,j}^{\beta}$ between different degenerate states from adjacent sites is necessary to account for the crossed features of quasidegenerate subbands as in the center of Fig. 2(b). However, overall, fourfold symmetry of the system implies that the values of the coefficients $W_{B;i,j}^{\beta}$ are opposite in orthogonal directions, i.e., $W_{B;x}^{\beta} = -W_{B;y}^{\beta}$; see details in Appendix C 1. To determine the dispersion relations, we again introduce Fourier-transform operators as in Eq. (13) for each state $|a\rangle$, $|B\rangle$, $|C\rangle$, and $|d\rangle$. The momentum-space Hamiltonian is then

$$\hat{H} = \sum_{\mathbf{k}} \varepsilon_{a}^{\beta}(\mathbf{k}) \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}} + \sum_{\mathbf{k}} \varepsilon_{d}^{\beta}(\mathbf{k}) \hat{d}_{\mathbf{k}}^{\dagger} \hat{d}_{\mathbf{k}} + \sum_{\mathbf{k}} \varepsilon_{B}^{\beta}(\mathbf{k}) (\hat{B}_{\mathbf{k}}^{\dagger} \hat{B}_{\mathbf{k}} + \hat{C}_{\mathbf{k}}^{\dagger} \hat{C}_{\mathbf{k}}) + \sum_{\mathbf{k}} w_{B}^{\beta}(\mathbf{k}) (\hat{B}_{\mathbf{k}}^{\dagger} \hat{C}_{\mathbf{k}} + \hat{C}_{\mathbf{k}}^{\dagger} \hat{B}_{\mathbf{k}}), \qquad (21)$$

with

$$\varepsilon_a^\beta(\mathbf{k}) = E_a^\beta - 2J_a^\beta(\cos k_x \ell + \cos k_y \ell), \qquad (22)$$

$$\varepsilon_B^{\beta}(\mathbf{k}) = E_B^{\beta} - 2J_B^{\beta}(\cos k_x \ell + \cos k_y \ell), \qquad (23)$$

$$w_B^{\beta}(\mathbf{k}) = -2W_B^{\beta}(\cos k_x \ell - \cos k_y \ell), \qquad (24)$$

$$\varepsilon_d^{\beta}(\mathbf{k}) = E_d^{\beta} - 2J_d^{\beta}(\cos k_x \ell + \cos k_y \ell).$$
(25)

To remove the nondiagonal operators of the form $\hat{B}_{\mathbf{k}}^{\dagger}\hat{C}_{\mathbf{k}}$ and $\hat{C}_{\mathbf{k}}^{\dagger}\hat{B}_{\mathbf{k}}$, we rewrite $\hat{B}_{\mathbf{k}}$ and $\hat{C}_{\mathbf{k}}$ in terms of new operators that diagonalize the coupling part, i.e.,

$$(\hat{B}_{\mathbf{k}}^{\dagger} \ \hat{C}_{\mathbf{k}}^{\dagger}) \begin{pmatrix} \varepsilon_{B}^{\beta}(\mathbf{k}) & w_{B}^{\beta}(\mathbf{k}) \\ w_{B}^{\beta}(\mathbf{k}) & \varepsilon_{B}^{\beta}(\mathbf{k}) \end{pmatrix} \begin{pmatrix} \hat{B}_{\mathbf{k}} \\ \hat{C}_{\mathbf{k}} \end{pmatrix}$$

$$= (\hat{b}_{\mathbf{k}}^{\dagger} \ \hat{c}_{\mathbf{k}}^{\dagger}) \begin{pmatrix} \varepsilon_{B}^{\beta}(\mathbf{k}) + w_{B}^{\beta}(\mathbf{k}) & 0 \\ 0 & \varepsilon_{B}^{\beta}(\mathbf{k}) - w_{B}^{\beta}(\mathbf{k}) \end{pmatrix} \begin{pmatrix} \hat{b}_{\mathbf{k}} \\ \hat{c}_{\mathbf{k}} \end{pmatrix},$$

$$(26)$$

where $\hat{b}_{\mathbf{k}} = \frac{\hat{B}_{\mathbf{k}} + \hat{C}_{\mathbf{k}}}{\sqrt{2}}$ and $\hat{c}_{\mathbf{k}} = \frac{\hat{B}_{\mathbf{k}} - \hat{C}_{\mathbf{k}}}{\sqrt{2}}$, allowing Hamiltonian (21) to be diagonalized as

$$\hat{H} = \sum_{\mathbf{k}} \varepsilon_{a}^{\beta}(\mathbf{k}) \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}} + \sum_{\mathbf{k}} \varepsilon_{d}^{\beta}(\mathbf{k}) \hat{d}_{\mathbf{k}}^{\dagger} \hat{d}_{\mathbf{k}} + \sum_{\mathbf{k}} \varepsilon_{b}^{\beta}(\mathbf{k}) \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}} + \sum_{\mathbf{k}} \varepsilon_{c}^{\beta}(\mathbf{k}) \hat{c}_{\mathbf{k}}^{\dagger} \hat{c}_{\mathbf{k}}, \qquad (27)$$

where $\varepsilon^{\beta}_{b,c}(\mathbf{k}) = \varepsilon^{\beta}_{B}(\mathbf{k}) \pm w^{\beta}_{B}(\mathbf{k})$, i.e.,

$$\varepsilon_b^{\beta}(\mathbf{k}) = E_B^{\beta} - 2\left(J_b^{\beta}\cos k_x \ell + J_c^{\beta}\cos k_y \ell\right), \qquad (28)$$

$$\varepsilon_c^{\beta}(\mathbf{k}) = E_B^{\beta} - 2\left(J_c^{\beta}\cos k_x \ell + J_b^{\beta}\cos k_y \ell\right), \qquad (29)$$

and

$$J_b^{\beta} = J_B^{\beta} + W_B^{\beta}$$
 and $J_c^{\beta} = J_B^{\beta} - W_B^{\beta}$. (30)

From this, there are four distinct dispersion relations, given by Eqs. (22), (25), (28), and (29), corresponding to four distinct subbands, $\alpha \in \{a, b, c, d\}$. Subbands a and d have the



FIG. 8. Plot of the (a1) density profile for a state in band 2 and (a2) the corresponding tight-binding model, taking spots as lattice sites (purple disks). The blue and red squares in (a2) are unit cells of length $\ell/2$, which contain two sites with nearest-neighbor coupling \mathcal{I}^{β} (black). The light-gray line in (a2) shows the original moiré cell from (a1), with the red and blue cells forming a superlattice structure in this unit cell.

standard dispersion relation, with different shifts $E_{a,d}^{\beta}$ and tunnelings $J_{a,d}^{\beta}$. In contrast, the subbands *b* and *c* have the same shift but different dispersion relations. Each one, $\varepsilon_b^{\beta}(\mathbf{k})$ and $\varepsilon_c^{\beta}(\mathbf{k})$, is anisotropic and breaks the fourfold rotational symmetry individually. However, the combination of both does not because they are rotated by an angle $\pi/2$ with respect to one another. In other words, if we rotate the whole system by $\pi/2$, we recover the same set of dispersion relations. Similar to band 1, the energy shifts E_{α}^{β} and band widths J_{α}^{β} can then be extracted by fitting them to the continuous dispersion relations; see Sec. V.

C. Band $\beta = 2$

In order to derive the tight-binding model for band 2, we follow a process similar to that of bands 3–5, where we separate strong and weak couplings. For band 2, however, the sites or spots are now located near the moiré unit cell boundaries, so that the dominant couplings are across these boundaries; see Fig. 8(a1). To derive the relevant tight-binding model, we use a superlattice of strongly coupled internal states, as depicted in Fig. 8(a2). The smaller blue and red cells, with length $\ell/2$, now contain pairs of sites with the strongest couplings. This allows us to treat intercell couplings in perturbation of intracell couplings, consistent with the prior discussions. Note that, however, there are two types of cells (blue and red), which are identical up to a $\pi/2$ rotation. Here, the inner Hamiltonian for each blue or red cell is

$$\hat{H}_{\text{cell}} = \begin{pmatrix} \epsilon^{\beta} & -\mathcal{I}^{\beta} \\ -\mathcal{I}^{\beta} & \epsilon^{\beta} \end{pmatrix}, \tag{31}$$

which has eigenvalues

$$E_A^{\beta} = \epsilon^{\beta} + \mathcal{I}^{\beta}, \quad E_B^{\beta} = \epsilon^{\beta} - \mathcal{I}^{\beta}, \tag{32}$$

and normalized eigenstates

$$|A\rangle = |A'\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\1 \end{pmatrix}, \quad |B\rangle = |B'\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\-1 \end{pmatrix}, \quad (33)$$



FIG. 9. Coupling of states from Eq. (31) between red-to-red, blue-to-blue, and red-to-blue cells of Fig. 8(a2). Black lines denote the states of each subband α , with corresponding energy E_{α}^{β} . Due to fourfold rotational symmetry, we have $E_{A}^{\beta} = E_{A'}^{\beta}$ and $E_{B}^{\beta} = E_{B'}^{\beta}$. The energy spacing between states is shown outside the right-hand cells.

where the eigenstates $(|A\rangle, |B\rangle)$ and $(|A'\rangle, |B'\rangle)$ belong to the blue and red cells in Fig. 8(a2), respectively. The implicit basis used to write the Hamiltonian and the eigenstates, given by Eqs. (31) and (33), is rotated with an angle $\pi/2$ for red cells with respect to blue cells. This creates two energy-separated subbands, A - A' on the one hand and B - B' on the other hand, with negligible couplings between the two. In contrast, couplings between A and A' states, which have degenerate onsite energies, must be taken into account. The same holds for B and B' states. By coupling the different cells as in Fig. 9 and retaining only the nearest-neighbor terms of each type, the Hamiltonian for band $\beta = 2$ can be expressed as

ε

$$H = H_A + H_B, \tag{34}$$

with

$$\hat{H}_{A} = E_{A}^{\beta} \sum_{i} (\hat{A}_{i}^{\dagger} \hat{A}_{i} + \hat{A}_{i}^{\prime \dagger} \hat{A}_{i}^{\prime}) - \sum_{\langle i,j \rangle \in R \leftrightarrow B} W_{A}^{\beta} \hat{A}_{i}^{\dagger} \hat{A}_{j}^{\prime} - \sum_{\langle i,j \rangle \in B \rightarrow B} J_{A;i,j}^{\beta} \hat{A}_{i}^{\dagger} \hat{A}_{j} - \sum_{\langle i,j \rangle \in R \rightarrow R} J_{A';i,j}^{\beta} \hat{A}_{i}^{\prime \dagger} \hat{A}_{j}^{\prime}, \quad (35)$$

and a similar formula for \hat{H}_B , where $\langle i, j \rangle \in B \leftrightarrow R$ denotes a sum over pairs of nearest-neighboring cells from both a blue cell to a red cell and a red cell to a blue cell, i.e., $\langle i, j \rangle \in$ $B \rightarrow B$ between blue cells and $\langle i, j \rangle \in R \rightarrow R$ between red cells. Since the red cells (corresponding to the primed symbols) are obtained from a $\pi/2$ rotation of blue cells (corresponding to the nonprimed symbols), we must have $J_{A;x}^{\beta} = J_{A';y}^{\beta}, J_{A;y}^{\beta} = J_{A';x}^{\beta}, J_{B;x}^{\beta} = J_{B';y}^{\beta}$, and $J_{B;y}^{\beta} = J_{B';x}^{\beta}$; see Appendix C 2. The unit cell with only blue-to-red intercell couplings has a smaller square length of $\ell/\sqrt{2}$, and larger square Brillouin-zone length of $2\sqrt{2\pi}/\ell$. In the following, we restrict the discussion to the subband A - A'. Since the Hamiltonians \hat{H}_A and \hat{H}_B have the same structure, all formulas for the subband B - B' are the same as for the subband A - A'

By transforming the operators to momentum space, the Hamiltonian reads

$$\hat{H}_{A} = \sum_{\mathbf{k}} \left[\varepsilon_{AA}^{\beta}(\mathbf{k}) \hat{A}_{\mathbf{k}}^{\dagger} \hat{A}_{\mathbf{k}} + \varepsilon_{A'A'}^{\beta}(\mathbf{k}) \hat{A}_{\mathbf{k}}'^{\dagger} \hat{A}_{\mathbf{k}}' \right] + \sum_{\mathbf{k}} w_{AA'}^{\beta}(\mathbf{k}) (\hat{A}_{\mathbf{k}}^{\dagger} \hat{A}_{\mathbf{k}}' + \hat{A}_{\mathbf{k}}'^{\dagger} \hat{A}_{\mathbf{k}}), \qquad (36)$$

where

$$\varepsilon_{AA}^{\beta}(\mathbf{k}) = E_{A}^{\beta} - 2\left(J_{A;x}^{\beta}\cos k_{x}\ell + J_{A;y}^{\beta}\cos k_{y}\ell\right),$$

$$\varepsilon_{A'A'}^{\beta}(\mathbf{k}) = E_{A}^{\beta} - 2\left(J_{A;y}^{\beta}\cos k_{x}\ell + J_{A;x}^{\beta}\cos k_{y}\ell\right), \qquad (37)$$

$$w_{AA'}^{\beta}(\mathbf{k}) = -4W_{A}^{\beta}\left(\cos\frac{k_{x}\ell}{2}\cos\frac{k_{y}\ell}{2}\right).$$

To diagonalize the problem, we then use a similar procedure as before and introduce new operators \hat{a} , \hat{a}' , \hat{a}^{\dagger} , and \hat{a}'^{\dagger} , which diagonalize terms coupling \hat{A} , \hat{A}' , \hat{A}^{\dagger} , and \hat{A}'^{\dagger} ,

$$(\hat{A}_{\mathbf{k}}^{\dagger} \ \hat{A}_{\mathbf{k}}^{\prime\dagger}) \begin{pmatrix} \varepsilon_{AA}^{\beta}(\mathbf{k}) & w_{AA'}^{\beta}(\mathbf{k}) \\ w_{AA'}^{\beta}(\mathbf{k}) & \varepsilon_{A'A'}^{\beta}(\mathbf{k}) \end{pmatrix} \begin{pmatrix} \hat{A}_{\mathbf{k}} \\ \hat{A}_{\mathbf{k}}' \end{pmatrix}$$

$$= (\hat{a}_{\mathbf{k}}^{\dagger} \ \hat{a}_{\mathbf{k}}^{\prime\dagger}) \begin{pmatrix} \varepsilon_{a}^{\beta}(\mathbf{k}) & 0 \\ 0 & \varepsilon_{a'}^{\beta}(\mathbf{k}) \end{pmatrix} \begin{pmatrix} \hat{a}_{\mathbf{k}} \\ \hat{a}_{\mathbf{k}}' \end{pmatrix},$$

$$(38)$$

(39)

where

and

$$\epsilon_{a'}^{\beta}(\mathbf{k}) = \frac{\varepsilon_{AA}^{\beta}(\mathbf{k}) + \varepsilon_{A'A'}^{\beta}(\mathbf{k}) - \sqrt{\left[\varepsilon_{AA}^{\beta}(\mathbf{k}) - \varepsilon_{A'A'}^{\beta}(\mathbf{k})\right]^{2} + 4w_{AA'}^{\beta}(\mathbf{k})^{2}}{2}.$$
(40)

 $\varepsilon_{a}^{\beta}(\mathbf{k}) = \frac{\varepsilon_{AA}^{\beta}(\mathbf{k}) + \varepsilon_{A'A'}^{\beta}(\mathbf{k}) + \sqrt{\left[\varepsilon_{AA}^{\beta}(\mathbf{k}) - \varepsilon_{A'A'}^{\beta}(\mathbf{k})\right]^{2} + 4w_{AA'}^{\beta}(\mathbf{k})^{2}}{2}$

Using these formulas and similar ones for the B - B' subband, we find that the final Hamiltonian is

$$\hat{H} = \sum_{\mathbf{k}} \varepsilon_{a}^{\beta}(\mathbf{k}) \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}} + \sum_{\mathbf{k}} \varepsilon_{a'}^{\beta}(\mathbf{k}) \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}}^{\prime} + \sum_{\mathbf{k}} \varepsilon_{b}^{\beta}(\mathbf{k}) \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}} + \sum_{\mathbf{k}} \varepsilon_{b'}^{\beta}(\mathbf{k}) \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}}^{\prime}.$$
(41)

We thus find four distinct subbands $\alpha \in \{a, a', b, b'\}$ within band $\beta = 2$.

We can then extract the energy shifts E_A^β and E_B^β , as well as the intercell tunnelings $J_{A;x}^\beta$, $J_{A;y}^\beta$, W_A^β , $J_{B;x}^\beta$, $J_{B;y}^\beta$, and W_B^β , by fitting them to the continuous-space dispersion relations; see Appendix D4. Note that these bands have nonstandard dispersion relations, given by Eqs. (39) and (40), with Eq. (37). In most cases, couplings between blue-to-red cells dominate over those between cells with the same due to the smaller distance; see Fig. 8(a2). We then have

$$\varepsilon_{a/a'}^{\beta}(\mathbf{k}) \approx E_{A}^{\beta} \pm w_{AA'}^{\beta}(\mathbf{k}) = E_{A}^{\beta} \mp 4J_{a}^{\beta} \left(\cos\frac{k_{x}\ell}{2}\cos\frac{k_{y}\ell}{2}\right),$$

$$\varepsilon_{b'/b'}^{\beta}(\mathbf{k}) \approx E_{B}^{\beta} \pm w_{BB'}^{\beta}(\mathbf{k}) = E_{B}^{\beta} \mp 4J_{b}^{\beta} \left(\cos\frac{k_{x}\ell}{2}\cos\frac{k_{y}\ell}{2}\right),$$
(42)

with $J_{a/b}^{\beta} = W_{A/B}^{\beta}$. The momentum dependence can be written as

$$4W^{\beta}\cos\frac{k_{x}\ell}{2}\cos\frac{k_{y}\ell}{2} = 2W^{\beta}\left(\cos\frac{\bar{k}_{x}\ell}{\sqrt{2}} + \cos\frac{\bar{k}_{y}\ell}{\sqrt{2}}\right), \quad (43)$$

with $\bar{k}_x = \mathbf{k} \cdot \bar{\mathbf{x}}$ and $\bar{k}_y = \mathbf{k} \cdot \bar{\mathbf{y}}$, where $\bar{\mathbf{x}} = (\hat{\mathbf{x}} + \hat{\mathbf{y}})/\sqrt{2}$ and $\bar{\mathbf{y}} = (\hat{\mathbf{x}} - \hat{\mathbf{y}})/\sqrt{2}$ are unit vectors of the smaller (rotated) square lattice. The subbands *a* and *a'* are thus centered around energy E_A^β and have almost opposite variations with \mathbf{k} . The



FIG. 10. Energy scales within twisted moiré potentials. On the left, we have degenerate harmonic bands with characteristic separation $\hbar\omega$, corresponding to the four sites (purple disks in the lower gray square) of an isolated moiré cell. By coupling the sites from a given unit cell, degenerate harmonic bands are split into subbands, with separation depending on the intracell tunneling \mathcal{I} . Finally, by coupling nearest-neighbor moiré cells, the energy spectrum will exhibit cosinelike dispersions for each subband, with width scaled to the intercell tunneling J.

same holds for subbands *b* and *b'*, but they are centered around a different energy E_B^{β} and the amplitude of variations is different from that of subbands *a* and *a'*.

V. EFFECTIVE TIGHT-BINDING PARAMETERS

So far, we have separated different energy scales in order to characterize the continuous-space spectra and devise effective tight-binding models. Figure 10 illustrates the different energy scales present in twisted moiré potentials as a reminder. First, we have the basic structure of well-separated bands, which are captured with a harmonic approximation around each minima. Next, by coupling different minima in a moiré cell together, degenerate harmonic states are split into distinct subbands, with intracell tunnelings governing the separation between each subband. Finally, by coupling different moiré cells together, we introduce the final energy scale of intercell couplings, which produces the cosinelike features in the dispersion relations.

We now compare the predictions of the effective tightbinding models constructed in Sec. IV with the exact results obtained in Sec. III from the continuous-space model. The parameters of tight-binding models (energy shifts E^{β}_{α} and band widths $\propto J_{\alpha}^{\beta}$) are obtained by fitting the tight-binding dispersion relation for each subband to the corresponding one for the continuous-space model. We show the momentum dependence, with the on-site energy offsets set to zero and modulations of cosine functions set to unity, of some example bands and subbands in Fig. 11, comparing continuous (upper row) and tight-binding (lower row) dispersion relations at the moiré angle of $\theta_{3,5}$. From the comparisons, we immediately see that the momentum dependence of the continuous-space dispersions is accurately captured with the tight-binding models. For the ground-state subband $\beta = 1$ in the first column of Fig. 11, the dispersion relation follows the standard dispersion of a 2D square lattice, given by Eq. (16). In the second and third columns, corresponding to $\beta = 2$, we show two quasidegenerate subbands $\alpha = (b, b')$. The dispersion relations are consistent with the nonstandard forms given in Eqs. (39) and (40), with Eq. (37). We also find good agreement with the approximation of Eq. (42). Next, in band $\beta = 3$, corresponding to the last three columns in Fig. 11, we have two nondegenerate subbands $\alpha = d$ (fourth column) and $\alpha = a$ (not shown), with dispersions again following that of a standard 2D square lattice. Finally, in the last two columns, we show the degenerate subbands $\alpha = c$ and $\alpha = b$, which have strongly anisotropic dispersions, due to the $\pi/2$ -rotational symmetry as discussed in the prior section, consistent with Eqs. (28) and (29).

More precisely, we quantify the agreement between the continuous-space and tight-binding models with a residual parameter γ_{α}^{β} , defined as the average difference between the tight-binding ε_{TBM} and continuous-space ε_{C}



FIG. 11. Momentum (**k**) dependence of the dispersion relations from the (a1)–(a6) continuous results when $V = 6E_r$ and (b1)–(b6) fitted tight-binding models. The color scales only show the momentum dependence of each dispersion relation, i.e., without an on-site energy offset and width scaling by tunneling rates. We consider bands and subbands (a1), (b1) $\beta = 1$; (a2), (b2) $\beta = 2$ and $\alpha = b$; (a3), (b3) $\beta = 2$ and $\alpha = b$; (a4), (b4) $\beta = 3$ and $\alpha = d$; (a5), (b5) $\beta = 3$ and $\alpha = c$; (a6), (b6) $\beta = 3$ and $\alpha = b$. In all cases, lattice and continuous results are in good agreement. Equivalent properties are also observed for the other bands and subbands.

dispersion relations,

$$\gamma_{\alpha}^{\beta} = \frac{\ell^2}{4\pi^2} \int_{-\pi/\ell}^{\pi/\ell} \int_{-\pi/\ell}^{\pi/\ell} dk_x \, dk_y \, |\varepsilon_{\text{TBM}}(\mathbf{k}) - \varepsilon_{\text{C}}(\mathbf{k})|. \tag{44}$$

Since the dispersions are scaled by the tunneling rates J_{α}^{β} , we consider the ratio $\gamma_{\alpha}^{\beta}/J_{\alpha}^{\beta}$ for each band and subband in order to provide meaningful comparisons. In Fig. 11, we find that the largest residuals are $\gamma_{\alpha}^{\beta}/J_{\alpha}^{\beta} \sim 0.04$, i.e., there are no noticeable differences between dispersion relations. These errors may be further reduced by including beyond-nearest-neighbor couplings within the tight-binding models. However, in the present work, we find it sufficient to consider only couplings with separation up to the moiré length ℓ for high accuracy across a range of potential depths.

For smaller potential depths V/E_r , it is to be expected that the effective tunneling rates of tight-binding models will increase, but at the same time the validity of the tight-binding approximation should progressively deteriorate. To understand the scaling of tight-binding parameters and the range of validity, we consider the moiré potential for a range of potential depths V and two twist angles, $\theta_{3,5}$ in Figs. 12(a1)– 12(a4) and $\theta_{2,1}$ in Figs. 12(b1)–12(b4). Here, different bands are colored according to the uth minima in Fig. 3 and labeled according to the equivalent harmonic energy $E_{n_{+},n_{-}}^{u}$. The matching between states is performed by comparing the structure and localization of a continuous state with harmonic eigenstates, e.g., continuous states that are Gaussian-like around some minima u are labeled as $E_{0,0}^{u}$ and likewise for higher excitations in n_{\pm} . As discussed, different minima correspond to different ladders of energy bands, which may cross at certain values of V/E_r . We then plot some of the lowest ground-state and excited bands to illustrate this. In particular, we plot ϵ^{β} , the intracell or on-site energy of band β , which is equivalent to the average shift of the subband energy; see Appendix D. We also plot $(\gamma/J)_{\max}^{\beta}$, which is defined as the largest value of $\gamma_{\alpha}^{\beta}/J_{\alpha}^{\beta}$ for band β . Finally, we also plot J_{max}^{β}



FIG. 12. Tight-binding parameters as a function of V/E_r , for angles (a1)–(a4) $\theta_{3,5}$ and (b1)–(b4) $\theta_{2,1}$. For different bands, we plot the (a1), (b1) on-site energy ϵ ; the (a2), (b2) largest residual $(\gamma/J)_{max}^{\beta}$; the (a3), (b3) largest intercell coupling J_{max}^{β} ; and the (a4), (b4) largest intracell coupling $\mathcal{I}_{max}^{\beta}$. Different bands are labeled according to the related harmonic energy $E_{n_{+},n_{-}}^{u}$ [see Eq. (11)], with colors for the *u*th minima as in Fig. 3, where squares are ground states and diamonds are excited states. Colored dashed lines are guides to the eye, with the gray line in (a2), (b2) showing $(\gamma/J)_{max}^{\beta} = 1$, the effective threshold for the tight-binding validity.

(the largest intercell tunneling of a band, in magnitude) and $\mathcal{I}_{\max}^{\beta}$ (the largest intracell tunneling of a band, in magnitude). Note that we take the absolute values of the tunnelings to determine the maximum since both positive and negative tunnelings exist within different bands. In Figs. 12(a1) and 12(b1), we observe a familiar structure of energy gaps in the spectrum close to that of Fig. 4, with crossings at larger $V \simeq 9E_{\rm r}$ (red and purple diamonds) and $V \simeq 11E_{\rm r}$ (green and purple diamonds) for the excited harmonic states. We find that the energy shifts increase with the potential depth. This is to be expected since they are governed by the energies at the potential minima (proportional to V) and the frequencies of the harmonic approximation (proportional to \sqrt{V}). The quasilinear behavior observed here suggests that the energy shifts are dominated by the former contribution, while the latter is negligible. To show that the tight-binding models are indeed valid across a range of V, we plot the largest residuals $(\gamma/J)_{\text{max}}^{\beta}$ in Figs. 12(a2) and 12(b2), which shows that $(\gamma/J)_{\rm max}^{\beta} \ll 1$ for the majority of bands. For bands generated from excited harmonic states (diamonds), the accuracy of the tight-binding model is not as good for the considered potential amplitudes, owing to larger on-site energies. We, however, expect to find good agreement for larger potential amplitude, consistent with the observed tendency of decreasing γ/J with V. The intercell (J_{max}^{β}) and intracell $(\mathcal{I}_{\text{max}}^{\beta})$ couplings decrease exponentially with V, as observed in Figs. 12(a3) and 12(b3), and Figs. 12(a4) and 12(b4). This is also to be expected since the potential barriers increase with V.

For large V/E_r , all tunnelings and γ_{α}^{β} become smaller. Each potential minima are decoupled and can be described more accurately via the harmonic approximation introduced in Sec. III. As V/E_r becomes smaller, coupling between potential minima or sites splits the degeneracies that are associated to the harmonic approximation. However, localized Wannier functions can still form in the low-energy bands, resulting in very small values of $(\gamma/J)_{\text{max}}^{\beta}$, so tight-binding theory can still be applied. Higher-energy bands have larger values of $(\gamma/J)_{\text{max}}^{\beta}$ due to the more extended behavior of the associated Wannier functions across space. While visible distortions of the full 2D dispersion are small, the continuous dispersion relation is no longer modulated by nearest-neighbor tunnel-ing alone, meaning that $(\gamma/J)_{\max}^{\beta}$ is more sensitive to small fluctuations. Finally, it is also important to note that at smaller $V/E_{\rm r}$, the subbands of certain bands are no longer isolated in energy from other bands, and hence the considered tightbinding framework cannot be applied. For $\theta_{3,5}$, this occurs for the u = 2, 3, 4 minima around $V/E_r \sim 3-4$. Similar properties also occur for excited states within different minima, e.g., $E_{0,1}^1$ and $E_{0,1}^2$ bands being absent for $V/E_r \lesssim 7$ (red and green diamonds).

The intercell tunnellings in Fig. 12(a3) usually grow in magnitude as the band index increases, giving the approximate ordering $J_{\alpha}^1 < J_{\alpha}^2 < J_{\alpha}^3 \dots$, and likewise for the intracell couplings in Fig. 12(a4). The reason behind this can be linked to the fact that higher band indices denote states that are either localized in higher-energy potential minima or excited Wannier states in the potential minima, which extend further away from the minima and thus enhance tunneling probabilities. Note that there are some special cases where this may not

occur, e.g., between bands 2 and 3 in Fig. 12(a3) (green and blue squares), where the nearest-neighbor intercell couplings have the separation $\sim \ell/\sqrt{2}$ (larger tunneling) rather than $\sim \ell$ (smaller tunneling) due to the superlattice structure. For more general or more exotic moiré potentials, a similar breakdown may also occur.

When considering different moiré angles, the distribution of tight-binding parameters can drastically change. In Figs. 12(b1)-12(b4), we plot the same results for the commensurate angle $\theta_{2,1}$. For this angle, we have two distinct minima as in Fig. 3(b), where bands and subbands can be modeled using the same tight-binding models as before, with red points equivalent to band 1 from Sec. IV A and green points equivalent to band 4 from Sec. IV B. The energy separation between minima for the commensurate angle $\theta_{2,1}$ is larger, allowing for the formation of more prominent spectral gaps in Fig. 12(b1). Furthermore, the spatial separation between minima is smaller, thus enhancing the observable tunneling rates in Figs. 12(b3) and 12(b4). This contrasts with the behavior observed for $\theta_{3,5}$ in Figs. 12(a1)–12(a4), in which the moiré cell is enlarged and has more distinct potential minima, with smaller relative separations in energy. This leads to more, but smaller gaps and tunnelings since the minima are distributed further across space.

VI. GENERALIZATION: CLASSIFICATION OF BANDS

So far, the bands we have studied for $\theta = \theta_{3,5}$ and $\theta = \theta_{2,1}$ fall into three distinct classes. For completeness, we now discuss the geometrical classification of bands for arbitrary θ . When V/E_r is deep enough, the low-energy eigenstates are well localized around distinct sets of potential minima. Each set forms a distinct geometry for an underlying tight-binding model, with examples from the prior sections.

Based on the fourfold rotational symmetry and the fact that there are, at most, four degenerate minima in the moiré cell, we may generally identify four unique classes of bands or geometrical arrangements that can appear in twisted square moiré potentials. These are shown in Fig. 13, with the green areas denoting regions of space where a site is closer to the moiré cell boundary than the center (defined up to a shift of the cell). In practice, we find that the shortest distance between sites determines the strongest couplings. It may, however, not be excluded that some short-distance couplings are suppressed by high potential barriers. Hence, more precisely, in our classification, sites in the white regions correspond to cases where intracell couplings dominate over intercell couplings (as for bands 1, 3, 4, and 5 discussed above), while, on the contrary, sites in the green regions correspond to cases where intercell couplings dominate over intracell couplings (as for band 2 discussed above). Note that the cases on the upper and lower rows of the same column in Fig. 13 are actually equivalent upon a shift or rotation of the unit moiré cell.

A. Class I

We start with the simplest case of class I in Fig. 13. Here, we effectively have one potential minima enclosed by the moiré cell, with components located at the cell center or at corners. The dispersion is that of a square lattice, which was



FIG. 13. Unique arrangements of potential minima in a moiré cell with fourfold rotational symmetry (blue and orange dotted lines are symmetry lines), ordered into classes of tight-binding models or bands. Green areas denote regions of space that will always be closer to an adjacent moiré cell than the center, defined up to a shift of the cell. For class I bands, we have one minima in the center of the cell or, by shifting the cell, a group of quarter minima at each of the four corners. For class II bands, we have a half minima at the midpoint of each edge or, by shifting the cell, one minima in the center with a group of quarter minima at the four corners. Class III bands have four minima in the cell along symmetry lines, outside the green regions. Finally, class IV bands have four minima inside the green regions or, by shifting the unit cell, a group of eight total half minima along the four edges.

discussed in Sec. IV A. Sites of class I bands are always located at the global minima of the potential. There is one subtle point to note about these bands, however. From the harmonic spectrum at larger V/E_r in Figs. 4(a1) and 4(b1), the *n*th excited states in these minima are implied to be (n + 1)fold degenerate, which would require a generalized matrix diagonalization procedure to describe the bands. In practice, anharmonic terms may split this degeneracy beyond that of the tunneling rates, allowing for each subband of the excited state to be treated by the model in Sec. IV A. For potential depths $V < 12E_r$ that are typical in cold-atom experiments, the largest excited state to appear isolated in the spectrum is the first excited state (see Fig. 12), although tunneling rates may now be larger than the degeneracy splitting. For such cases, the dispersions of the first excited class I subbands will then be similar to Eqs. (28) and (29).

B. Class II

In Fig. 13, we also show the configuration of class II bands. Here, we have four potential minima at the midpoints of the unit cell edges. In other words, there are two effective minima enclosed by the cell, which would produce two subbands. At present, this class has not been observed in the considered cases with square lattices, including other commensurate angles with moiré lengths $\ell_{m,n} < 10a$. While a class II band can form if larger supercells are used as the unit cell, the lattice points of a class II band are then that of the global potential minima. In other words, we can always form a smaller, square cell and reduce a class II band to a class I band. In general, however, we cannot fully rule out the possibility of forming

this class for larger moiré lengths and/or nonsquare lattices, hence why we include a brief discussion for completeness. The model of this band structure is a simplified version of the one covered in Sec. IV C. Here a superlattice similar to that of Fig. 8(a2) is formed, but with a single site in each nonempty superlattice cell. For this reason, there is a single type of state in each cell: $|A\rangle$ in blue cells and $|A'\rangle$ in red cells. The Hamiltonian is

$$\hat{H} = \epsilon^{\beta} \sum_{i} (\hat{A}_{i}^{\dagger} \hat{A}_{i} + \hat{A}_{i}^{\prime \dagger} \hat{A}_{i}^{\prime})$$

$$- W_{A}^{\beta} \sum_{\langle i, j \rangle \in R \leftrightarrow B} \hat{A}_{i}^{\dagger} \hat{A}_{j}^{\prime}$$

$$- J_{A}^{\beta} \sum_{\langle i, j \rangle \in B \rightarrow B} \hat{A}_{i}^{\dagger} \hat{A}_{j} - J_{A}^{\beta} \sum_{\langle i, j \rangle \in R \rightarrow R} \hat{A}_{i}^{\prime \dagger} \hat{A}_{j}^{\prime}.$$

$$(45)$$

Note that the on-site energy is directly ϵ^{β} and the hopping is not directional. The latter can be diagonalized as \hat{H}_A in Sec. IV C, and we find two bands,

$$\varepsilon_{a}^{\beta}(\mathbf{k}) = \epsilon^{\beta} - 2J_{A}^{\beta}(\cos k_{x}\ell + \cos k_{y}\ell) + 4W_{A}^{\beta}\left(\cos \frac{k_{x}\ell}{2}\cos \frac{k_{y}\ell}{2}\right), \varepsilon_{a'}^{\beta}(\mathbf{k}) = \epsilon^{\beta} - 2J_{A}^{\beta}(\cos k_{x}\ell + \cos k_{y}\ell) - 4W_{A}^{\beta}\left(\cos \frac{k_{x}\ell}{2}\cos \frac{k_{y}\ell}{2}\right).$$
(46)

These formulas are similar to Eqs. (39) and (40) for $J_{A;x}^{\beta} = J_{A;y}^{\beta}$ and thus $\varepsilon_{AA}^{\beta}(\mathbf{k}) = \varepsilon_{A'A'}^{\beta}(\mathbf{k})$.

C. Class III

The next class III geometries in Fig. 13 describe a wider variety of bands in twisted moiré potentials. For these cases, four potential minima are now located within the unit cell. The minima are located outwith the green, superlattice cell, i.e., they are localized towards the unit cell center. The resulting class III bands can then be modeled using the procedures outlined in Sec. IV B.

D. Class IV

The final set of class IV bands in Fig. 13 describes a more complex series of bands that must be described by a superlattice structure. There are again four potential minima in the cell, but now located within the green, superlattice cells. In other words, intercell couplings dominate over intracell ones. This situation can be treated using the superlattice scheme discussed in Sec. IV C for band $\beta = 2$.

VII. CONCLUSIONS

In summary, we have discussed the single-particle spectrum of twisted moiré potentials across a range of potential depths and described how effective tight-binding models are constructed in different bands. Our construction is mainly based on energy separation, as illustrated in Fig. 10. If the moiré potentials are deep enough, each distinct minima of the potential contributes to unique sets of bands within the overall spectrum, with the exact form derived from the anisotropic harmonic approximation. As the potential depth is decreased, couplings between potential minima become significant. Localized Wannier states can still form at potential minima, allowing for bands and subbands to be characterized by one of four distinct classes of tight-binding geometries. The latter are determined by a hierarchy of energy scales encompassing strong local couplings, and weak couplings that support long-range coherence. This allows us to build various effective tight-binding models, the parameters of which (tunneling and on-site energies) can be fitted to the exact continuous-space spectrum. Furthermore, the accuracy between the continuousspace and tight-binding dispersions is then related to the localization of eigenstates. If an eigenstate is too extended across space, i.e., at very small potential depths, the introduction of longer-range coupling and overlapping bands reduces the accuracy of the models. Otherwise, for larger potential depths, eigenstates become more localized, in agreement with the harmonic approximation.

In this work, we have focused on single-particle energy spectra, but our findings are also directly relevant to the many-body, bosonic counterpart of Hamiltonian (1) with 2D contact interactions [38]. In the strongly interacting regime, spectral gaps can be mapped to insulating phases, and bands of states to compressible phases. For the compressible domains, we may have either a superfluid (SF) or normal fluid (NF), and the calculated tunnelings serve as a typical temperature scale for which the system transitions from one to the other: If the temperature *T* of the many-body system is such that $k_BT \lesssim J^{\beta}_{\alpha}$ for the given band, then the compressible phase will be that of a SF. Otherwise, for $k_BT \gtrsim J^{\beta}_{\alpha}$, we will have a thermal, NF phase. Our results therefore illustrate the thermal

stability of SF order in twisted moiré potentials. In realistic experiments with a typical $T \sim 10nK$, we have $k_BT \sim 10^{-2}E_r$ for most atomic species. For most of the low-energy bands, we then have $J_{\alpha}^{\beta} \ll 10^{-2}$, so SF order will generally not be stable for small chemical potentials μ/E_r . There are, however, some exceptions, notably for moiré potentials with smaller unit cells, in which effective couplings are enhanced by virtue of the smaller separation between sites [38].

Our work may be extended in various directions. For instance, while we have focused on square-lattice examples, the framework and procedures that we have introduced here can also be applied to other, more general twisted potentials as well, provided one can identify a separation of energy scales similar to that of Fig. 10. Finally, the physics of twisted moiré potentials can be extended to twisted bilayer or multilayer systems for strong interlayer couplings [37]. This includes, for instance, twisted bilayer graphene, which can be modeled using state-dependent, hexagonal rather than square optical potentials with a twist [35].

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APPENDIX A: GEOMETRICAL PROPERTIES OF MOIRÉ POTENTIALS

Here, we provide further details and derivations on the geometrical properties of twisted moiré potentials. To begin, we discuss the origin of moiré angles. Given two square-lattice vectors,

$$\mathbf{a}_{m,n}/a = m\hat{\mathbf{x}} + n\hat{\mathbf{y}}, \quad \mathbf{b}_{m',n'}/a = m'R_{\theta}\hat{\mathbf{x}} + n'R_{\theta}\hat{\mathbf{y}}, \quad (A1)$$

where $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ are unit vectors along the *x* and *y* axes, and R_{θ} is the rotation matrix with angle θ ,

$$R_{\theta} = \begin{pmatrix} \cos\theta & -\sin\theta\\ \sin\theta & \cos\theta \end{pmatrix}, \tag{A2}$$

a commensurate angle is defined when the lattice vectors coincide, i.e.,

$$\mathbf{a}_{m,n} = \mathbf{b}_{m',n'}, \quad \binom{m}{n} = \binom{m'\cos\theta - n'\sin\theta}{n'\cos\theta + m'\sin\theta}, \quad (A3)$$

from which it follows that

$$\cos \theta = \frac{mm' + nn'}{m'^2 + n'^2}, \quad \sin \theta = \frac{m'n - mn'}{m'^2 + n'^2}.$$
 (A4)

The numbers in the numerators and denominators of Eq. (A4),

$$Z_{1} = mm' + nn',$$

$$Z_{2} = m'n - mn',$$

$$Z_{3} = m'^{2} + n'^{2},$$
 (A5)

are all integers since m, m' n, and n' are integers. The numbers Z_1 , Z_2 , and Z_3 thus form a Pythagorean triple, which constrains m and n to be coprime integers, with m' = n and n' = m. Align (A4) can then be simplified into

$$\cos \theta_{m,n} = \frac{2mn}{m^2 + n^2}, \quad \sin \theta_{m,n} = \frac{n^2 - m^2}{m^2 + n^2},$$
 (A6)

where $\theta_{m,n}$ is the moiré angle, as in Eq. (4).

Two twisted lattices will therefore intersect at points $\mathbf{r}/a =$ (0, 0) and $\mathbf{r}/a = (m, n)$, separated by a distance $\sqrt{m^2 + n^2}/a$. One would then expect, in general, that this distance is the period of the moiré lattice $\ell_{m,n}$. However, some care has to be taken when considering the parities of m or n, and the uniqueness of $\theta_{m,n}$. The full set of moiré angles can be defined in the range $[0 \dots 45^\circ]$. Any moiré angle outside this range must be mapped into one within the range. As an example, let us choose the smallest, nontrivial moiré angle $\theta_{2,1} \approx 36.87^{\circ}$, which we have studied in the main text. Note that a nontrivial moiré angle refers to an angle in which the resulting optical lattice is not that of a simple square lattice. We also have $\theta_{3,1} \approx 53.13^{\circ} = -36.87^{\circ}$, i.e., $\cos \theta_{2,1} = \sin \theta_{3,1}$. Both $\theta_{2,1}$ and $\theta_{3,1}$ are geometrically equivalent, but care has to be taken in the way the unit cell is defined with m and n. Let us consider two cases: m + n an odd or even number. For m + nodd, e.g., $\theta_{2,1}$ with m + n = 3, $m^2 + n^2 = 5$ is also an odd and prime number. For m + n even, e.g., $\theta_{3,1}$ with m + n = 4, $m^2 + n^2 = 10$ is an even number. Clearly, the true moiré period must be $\ell_{2,1} = \sqrt{5} \equiv \ell_{3,1} = \sqrt{10/2}$. In summary, given a moiré angle θ_{m_0,n_0} where $m_0 + n_0$ is an odd number, there is a geometrically equivalent moiré angle θ_{m_e,n_e} for $m_e + n_e$ as an even number, which are related via

$$m_{\rm o}^2 + n_{\rm o}^2 = \frac{m_{\rm e}^2 + n_{\rm e}^2}{2}.$$
 (A7)

Given this condition, the true moiré period $\ell_{m,n}$ is then written as

$$\ell_{m,n}/a = \begin{cases} \sqrt{(m^2 + n^2)/2} & \text{if } m + n \text{ even,} \\ \sqrt{m^2 + n^2} & \text{if } m + n \text{ odd,} \end{cases}$$
(A8)

as in Eq. (5).

By superimposing two square optical potentials, we can then generate a twisted moiré potential by tuning the twist angle to $\theta_{m,n}$. This generates an intricate superlattice structure, with distinct sets of potential minima in the moiré cell. The total number of distinct minima in a moiré potential follows the relation given in Eq. (6). Note that this relation is empirical. The formal derivation of the number of distinct minima requires solutions to the problem $\partial V(\mathbf{r})/\partial x = \partial V(\mathbf{r})/\partial y = 0$. However, to the best of our knowledge, no analytical solutions to this problem exist. However, Eq. (6) always produces an integer number, which can be shown as follows. As m and *n* are two coprime integers, we may distinguish two cases: (i) one is an odd number and the other is an even number; (ii) both are odd numbers. For case (i), m and n have different parities and we may suppose *m* is odd and *n* is even, without loss of generality. For three integers a, b, c, it can be shown that if $a \equiv b \mod c$, then $a^2 \equiv b^2 \mod c$. Since m is an odd number, $m \equiv 1 \mod 4$ or $m \equiv 3 \mod 4$. Furthermore, since $3^2 \equiv 1 \mod 4$, we always have $m^2 \equiv 1 \mod 4$.

Finally, since m + n is odd, according to Eq. (5), $\ell_{m,n}/a = \sqrt{m^2 + n^2}$. So $\ell_{m,n}^2/a^2 = m^2 + n^2 \equiv 1 \mod 4$, which means that $\mathcal{M}_{m,n}$ [Eq. (6)] is an integer. For case (ii), *m* and *n* are both odd numbers. Since *m* is an odd number, $m \equiv 1$ or 3 or 5 or 7 mod 8, then $m^2 \equiv 1^2 \equiv 3^2 \equiv 5^2 \equiv 7^2 \equiv 1 \mod 8$. Similarly, when *n* is an odd number, we also have $n^2 \equiv 1 \mod 8$. Thus, we have $m^2 + n^2 \equiv 2 \mod 8$ so that $\frac{m^2 + n^2}{2} \equiv 1 \mod 4$. As m + n is even, according to Eq. (5), $\ell_{m,n}^2/a^2 = \frac{m^2 + n^2}{2}$. So in this case also, $\mathcal{M}_{m,n}$ [Eq. (6)] must also be an integer.

APPENDIX B: BUILDING TIGHT-BINDING MODELS

In this Appendix, we outline the general construction of tight-binding models. We start from a wave function written in the Bloch form,

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u(\mathbf{r});\tag{B1}$$

see Sec. III A. For a sufficiently deep potential $V(\mathbf{r})$, the function $u(\mathbf{r})$ in Eq. (B1) is distributed around potential minima on a length scale of the order of $\delta r \ll a$. It then follows $|\nabla^2 u| \gg |\mathbf{k} \cdot \nabla u| \gg |\mathbf{k}^2 u|$ and, according to Eq. (7), $u(\mathbf{r})$ is almost independent of \mathbf{k} . We may then write

$$u(\mathbf{r}) \simeq \frac{1}{\sqrt{N}} \sum_{j} w_j(\mathbf{r}),$$
 (B2)

where *j* spans the set of *N* local potential minima and $w_j(\mathbf{r})$ are normalized functions that are localized around each minimum *j* on a length scale $\delta r \ll a$. The eigenfunctions of the Hamiltonian \hat{H} then take the form

$$\psi(\mathbf{r}) \simeq \sum_{j} w_{j}(\mathbf{r})\psi_{j},$$
(B3)

where ψ_j are complex numbers normalized by $\sum_j |\psi_j|^2 = 1$. By substituting this relation into the Schrödinger align, we reduce the eigenvalue align to a tight-binding form,

$$E\psi_j = \epsilon_j \psi_j - \sum_{\ell \neq j} \mathcal{J}_{j,\ell} \psi_\ell, \qquad (B4)$$

where $\epsilon_j = \int d\mathbf{r} \ w_j^*(\mathbf{r}) \hat{H} w_j(\mathbf{r})$ is the on-site energy at site *j* and $\mathcal{J}_{j,\ell} = -\int d\mathbf{r} \ w_j^*(\mathbf{r}) \hat{H} w_\ell(\mathbf{r})$ is the tunneling energy between the sites *j* and ℓ . Note that in our notations for this work, \mathcal{J} is used to designate tunnelings in the basis of lattice sites or minima, and *J* is used for tunnelings in a composite eigenstate basis for specific classes of energy bands and subbands. Conversion between each basis can be performed using the relations in Appendix C. The coefficients ϵ_j and $\mathcal{J}_{j,\ell}$ may then be used as fitting parameters for the energy spectrum. The solution of Eq. (B4) yields the eigenenergy *E* as well as the eigenfunction coefficients ψ_j . The latter can be used to reconstruct the continuous-space wave functions via Eq. (B3), where the functions $w_j(\mathbf{r})$ are found from Eq. (B2).

Finally, in the second-quantization formalism, the field operator can also be written as $\hat{\psi}(\mathbf{r}) \simeq \sum_{j} w_{j}(\mathbf{r})\hat{a}_{j}$, leading to the Hamiltonian

$$\hat{H} \simeq \sum_{j} \epsilon_{j} \hat{a}_{j}^{\dagger} \hat{a}_{j} - \sum_{\langle j,\ell \rangle} \mathcal{J}_{j,\ell} \hat{a}_{j}^{\dagger} \hat{a}_{\ell},$$
 (B5)



FIG. 14. Origin of inhomogeneous eigenstate couplings. Here, we show sites in the lattice site basis (black numbers), in a red central cell and four black neighboring cells. Real-space tunnelings $\mathcal{J}_{u,v}^{\beta}$ between a site *u* in the red cell and *v* in a black cell must preserve the fourfold rotational symmetry of the moiré potential. As an example, this implies that all of the marked, blue tunnelings must be equal. These conditions then impose constraints on the corresponding eigenstate-basis couplings J_{α}^{β} , according to Eq. (C1).

where \hat{a}_j is the annihilation operator for a particle in the state w_j , or site j and $\langle j, \ell \rangle$ denotes a sum between pairs of minima ℓ and j, i.e., connected sites or minima with $|\mathcal{J}_{j,\ell}| > 0$.

APPENDIX C: EIGENSTATE BASIS TO LATTICE SITE BASIS

When constructing tight-binding models, it is also interesting to consider their representation in the basis of lattice sites, rather than the eigenstate basis. These representations are also important to understand the origin of anisotropic tunneling rates in the eigenstate basis. For band $\beta = 1$ (more generally, class I and II bands in Fig. 13), each moiré cell or superlattice cell will, respectively, contain one lattice site, and hence no conversion is necessary for these bands. However, for the other bands (classes III and IV), the situation is different since the intracell Hamiltonians contain more than one unique eigenstate.

1. Class III Bands

As discussed in Sec. IV B, tunneling rates $W_{B;i,j}^{\beta}$ must be equal for a class III band, but with flipped sign to preserve global fourfold rotational symmetry. To show this, we rewrite Hamiltonian (20) in the basis of lattice sites. This can be done by representing the eigenstates in Eq. (18) with operators that create or destroy particles at each of the four intracell sites. For example, we have $\hat{a}_i = (\hat{s}_i + \hat{t}_i + \hat{u}_i + \hat{v}_i)/2$, where the operators \hat{s}_i , \hat{t}_i , \hat{u}_i , and \hat{v}_i destroy a particle at sites 1, 2, 3, and 4 in Fig. 14, respectively. The other eigenstate operators \hat{B}_i , \hat{C}_i , \hat{d}_i can be represented in a similar way. When we convert Hamiltonian (20) to the lattice site basis, we get terms such as $\hat{s}_i^{\dagger} \hat{t}_i$, e.g., a tunneling operator from site 1 to site 2 of an adjacent cell, etc. Each site of a cell couples to four sites of an adjacent cell, producing 16 distinct tunneling rates and on-site terms in the lattice site basis. For the tunneling operators, the coefficients between a site u in one cell and a site v in an adjacent cell can be computed as

$$\begin{aligned} \mathcal{J}_{u,v}^{\beta} &= J_{a}^{\beta} a_{u} a_{v} + J_{d}^{\beta} d_{u} d_{v} + J_{B}^{\beta} (B_{u} B_{v} + C_{u} C_{v}) \\ &+ W_{B;u,v}^{\beta} (B_{u} C_{v} + C_{u} B_{v}), \end{aligned} \tag{C1}$$

where the coefficients a_i are the components of eigenstate $|a\rangle$ at index *i*. Likewise, the intracell and on-site couplings between sites *u* and *v* will be

$$\eta_{u,v}^{\beta} = E_a^{\beta} a_u a_v + E_d^{\beta} d_u d_v + E_B^{\beta} (B_u B_v + C_u C_v).$$
(C2)

One can then verify that for each u and v, $\eta_{u,v}^{\beta}$ will simply be equal to one of the intracell parameters of the original, decoupled Hamiltonian in Eq. (17), i.e., $\eta_{1,1}^{\beta} = \epsilon^{\beta}$, $\eta_{1,2}^{\beta} = \mathcal{I}^{\beta}$, etc. Based on the geometry of the moiré potential, the real-space tunnelings $\mathcal{J}_{u,v}^{\beta}$ must preserve fourfold rotational symmetry; see Fig. 14. As an example, this implies that $\mathcal{J}_{1,4}^{\beta}$ across the +y direction must be equal to $\mathcal{J}_{3,4}^{\beta}$ across the +x direction. Each tunneling can be explicitly written as

$$\mathcal{J}_{1,4}^{\beta} = \frac{1}{2} J_a^{\beta} - \frac{1}{2} J_d^{\beta} - \frac{1}{4} W_{B;1,4}^{\beta},$$

$$\mathcal{J}_{3,4}^{\beta} = \frac{1}{2} J_a^{\beta} - \frac{1}{2} J_d^{\beta} + \frac{1}{4} W_{B;3,4}^{\beta}.$$
 (C3)

For rotational symmetry to be preserved, we must have $W_{B;1,4}^{\beta} = -W_{B;3,4}^{\beta}$. More generally, $W_{B;x}^{\beta} = -W_{B;y}^{\beta} = W_{B}^{\beta}$, where *x* and *y* refer to the direction of the considered bound.

2. Class IV Bands

A similar process can be performed for class IV bands, such as $\beta = 2$. Each superlattice cell has two sites, giving four unique couplings between two different cells. The realspace tunneling rates between the different types of cells are given by

$$\mathcal{J}_{u,v}^{B \to B} = J_{A;u,v}^{\beta} A_u A_v + J_{B;u,v}^{\beta} B_u B_v,$$

$$\mathcal{J}_{u,v}^{R \to R} = J_{A';u,v}^{\beta} A_u A_v + J_{B';u,v}^{\beta} B_u B_v,$$

$$\mathcal{J}_{u,v}^{B \leftrightarrow R} = W_A^{\beta} A_u A_v + W_B^{\beta} B_u B_v.$$
(C4)

The intracell and on-site couplings can also be expressed as

$$\eta_{u,v}^{\beta} = 2\left(E_A^{\beta}A_uA_v + E_B^{\beta}B_uB_v\right),\tag{C5}$$

which are again equal to the intracell parameters of Hamiltonian (31). The couplings $\mathcal{J}_{u,v}^{B\to B}$ and $\mathcal{J}_{u,v}^{R\to R}$ have a similar form and unit cell, but are aligned across different directions. In order to preserve fourfold rotational symmetry, we require that $J_{A;x}^{\beta} = J_{A';y}^{\beta}, J_{A;y}^{\beta} = J_{A';x}^{\beta}, J_{B;x}^{\beta} = J_{B';y}^{\beta}$, and $J_{B;y}^{\beta} = J_{B';x}^{\beta}$.

APPENDIX D: EXTRACTING TIGHT-BINDING PARAMETERS FROM CONTINUOUS DISPERSIONS

Here, we outline the extraction of tight-binding parameters for the different classes of bands in Fig. 13.

1. Class I

Class I bands, such as band $\beta = 1$ in Sec. IV A for $\theta_{3,5}$, have a standard cosine dispersion as in Eq. (16). The average and amplitude of the dispersion relations can be calculated to extract ϵ^{β} and J^{β} .

2. Class II

For class II bands in Eq. (46), we have two aligns and three parameters to fit. First, we consider the average dispersion,

$$\frac{\varepsilon_a^{\beta}(\mathbf{k}) + \varepsilon_{a'}^{\beta}(\mathbf{k})}{2} = \epsilon^{\beta} - 2J_A^{\beta}(\cos k_x \ell + \cos k_y \ell), \qquad (D1)$$

from which ε_a^{β} and J_A^{β} can be found as for a class I band, independent from W_A^{β} . Instead, W_A^{β} is calculated by fitting the difference of dispersions,

$$\frac{\varepsilon_a^{\beta}(\mathbf{k}) - \varepsilon_{a'}^{\beta}(\mathbf{k})}{2} = -4W_A^{\beta} \left(\cos\frac{k_x\ell}{2}\cos\frac{k_y\ell}{2}\right), \qquad (D2)$$

which is independent of ε_a^{β} and J_A^{β} .

3. Class III

For class III bands, such as those considered in Sec. IV B, we must extract three intracell parameters and four intercell couplings from four dispersion relations. For the two nondegenerate subbands *a* and *d*, eigenvalues $E_{a,d}^{\beta}$ and tunnelings $J_{a,d}^{\beta}$ can be extracted from the standard cosine dispersions as for class I. For degenerate bands *b* and *c*, we consider average and difference functions,

$$\frac{\varepsilon_b^\beta(\mathbf{k}) + \varepsilon_c^\beta(\mathbf{k})}{2} = E_B^\beta - 2J_B^\beta(\cos k_x \ell + \cos k_y \ell) = \varepsilon_B^\beta(\mathbf{k})$$
(D3)

and

$$\frac{\varepsilon_b^\beta(\mathbf{k}) - \varepsilon_c^\beta(\mathbf{k})}{2} = -2W_B^\beta(\cos k_x \ell - \cos k_y \ell) = w_B^\beta(\mathbf{k}),$$
(D4)

which yield E_B^{β} and J_B^{β} , on the one hand, and W_B^{β} , on the other hand, from independent fits. The effective tunneling energies J_b^{β} and J_c^{β} associated to the final dispersion relations are then found from Eq. (30). Finally, the eigenvalues E_{α}^{β} of the intracell Hamiltonian are simply the energy shifts to each dispersion relation, allowing for the intracell parameters to be

calculated as

$$\epsilon^{\beta} = \frac{1}{4} \left(E_{a}^{\beta} + E_{d}^{\beta} + 2E_{B}^{\beta} \right),$$

$$\mathcal{I}^{\beta} = \frac{1}{4} \left(E_{a}^{\beta} - E_{d}^{\beta} \right),$$

$$\mathcal{I}^{\prime\beta} = \frac{1}{4} \left(-E_{a}^{\beta} - E_{d}^{\beta} + 2E_{B}^{\beta} \right),$$
 (D5)

which is equivalent to Eq. (19).

4. Class IV

Finally, for class IV bands, such as the one considered in Sec. IV C, we first consider the average dispersion for each degenerate set of subbands,

$$\frac{\varepsilon_{a}^{\beta}(\mathbf{k}) + \varepsilon_{a'}^{\beta}(\mathbf{k})}{2} = \frac{\varepsilon_{AA}^{\beta}(\mathbf{k}) + \varepsilon_{A'A'}^{\beta}(\mathbf{k})}{2}$$
$$= E_{A}^{\beta} - 2(J_{A;x}^{\beta} + J_{A;y}^{\beta})(\cos k_{x}\ell + \cos k_{y}\ell).$$
(D6)

Here we focus on subbands A - A', and similar formulas are found for subbands B - B'. In this way, we can fit the values for E_A^β and E_B^β , and determine the intracell parameters from the energy shifts,

$$\epsilon^{\beta} = \frac{1}{2} \left(E_A^{\beta} + E_B^{\beta} \right),$$

$$\mathcal{I}^{\beta} = \frac{1}{2} \left(E_A^{\beta} - E_B^{\beta} \right),$$
 (D7)

as well as the widths $J_{A;x}^{\beta} + J_{A;y}^{\beta}$ and $J_{B;x}^{\beta} + J_{B;y}^{\beta}$. Next, we take the differences,

$$\varepsilon_{a}^{\beta}(\mathbf{k}) - \varepsilon_{a'}^{\beta}(\mathbf{k}) = \sqrt{\left[\varepsilon_{AA}^{\beta}(\mathbf{k}) - \varepsilon_{A'A'}^{\beta}(\mathbf{k})\right]^{2} + 4w_{AA'}^{\beta}(\mathbf{k})^{2}}.$$
 (D8)

First, we consider a **k** direction in which $w_{AA'}^{\beta}(\mathbf{k}) = 0$, e.g., $k_y/\ell = \pi$. We then have

$$\begin{split} \tilde{\varepsilon}_{a}^{\beta}(\mathbf{k}) - \tilde{\varepsilon}_{a'}^{\beta}(\mathbf{k}) &= \left| \varepsilon_{AA}^{\beta}(\mathbf{k}) - \varepsilon_{A'A'}^{\beta}(\mathbf{k}) \right| \\ &= -2 \left| \left(J_{A;x}^{\beta} - J_{A;y}^{\beta} \right) (\cos k_{x}\ell + \cos k_{y}\ell) \right|, \end{split}$$
(D9)

from which we may extract the widths $J_{A;x}^{\beta} - J_{A;y}^{\beta}$. We can then solve the individual couplings $J_{A;x}^{\beta}$ and $J_{A;y}^{\beta}$ by using the results from Eq. (D6). Finally, we can consider a **k** direction in which $\varepsilon_{AA}^{\beta}(\mathbf{k}) = \varepsilon_{A'A'}^{\beta}(\mathbf{k})$, i.e., $k_x = k_y$. This yields

$$\varepsilon_{a}^{\beta}(\mathbf{k}) - \varepsilon_{a'}^{\beta}(\mathbf{k}) = 2w_{AA'}^{\beta}(\mathbf{k}) = -8W_{A}^{\beta}\left(\cos\frac{k_{x}\ell}{2}\cos\frac{k_{y}\ell}{2}\right),$$
(D10)

allowing for W_A^β to be extracted from the widths. The parameters for the B - B' subbands are similarly found.

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