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Supplementary information

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Localization and delocalization of light in photonic moiré lattices

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I. ON THE CONCEPT OF ALMOST PERIODIC FUNCTIONS

The concept of an almost periodic (AP) function of one variable was introduced by H. Bohr about a century ago [1]. Soon after that, the concept was extended to functions of two variables [2]. By definition, an AP function of two variables, $F(\boldsymbol{r})$, where $\boldsymbol{r} = (x, y)$, is characterized by, (i) the existence of translation vectors $\boldsymbol{a}$, such that $|F(\boldsymbol{r} + \boldsymbol{a}) - F(\boldsymbol{r})| < \varepsilon$ for some positive ε, and (ii) the existence of an area Ω_L of a characteristic linear size L (respectively characteristic area $\propto L^2$), such that for any its location in the (x, y) plane and for any ε one can find at least one translation vector $\boldsymbol{a}$ connecting the origin with a point inside Ω_L. A particular geometry of Ω_L is not specified. For example, a periodic crystal is at the same time an AP function, with Ω_L being the respective primitive cell and the translation vectors being the lattice vectors.

Optical potentials considered in our experiments (see Table I in Methods) are AP functions. This follows from the property [2]: *the sum, the product, and the quotient of two AP functions is still an AP function*. Since the optical potential in Eq. (1) of the main text, i.e.,

$$\mathcal{U}_\theta(\boldsymbol{r}) \equiv \frac{E_0}{1 + |p_1 V(\boldsymbol{r}) + p_2 V(S(\theta)\boldsymbol{r})|^2} \tag{1}$$

is obtained from periodic functions $V(\boldsymbol{r})$ and $V(S\boldsymbol{r})$ using these operations, it is an AP function.

II. THE EFFECTIVE-CELL METHOD AND FLAT-BAND INTERPRETATION

In this section we describe the details of the "effective-cell" approach, which is based on the relation between specially chosen periodic and AP functions. We use this approach to calculate the spectrum of the moiré potential with any desired accuracy and to interpret the wave localization in moiré potential in terms of flat bands.

A. Statement of the problem

Our goal is to compute the spectrum of the Hamiltonian with the potential (1), where θ is non-Pythagorean, i.e., corresponding to an incommensurable AP lattice. To this end we look for an effective Pythagorean lattice, defined by a Pythagorean angle θ_{mn}, where

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

which would reproduce a prescribed part of the spectrum of the AP lattice as close as necessary. This is impossible to achieve for the whole spectrum of an infinite AP lattice because for any deviation of the rotation angle θ from a Pythagorean value θ_{mn}, the deviation of the effective potential $\mathcal{U}_{mn}$ (we denote $\mathcal{U}_{\theta_{mn}} = \mathcal{U}_{mn}$ from here on for brevity) generated by θ_{mn}, from the incommensurable moiré potential $\mathcal{U}_\theta$, i.e., $|\mathcal{U}_\theta - \mathcal{U}_{mn}|$, cannot be kept small for sufficiently large $\boldsymbol{r}$. However, if we are interested only in a finite area of an AP lattice, like the one used in the experiment, we can search for approximation of only a part of the spectrum of the AP lattice by a respective part of the spectrum of the effective Pythagorean lattice by approaching θ_{mn} to θ close enough. In the experiment these are the parts of the spectra corresponding to higher eigenvalues of the optical potential.

Let us elaborate this approach for the AP lattice limited by the square of the area $4L^2$ where $2L$ is the length of a side of the square Ω_L. Since $\sqrt{2}L$ determines the largest distance of a point in Ω_L from the origin, we pose a problem of finding a Pythagorean triplet $(a,b,c) = (n^2-m^2, 2mn, m^2+n^2)$, i.e., of finding of m and n, such that

$$|\mathcal{U}_\theta - \mathcal{U}_{mn}| < \varepsilon \quad \text{for } |\theta-\theta_{mn}| < \nu(\varepsilon) \text{ and } |\boldsymbol{r}| < \sqrt{2}L, \tag{3}$$

where $\nu(\varepsilon)$ vanishes when $\varepsilon \to 0$. Due to the C_4 symmetry of the potential with respect to rotations, in the following the rotation angles are assumed to be restricted to the first quadrant: $\theta, \theta_{mn} \in (0, \pi/4)$.

B. Approximation of a non-Pythagorean angle by a Pythagorean one

First of all, we prove that the above statement makes sense, i.e., that by changing m and n one can make $\nu(\varepsilon)$ as small as necessary. To this end we recall that any irrational number, say, $\sin\theta$ where θ is a non-Pythagorean angle, can be approximated by rational ones, with a desired accuracy. In particular, for any positive integer $\tilde{n}$ one can find a positive integer $\tilde{m}$ ($0 < \tilde{m} < \tilde{n}$) such that the following inequality holds [3]

$$C = \frac{\tilde{m}}{\tilde{n}} - \frac{1}{\sqrt{5}\tilde{n}^2} < \sin\theta < \frac{\tilde{m}}{\tilde{n}} + \frac{1}{\sqrt{5}\tilde{n}^2} \tag{4}$$

Here the left expression is denoted by C for the sake of convenience. Generally speaking, in this estimate $\tilde{n}$ and $\tilde{m}$ may be non-Pythagorean, i.e. $\sqrt{\tilde{m}^2 + \tilde{n}^2}$ is not necessarily an integer. Thus for our purpose we have to refine this estimate by searching Pythagorean pairs $(\tilde{m}, \tilde{n})$ which define Pythagorean angles θ_{mn} approaching θ.

Taking into account the relations (2) we denote $\alpha = m/n$, where m and n are positive integers ordered as $0 < m < n$, and introduce a Pythagorean angle θ_{mn} defined as (c.f. (2))

$$\sin\theta_{mn} = \frac{2\alpha}{1+\alpha^2} =: f(\alpha) \tag{5}$$

Since α is rational, the function $f(\alpha)$ is rational, as well. Note that $\alpha \in (0,1)$, $f(0) = 0$, and values $f(\alpha) \in (0,1)$ represent a growing sequence of rational numbers, i.e., $f(\alpha) < f(\alpha')$ for $\alpha < \alpha'$. Thus, for any $\tilde{m}/\tilde{n} \in (0,1)$ and $\tilde{n} > 1/(\sqrt{5}\tilde{m})$ (the last inequality ensuring that $C > 0$) one can find α such that

$$f(\alpha) \le C \le f\left(\alpha + \frac{1}{n}\right) \tag{6}$$

or explicitly

$$\frac{2\alpha}{1+\alpha^2} \le \frac{\tilde{m}}{\tilde{n}} - \frac{1}{\sqrt{5}\tilde{n}^2} \le \frac{2\alpha}{1+\alpha^2} + \frac{2}{n(1+\alpha^2)}. \tag{7}$$

Now condition (4) can be rewritten in the form

$$\frac{2\alpha}{1+\alpha^2} < \sin\theta < \frac{2\alpha}{1+\alpha^2} + \frac{2}{n(1+\alpha^2)} + \frac{2}{\sqrt{5}\tilde{n}^2} \tag{8}$$

and subsequently using the definitions (2) and (5) as

$$0 < \sin\theta - \sin\theta_{mn} < \frac{2}{n} + \frac{2}{\sqrt{5}\tilde{n}^2}. \tag{9}$$

Hence,

$$\nu_{mn} := \theta - \theta_{mn} > 0. \tag{10}$$

So far, n was arbitrary (since we fixed only $\alpha = m/n$). Thus we can require that $n = \tilde{n}^2$ and rewrite (9) as

$$\sin\theta - \sin\theta_{mn} < \left(1 + \frac{1}{\sqrt{5}}\right)\frac{2}{n}. \tag{11}$$

Since $\theta, \theta_{mn} \in (0, \pi/4)$, we have

$$\sin\theta - \sin\theta_{mn} \geq 2\sin\left(\frac{\theta - \theta_{mn}}{2}\right)\cos\theta. \tag{12}$$

Finally, we use that $\sin x \geq 2x/\pi$ for all $x \in [0, \pi/2]$, and combining (11) and (12) obtain that for the chosen integers m and n the following inequality takes place

$$\theta - \theta_{mn} \leq \frac{\sqrt{5}+1}{\sqrt{5}}\frac{\pi}{n\cos\theta} =: \nu\left(\frac{1}{n}\right). \tag{13}$$

This formula defines $\nu(\varepsilon)$ with $\varepsilon = 1/n$ used in Eq. (3). We also notice that although this definition of $\nu(\varepsilon)$ explicitly contains only n. This however, does not mean that m is any arbitrary: it is given by $m = \alpha n$ where α must be chosen to satisfy (7) (or (6)).

C. Approximation of an incommensurable moiré lattice by a Pythagorean one

Having approximated of a non-Pythagorean angle by a Pythagorean one, we turn to calculation of the spectrum within the framework of the effective-cell approximation. The main idea consists in approaching a finite domain of an aperiodic moiré lattice by the primitive cell of an effective Pythagorean one. Since the spectrum of a periodic Pythagorean lattice can be

computed using Floquet-Bloch theory and has band-gap structure, this will allow us to confirm the direct simulations of the energy spectrum of an aperiodic lattice and, what is even more importantly, to uncover the physical mechanism of the localization.

To this end we consider the standard 2D rotation through the angle θ performed by the matrix

$$S(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}. \tag{14}$$

As it was shown in Subsection II B, any non-Pythagorean angle θ can be approximated by a Pythagorean one, $\theta_{m,n}$. Thus, neglecting terms of order of ν_{mn}^2, one can approximate

$$S(\theta) - S(\theta_{mn}) \approx S'_{mn}\nu_{mn}, \quad S'_{mn} = \begin{pmatrix} -\sin\theta_{mn} & -\cos\theta_{mn} \\ \cos\theta_{mn} & -\sin\theta_{mn} \end{pmatrix}. \tag{15}$$

Now our goal is to make $|\mathcal{U}_\theta - \mathcal{U}_{mn}|$ small enough. Let us assume that this is achieved for any $\boldsymbol{r} \in \Omega_L$ by requiring $|L\nu_{mn}| \ll 1$. Then, for $\boldsymbol{r} \in \Omega_L$ the following approximation is valid:

$$\mathcal{U}_\theta - \mathcal{U}_{mn} \approx \mathcal{U}_{mn}\nu_{mn}\frac{2p_2\left[p_1V(\boldsymbol{r}) + p_2V(\boldsymbol{r}_{mn})\right]}{1 + \left[p_1V(\boldsymbol{r}) + p_2V(\boldsymbol{r}_{mn})\right]^2}\tilde{\boldsymbol{r}}_{mn} \cdot (\nabla V)_{\boldsymbol{r}_{mn}} \tag{16}$$

where we use notations $\boldsymbol{r}_{mn} = S(\theta_{mn})\boldsymbol{r}$ and $\tilde{\boldsymbol{r}}_{mn} = S'_{mn}\boldsymbol{r}$. The neglected terms are of order of $(L\nu_{mn})^2$ or less.

Next we recall the result obtained in [4]: *for an arbitrary Pythagorean lattice one can choose a square primitive cell*. This suggests the following algorithm. If θ_{mn} is a Pythagorean angle defined by (2), then the Pythagorean moiré lattice is rotated with respect to the original x and y axes through the angle $\theta_{mn}/2$. The primitive vectors of the respective periodic Pythagorean lattice (see Figs. 1 and 2 in [4], although note that the meaning of m and n in this text is different) is given either by

$$\boldsymbol{b}_1 = \pi(m, n), \quad \boldsymbol{b}_2 = \pi(-n, m) \tag{17}$$

or by

$$\boldsymbol{b}_1 = \frac{\pi}{D}(n^2 - m^2, (n-m)^2), \quad \boldsymbol{b}_2 = \frac{\pi}{D}(-(n-m)^2, n^2 - m^2) \tag{18}$$

where D is the largest common divisor of $n^2 - m^2$ and $(n-m)^2$. Among these two bases we choose the one which guarantees the smallest value of $|\boldsymbol{b}_1| = |\boldsymbol{b}_2|$.

Let us consider the example from the main text. The AP lattice is created by the twist angle $\theta = \pi/6$. Now $\sin\theta = 1/2$ and we have to approximate θ by a Pythagorean angle. Thus we have to approximate $1/2$ by $f(\alpha)$ where $\alpha = m/n$. To this end we solve $f(\alpha) = 1/2$ and find $\alpha = 2 - \sqrt{3}$ (recall that we have to choose the root from the interval $0 < \alpha < 1$). The results for the Pythagorean lattice approximations are presented in Table I. The accuracy of the approximation is determined by the number of digits of ν_{mn} (the first column in the Table I) and by the choice of the integers m and n (the second and third columns in the Table I)). The forth column of the table shows the respective primitive Pythagorean triples, while the last two columns determine the lengths of lattice vectors obtained from (18) and (17): for the construction of the effective cell one has to choose the smallest one.

digits of accuracy	m	n	primitive (a, b, c)	$\lvert\boldsymbol{b}_{1,2}\rvert$ from (18)	$\lvert\boldsymbol{b}_{1,2}\rvert$ from (17)
2	1	4	(8, 15, 17)	$\sqrt{34}\pi \approx 6\pi$	$\sqrt{17}\pi \approx 4.1\pi$
3	4	15	(120, 209, 241)	$\sqrt{482}\pi \approx 22\pi$	$\sqrt{241}\pi \approx 15.5\pi$
4	15	56	(1680, 2911, 3361)	$\sqrt{6722}\pi \approx 82\pi$	$\sqrt{3361}\pi \approx 60\pi$

TABLE I: The choice between two possible $\boldsymbol{b}_1$ is based on the smallest norm $|\boldsymbol{b}_1|$.

It follows form Tab. I that when one uses, say 4–digits approximation, the achieved accuracy of the approximation of the incommensurable potentail by an effective Pythagorean lattice, according to (16), is determined by $\nu_{4,15} = 1/56 \approx 0.0179$ (the bottom line of the table). We notice that 6–digits approximation allows one to achieve the accuracy $\nu_{6,153} = 1/571 \approx 0.00175$ (not shown here).

Since, roughly speaking, the accuracy of the approximation of the AP moiré lattice by an effective-cell lattice is determined by $\varepsilon = 1/n$, in terms of the pair of integers (m, n) the size of the primitive cell of the Pythagorean lattice is of order of n^2. Thus *the primitive cell of the effective Pythagorean lattice must have an area much larger than the area of the incommensurable moiré lattice used in the experiment.*

III. ON THE DECAY LAW OF THE LOCALIZED STATES

The numerical analysis of the localized states reported in the main text revealed their exponential decay, illustrated in the inset of Fig. 2(c). To understand the observed decay law, we take into account the effective-cell approximation, developed in Sec. II C, and recall that any solution of Eq. (1) from the main text, with a periodic Pythagorean lattice $\mathcal{U}_{mn}$, i.e., of the equation

$$i\frac{\partial\psi}{\partial z} = H\psi, \qquad H = -\frac{1}{2}\nabla^2\psi + \mathcal{U}_{mn}, \tag{19}$$

can be expanded over a complete set of Wannier functions $w_n(\boldsymbol{r}-\boldsymbol{a})$. Consider the Bloch states $\varphi_{\alpha\boldsymbol{k}}(\boldsymbol{r})$ of the Hamiltonian H, $H\varphi_{\alpha\boldsymbol{k}} = -b_\alpha(\boldsymbol{k})\varphi_{\alpha\boldsymbol{k}}$ (recall that in optics the eigenvalue $b_\alpha(\boldsymbol{k})$ corresponds to the propagation constant). Then the Wannier functions are determined through the realtions

$$w_\alpha(\boldsymbol{r}-\boldsymbol{a}) = \frac{\Omega_L}{(2\pi)^2}\int_{\mathrm{BZ}} \varphi_{\alpha\boldsymbol{k}}(\boldsymbol{r})d\boldsymbol{k}, \quad \varphi_{\alpha\boldsymbol{k}}(\boldsymbol{r}) = \sum_{\boldsymbol{a}} e^{i\boldsymbol{k}\cdot\boldsymbol{a}} w_\alpha(\boldsymbol{r}-\boldsymbol{a}) \tag{20}$$

where Ω_L is the area of the 2D primitive cell (which is an effective cell in our case, i.e., $\Omega_L = 4L^2$ as defined above), α is the band number, the integral is performed over the first Brillouin zone (BZ), while the sum is over all lattice vectors $\boldsymbol{a}$ of the periodic potential $\mathcal{U}_{mn}(\boldsymbol{r})$.

The Wannier functions are not eigenmodes of H (unlike the Bloch functions). However, for extremely flat bands, like in the case of the effective Pythogorean lattice shown in Fig. 1 (f) of

the main text, they can be considered as *quasi*-modes. Indeed, one has

$$Hw_\alpha(\boldsymbol{r}-\boldsymbol{a}) = -b_\alpha(\boldsymbol{k})w_\alpha(\boldsymbol{r}-\boldsymbol{a}) - \frac{\Omega_L}{(2\pi)^2}\int_{\mathrm{BZ}}[b_\alpha(\boldsymbol{k}')-b_\alpha(\boldsymbol{k})]\varphi_{\alpha\boldsymbol{k}'}(\boldsymbol{r})d\boldsymbol{k}'. \tag{21}$$

Suppose now that the band is extremely flat and that $b_\alpha(0)$ is nonzero. Then for any point $\boldsymbol{k}$ in the first Brillouin zone $|b_\alpha(\boldsymbol{k})-b_\alpha(0)| \ll |b_\alpha(0)|$ (i.e., $b_\alpha(\boldsymbol{k})$ very weakly depends on $\boldsymbol{k}$), and one can approximate

$$Hw_\alpha(\boldsymbol{r}-\boldsymbol{a}) \approx -b_\alpha(0)w_\alpha(\boldsymbol{r}-\boldsymbol{a}). \tag{22}$$

Subject to quite general conditions on the periodic potential (in particular trivial topology of the lattice, as this is the case of Pythagorean lattices we are dealing with), the respective 2D Wannier functions can be chosen exponentially localized [5]. Since quasi-stationary states of flat bands are approximately described by the Wannier functions of a flat band, they are expected to display exponential localization withing the primitive (effective) cell. The obtained estimates explain the exponential localization observed in the experiment.

IV. ON A PYTHAGOREAN MOIRÉ LATTICE AS AN OPTICAL POTENTIAL.

The minima of the optical potential in Eq. (1) are determined by the maxima of the lattice $I(\boldsymbol{r})$. Obviously $I(\mathbf{0}) = \max_{\boldsymbol{r}} I(\boldsymbol{r}) = 2(p_1+p_2)$. If θ is not a Pythagorean angle, then $I(\boldsymbol{r}) < I(\mathbf{0})$ for any $\boldsymbol{r} \neq \mathbf{0}$, i.e. $\boldsymbol{r} = \mathbf{0}$ is the location of an absolute maximum of the refractive index. Indeed, suppose the opposite, i.e. suppose that there exists $\boldsymbol{r}_0 \neq \mathbf{0}$, such that $I(\boldsymbol{r}_0) = 2(p_1+p_2)$. This is only possible if $V(\boldsymbol{r}_0) = V(\mathbf{0}) = 2$ and $V(S\boldsymbol{r}_0) = V(\mathbf{0}) = 2$. Thus one has to conclude that θ is a Pythagorean angle because the rotation $S(\theta)$ transforms the lattice site of one of the sublattices to the lattice site of the other sublattice (the characteristic property of commensurate Pythagorean lattice [4]). This is, however, contradicts to the supposition made.

The first terms of the Taylor expansion of the optical potential in the vicinity of the origin read:

$$\frac{E_0}{1+|p_1V(\boldsymbol{r})+p_2V(S(\theta)\boldsymbol{r})|^2}=\frac{8E_0(p_1+p_2)^2}{[4(p_1+p_2)^2+1]^2}|\boldsymbol{r}|^2+\mathcal{O}((x+y)^4) \tag{23}$$

Thus, the dependence on the twist angle θ appears only in the fourth-order terms $\mathcal{O}((x+y)^4)$. This explains weak dependence on the angle of the LDT transition reported in Fig. 2(a) of the main text.

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