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# Localization in one-dimensional incommensurate lattices beyond the Aubry-André model

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Localization properties of particles in one-dimensional incommensurate lattices without interaction are investigated with models beyond the tight-binding Aubry-André (AA) model. Based on a tight-binding $t_1$-$t_2$ model with finite next-nearest-neighbor hopping $t_2$, we find the localization properties qualitatively different from those of the AA model, signaled by the appearance of mobility edges. We then further go beyond the tight-binding assumption and directly study the system based on the more fundamental single-particle Schrödinger equation. With this approach, we also observe the presence of mobility edges and localization properties dependent on incommensuration.

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The physics of quantum transport in random disordered potentials has been a subject of substantial interest for condensed-matter physicists for decades. The extended Bloch waves in a periodic lattice could undergo a quantum interference induced transition into localized states due to random disorder by a mechanism commonly referred to as Anderson localization [1]. Matter waves can also be localized in deterministic potentials that exhibit some similarities to random disorder [2–5]. Quasiperiodic potentials, such as incommensurate lattices (the superposition of two or more lattices with incommensurate periods), are notable examples and have been extensively studied with the Aubry-André (AA) model [2]. Such potentials have been shown to exhibit interesting quantum transport phenomena in themselves. Incommensurate potentials, for example, are theorized to have fractal spectra [6]. However, it remains challenging to study these phenomena in solid-state experiments, as it is difficult to systematically control the disorder in solid-state systems. In contrast to the solid-state systems, ultracold atoms loaded in optical lattices offer a remarkable controllability over the system parameters, making it an attractive platform for the study of the localization of matter waves. Recently, Anderson localization of noninteracting Bose-Einstein condensates (BECs) has been observed in a one-dimensional (1D) matter waveguide with a random potential introduced with laser speckles [7]. Similar experiments have also been done in quasiperiodic optical lattices [8,9].

Localization of noninteracting particles in one-dimensional incommensurate lattices is often studied with the AA model with nearest-neighbor (nn) hopping, where one of the lattices is assumed to be relatively weak and can be treated as a perturbation. Within the framework of the AA model, there is a duality point, at which a sharp transition from all eigenstates being extended to all being localized occurs. However, in ultracold atom experiments, one can tune the depth of each lattice in a controllable way and bring the system out of the tight-binding regime. To explore the physics of localization for shallow lattices, it is of interest to go beyond the AA model and the tight-binding assumption [10].

In this work, we first study the tight-binding $t_1$-$t_2$ model, which extends the AA model by including the next-nearest-neighbor (nnn) hopping. The inclusion of the nnn hopping destroys the self-duality possessed by the AA model and the localization properties of the system become more complex through the emergence of mobility edges. We then examine the system directly with the single-particle Schrödinger equation. We discretize the equation and solve it numerically without any further assumption. Within this formalism, we also find the existence of mobility edges, consistent with the $t_1$-$t_2$ model results, and we find localization properties with nontrivial dependence on incommensuration.

Consider diffuse noninteracting ultracold atoms in a one-dimensional incommensurate lattice, where the atoms can only move along the $x$ axis. The lattice potential is given by

$$V(x) = \frac{V_0}{2}\cos(2k_L x) + \frac{V_1}{2}\cos(2\alpha k_L x + \delta), \tag{1}$$

where $V_0$ and $V_1$ describe the depth of the primary and the secondary lattices, respectively; $k_L$ is the wave vector of the primary lattice along the $x$ axis; $\alpha$ is an irrational number characterizing the degree of incommensurability between the periods of the two lattices; and $\delta$ is an arbitrary phase (in our calculations it is chosen to be zero for convenience, without loss of generality). When the depth of the primary lattice is sufficiently large as compared with the recoil energy $E_r \equiv (\hbar k_L)^2/2m$ as well as the depth of the secondary lattice $V_1$, the physical properties of the system can be studied with the well-known single-band tight-binding Aubry-André model

$$t(u_{n-1} + u_{n+1}) + V_n u_n = E u_n, \tag{2}$$

in which only the coupling between nn's is retained and the incommensurate modulating potential $V_n = V\cos(2\pi\alpha n)$. The duality point is given by $V/t = 2$. The nn hoping term $t$ is determined by the primary potential and can be approximated by the expression

$$t \approx \frac{4}{\sqrt{\pi}} E_r \left(\frac{V_0}{E_r}\right)^{3/4} \exp\left(-2\sqrt{\frac{V_0}{E_r}}\right). \tag{3}$$

The lattice potential and its magnitude can be roughly estimated by applying Gaussian approximation for the Wannier states,

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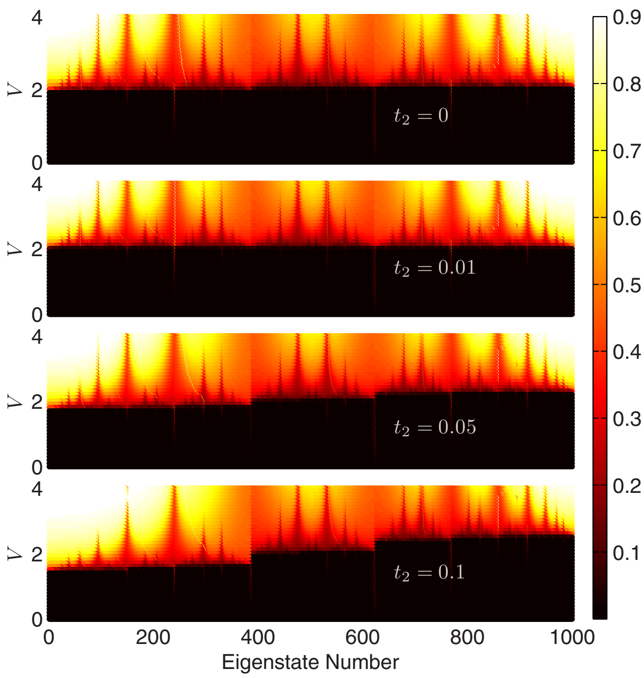


FIG. 1. (Color online) Inverse participation ratio of all eigenstates for $t_1$-$t_2$ model with $\alpha=(\sqrt{5}-1)/2$. The size of the system is chosen to have 1000 sites. The four panels correspond to $t_2=0$, 0.01, 0.05, and 0.1, respectively. ($t_1$ is the unit for energy.) Darker shading corresponds to more extended states while lighter shading corresponds to more localized states.

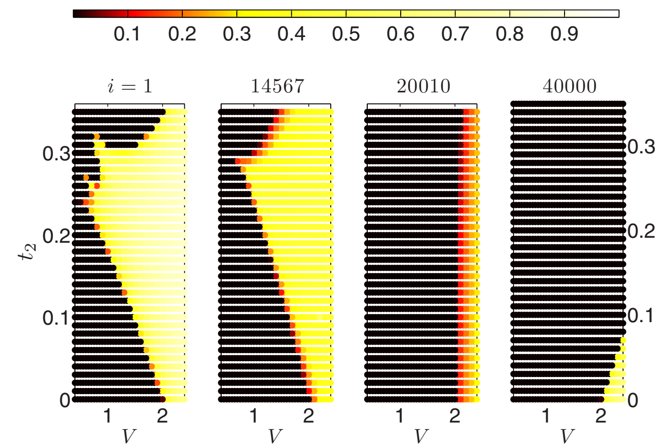


FIG. 2. (Color online) Inverse participation ratio on the $t_2$-$V$ plane for $\alpha=(\sqrt{5}-1)/2$ based on the $t_1$-$t_2$ model. The four panels correspond to four eigenstates labeled by $i$, with ascending eigenenergies. Darker shading corresponds to more extended states while lighter shading corresponds to more localized states.

$$V \approx \frac{V_1}{2}\exp\left(-\frac{\alpha^2}{\sqrt{V_0/E_r}}\right). \quad (4)$$

We note that $V$ depends on $V_1$, $\alpha$, and $V_0/E_r$. As a naive extension to the AA model, we ask what will happen if the coupling between next-nearest neighbors is included. To answer this question, we consider the model

$$\sum_{d=1,2} t_d(u_{n-d}+u_{n+d}) + V_n u_n = E u_n, \quad (5)$$

where $V_n = V\cos(2\pi \alpha n)$. We solve the equation by direct diagonalization. To quantify the localization of the wave function, we compute the inverse participation ratio (IPR) as follows:

$$\mathrm{IPR}^{(i)} = \frac{\sum_n |u_n^{(i)}|^4}{\left(\sum_n |u_n^{(i)}|^2\right)^2}, \quad (6)$$

where the superscript $i$ denotes the $i$th eigenstate (ordered according to energy from low to high). For spatially extended states, IPR approaches zero whereas it is finite for localized states [11].

Figure 1 shows the IPR values of all eigenstates as a function of the effective strength $V$ of the secondary lattice based on the tight-binding $t_1$-$t_2$ model with $\alpha=(\sqrt{5}-1)/2$ for various values of $t_2$ ($t_1$ is chosen to be the unit of energy). The calculation for Fig. 1 is done for a system with 1000 sites in the primary lattice. For small values of $t_2$ (e.g., $t_2=0.01$), the localization properties of the system have essentially the same features as those determined by the AA model. However, when $t_2=0.05$ or higher, the AA duality is clearly destroyed and localization transitions appear to be energy dependent. For lower energies, the transition can appear for $V<2t_1$ and, for higher energies, the transition can appear for $V>2t_1$.

In order to demonstrate the dependence of the localization transition on $t_2$, we show the distribution of IPR on the $t_2$-$V$ plane for four different eigenfunctions with $\alpha=(\sqrt{5}-1)/2$ in Fig. 2. For the calculation, the size of the system is chosen to be 40 000. At $t_2=0$, the $t_1$-$t_2$ model reduces to the AA model, and from Fig. 2 one can see the sharp transition when $V$ is increased across the duality point $V=2$. However, the localization property of the system is greatly complicated when $t_2$ is finite. Besides the appearance of mobility edges, our results also reveal that the dependence of the localization property on $t_2$ is not monotonic, e.g., at fixed $V<2$ when $t_2$ is increased the ground state could be tuned from extended to localized, but further increasing of $t_2$ could bring the ground state into an extended state again.

We infer from the results presented in Figs. 1 and 2 that (1) the AA duality is destroyed by having $t_2\neq 0$; (2) instead of the $V=2t_1$ dual point, the system has energy-dependent mobility edges for $t_2\neq 0$; and (3) the precise localization condition deviates up or down from the $V=2t_1$ AA condition depending on the energy of the eigenstate and the value of $t_2$. As illustrated by Figs. 1 and 2, the $t_1$-$t_2$ model itself could be of interest. However, for the study of localization properties in 1D incommensurate lattices, its validity must be dealt with caution, especially when $t_2$ is not sufficiently small as compared with $t_1$. The tight-binding nn and nnn hoping integrals $t_1$ and $t_2$ can be estimated with the Wannier basis, which is fully determined by the primary lattice. One can easily estimate that, when $V_0=3E_r$, the ratio of $t_2/t_1$ is on the order of 10%. To get a higher $t_2/t_1$ ratio, one will need to tune the lattice potential shallower and should expect the tight-binding approximation to break down at some point. Alter-

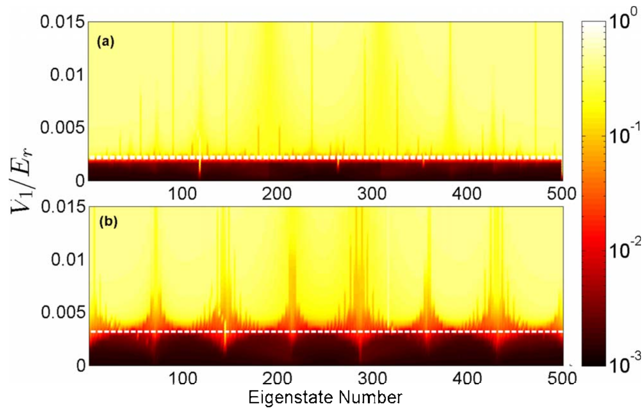


FIG. 3. (Color online) Inverse participation ratio obtained by solving the Schrödinger equation and calculated AA duality point (dashed line) at $V_0=30E_r$; (a) $\alpha=(\sqrt{5}-1)/2$ and (b) $\alpha=\pi/2$.

natively, to study the interesting physics of localization in this regime, we numerically solve the single-particle Schrödinger equation without any tight-binding approximation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right)\psi(x)=E\psi(x). \tag{7}$$

To achieve this goal, we discretize the Schrodinger equation in the position basis with a finite system size of length $L=Na$, where $a$ is the lattice constant of the primary lattice associated with $V_0$. The continuous Schrödinger equation is now cast into the following form:

$$\left(-\frac{\hbar^2}{2m}\right)\frac{\psi_{n+1}-2\psi_n+\psi_{n-1}}{\delta^2}+[V_0\cos(2k_Ln\delta)$$
$$+V_1\cos(2k_L\alpha n\delta)]\psi_n=E\psi_n, \tag{8}$$

where $\delta=Na/M$ is the step interval for the discretization with $M$ denoting the total number of steps. Then we proceed by diagonalizing the $M\times M$ matrix of the discretized Hamiltonian and study the first $N$ eigenstates with smallest energy eigenvalues. These states would correspond to the ground band for the case with no secondary lattice (i.e., $V_1=0$). In our calculations for the following results, we have set $N=500$, $M=80\,000$, and $2k_L=1$.

IPR values [obtained with Eq. (6) by replacing $u_n$ with $\psi_n$] of the first $N$ eigenstates as a function of the secondary lattice strength $V_1$ are shown in Fig. 3 for a primary lattice strength of $V_0=30E_r$. In Fig. 3(a) the irrational ratio $\alpha$ is set to be the inverse golden mean $(\sqrt{5}-1)/2$ whereas, in Fig. 3(b), $\alpha=\pi/2$. The bold-dashed line represents the AA duality point calculated with Eqs. (3) and (4). We can see that the localization properties shown in Fig. 3 closely resemble the well-known results from the AA model (see top panel in Fig. 1). We do note, however, that the IPR results of Fig. 3 indicate a dependence on the specific value of $\alpha$ with $\alpha=(\sqrt{5}-1)/2$, providing a sharper AA duality than $\alpha=\pi/2$.

In Fig. 4(a) we show the IPR values for the case of $V_0=2E_r$ and $\alpha=(\sqrt{5}-1)/2$. In this case, the eigenstates no longer appear to localize all at once, but in discrete steps

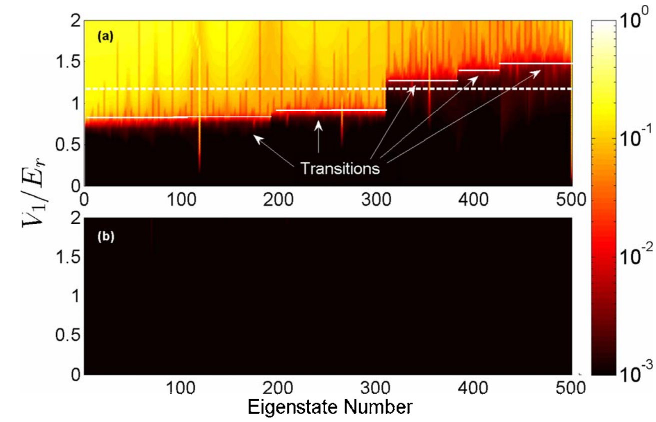


FIG. 4. (Color online) (a) Inverse participation ratio obtained by solving the Schrödinger equation and calculated AA duality point (dashed line) at $V_0=2E_r$; (a) $\alpha=(\sqrt{5}-1)/2$, solid lines are the estimated location of localization transitions, and (b) $\alpha=\pi/2$.

(represented by the solid lines in the figure). This localization behavior is similar to what we observed in the $t_1$-$t_2$ model (see bottom panel in Fig. 1). Also the transitions occur at fairly large values for $V_1$, where the secondary lattice can no longer be treated as a perturbation. We have also studied the cases where $V_0=2E_r$, $\alpha=\pi/2$ [Fig. 4(b)], and $\alpha=(\sqrt{5}+1)/2$ (not shown in the figure). In these cases no localization was observed in the eigenfunctions for any value of $V_1$ investigated (up to $V_1=V_0$). This suggests that incommensurability between the lattices is not a sufficient condition to observe localization for shallow cases.

To examine the dependence of the localization transitions on $\alpha$, we set $V_0=V_1$ and calculate the IPR of the ground state for various values of $V_0$ and $\alpha$ [the values of $\alpha$ examined are all proportional to $(\sqrt{5}-1)/2$]. These results are shown in Fig. 5. We see fairly distinct regions of localized and extended states, with localization tending toward areas of larger values for $V_0$ and smaller magnitudes for $\alpha$. The solid curve in Fig. 5 represents the set of points $(\alpha, V_0)$ such that the AA duality point [calculated from Eqs. (3) and (4)] is equal to

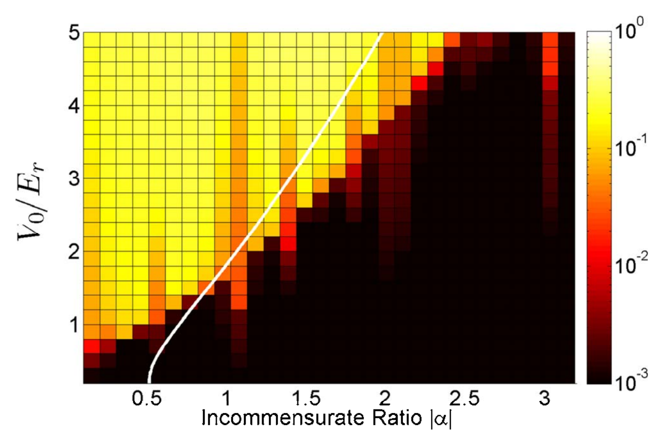


FIG. 5. (Color online) Inverse participation ratios of the ground-state wave function for the case $V_0=V_1$ and $\alpha$ equal to fractional multiples of $(\sqrt{5}-1)/2$. The solid line represents an approximate analytical boundary between localized and extended regions based on the AA duality point.

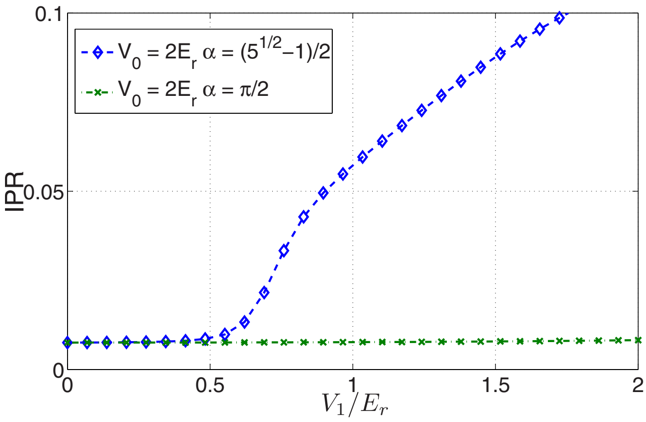


FIG. 6. (Color online) Inverse participation ratio of ground-state wave function at time $T_0 \approx \hbar / E_r$ after the trap potential $V_{trap} = \Omega x^2$ has been turned off ($\Omega / E_r \approx 10^{-7}$).

the lattice strength $V_0$. These sets of points serve as a simple heuristic estimation of the boundary between localized and extended states based on the AA duality condition. Although in principle we should not expect the AA duality point obtained from Eqs. (3) and (4) to be applicable in the case of shallow lattices, this simple analytical result is in good qualitative agreement with our numerical findings.

We now briefly discuss how some of these results may be observed in cold-atom experiments. We consider a diffuse BEC that is loaded into an incommensurate optical lattice, confined by a harmonic trap $V_{trap} = \Omega x^2$. We assume that the diffuse gas is prepared in the ground state. At time $T=0$, the harmonic trap is suddenly turned off and the BEC is allowed to diffuse. Localization can be observed by monitoring the IPR of the density wave function over time. In Fig. 6, we present the calculated values for the IPR as a function of $V_1$ for the wave function after a fixed period of time $T_0 \approx \hbar / E_r$ has passed since the trap was turned off for the cases with $V_0 = 2E_r$, $\Omega / E_r \approx 10^{-7}$, $\alpha = (\sqrt{5}-1)/2$, and $\alpha = \pi/2$. In the figure, we see that the two cases are similarly delocalized for small values of $V_1$. But for larger values of $V_1$, the IPR for the $\alpha = (\sqrt{5}-1)/2$ case begins to grow, showing an increasing degree of localization, while in the $\alpha = \pi/2$ case it remains constant.

In conclusion, we have studied the localization properties of noninteracting particles in a one-dimensional incommensurate optical lattice system based on a tight-binding $t_1$-$t_2$ model with nearest-neighbor as well as next-nearest-neighbor hopping. We reveal the emergence of mobility edges when the next-nearest-neighbor hopping is finite. We have also gone beyond the tight-binding approximation by directly modeling the system with the fundamental single-particle Schrödinger equation, which is expected to provide more reliable theoretical description of the system especially for the case with a shallow primary lattice potential. By diagonalizing the discretized Hamiltonian, we numerically solve the Schrödinger equation. Our results clearly show the existence of mobility edges. Our study also reveals that the emergence of localization is sensitive to the magnitude of the irrational ratio $\alpha$ of the incommensurate lattice potentials when the system is well outside the tight-binding regime. Our results also establish the fragile nature of the AA duality, which gives way to mobility edges as soon as longer-range hopping, even at the nnn level, is turned on. It will be interesting to verify our predictions about the sensitive qualitative dependence of 1D incommensurate localization on $V_0$, $V_1$, $E_r$, and $\alpha$ through experiments in cold atomic systems [7–9].

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[1] P. W. Anderson, Phys. Rev. **109**, 1492 (1958).
[2] S. Aubry and G. André, Ann. Israel Phys. Soc **3**, 133 (1980).
[3] S. Das Sarma, S. He, and X. C. Xie, Phys. Rev. B **41**, 5544 (1990).
[4] S. Das Sarma, S. He, and X. C. Xie, Phys. Rev. Lett. **61**, 2144 (1988).
[5] D. J. Thouless, Phys. Rev. Lett. **61**, 2141 (1988).
[6] A. Saul, A. M. Llois, and M. Weissmann, J. Phys. C **21**, 2137 (1988).
[7] J. Billy, V. Josse, Z. Zuo, A. Bernard, B. Hambrecht, P. Lugan, D. Clément, L. Sanchez-Palencia, P. Bouyer, and A. Aspect, Nature (London) **453**, 891 (2008).
[8] E. E. Edwards, M. Beeler, T. Hong, and S. L. Rolston, Phys. Rev. Lett. **101**, 260402 (2008).
[9] G. Roati, C. D'Errico, L. Fallani, M. Fattori, C. Fort, M. Zaccanti, G. Modugno, M. Modugno, and M. Inguscio, Nature (London) **453**, 895 (2008).
[10] R. B. Diener, G. A. Georgakis, J. Zhong, M. Raizen, and Q. Niu, Phys. Rev. A **64**, 033416 (2001).
[11] B. Kramer and A. MacKinnon, Rep. Prog. Phys. **56**, 1469 (1993).