Periodic wave packet reconstruction in truncated tight-binding lattices

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A class of truncated tight-binding Hermitian and non-Hermitian lattices with commensurate energy levels, showing periodic reconstruction of the wave packet, is presented. Examples include exact Bloch oscillations on a finite lattice, periodic wave packet dynamics in non-Hermitian lattices with a complex linear site-energy gradient, and self-imaging in lattices with commensurate energy levels quadratically-varying with the quantum number.

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Introduction. Tight-binding lattice models provide a simple tool to investigate the transport properties of different physical systems, such as electronic transport in semiconductor superlattices or coupled quantum dots, photonic transport in waveguide arrays or coupled optical cavities, and transport of cold atoms in optical lattices. In certain conditions, the dynamics of a wave packet in the lattice turns out to be periodic. Such a special regime is attained, for example, in an infinitely-extended periodic lattice with a superimposed dc field, leading to the formation of an equally-spaced Wannier-Stark ladder energy spectrum and to the appearance of Bloch oscillations (BOs) [1]. Another important case is that of an infinitely-extended periodic lattice with an applied ac field, for which quasi-energy band collapse leading to dynamic localization can be found at special ratios between amplitude and frequency of the ac modulation [2,3]. Such periodic dynamical behaviors realize wave self-imaging, i.e. a periodic reconstruction of the initial wave packet distribution. Self-imaging phenomena in tight-binding lattices have been observed in different physical systems (see, for instance, [4–8]). Even in an infinite periodic lattice without any external applied field periodic self-imaging can be observed for special periodic initial wave distributions owing to the discrete analogue of the Talbot effect [9]. Unfortunately, lattice truncation, defects and edge effects generally destroy the periodic wave packet dynamics because of incommensurate frequencies of the eigenstates. As a consequence, the system never revives fully to its initial state, and phenomena like wave packet collapse and revivals are generally found [10]. Recently, a few examples of lattice engineering that enables to restore exact periodic wave packet dynamics have been proposed [11–13], including harmonic oscillations in a finite lattice with engineered hopping rates [11,12] and Bloch oscillations on a semi-infinite lattice with linearly-increasing hopping rates [14]. In this Report we introduce a more general class of truncated tight-binding lattices -not necessarily Hermitian- that sustain a periodic dynamics of the wave packet and that include the Hermitian lattices of Refs. [11–13,14] as special cases. In particular, we prove the existence of Bloch oscillations on engineered finite lattices, either Hermitian or non-Hermitian, and show self-imaging phenomena in a novel class of finite lattices with commensurate energy levels that depend quadratically on the quantum number.

Lattice synthesis. Let us consider a tight-binding one-dimensional lattice with site energies $V_n$ and hopping amplitude $\kappa_n$ between adjacent sites $|n\rangle$ and $|n+1\rangle$. In the nearest-neighbor approximation, indicating by $\psi(n)$ the occupation amplitude at lattice site $|n\rangle$, the energies $E$ of the lattice Hamiltonian $\mathcal{H}$ are found as eigenvalues of the second-order difference equation

$$\mathcal{H}\psi(n) \equiv \kappa_{n-1}\psi(n-1) + \kappa_n\psi(n+1) + V_n\psi(n) = E\psi(n) \quad (1)$$

Lattice truncation is realized by assuming $\kappa_{-1} = 0$ for a semi-infinite lattice comprising the sites $|0\rangle, |1\rangle, |2\rangle \ldots$, or $\kappa_{-1} = \kappa_N = 0$ for a finite lattice comprising the $(N+1)$ sites $|0\rangle, |1\rangle, |2\rangle \ldots |N\rangle$. Note that the Hamiltonian $\mathcal{H}$ is Hermitian provided that $V_n$ and $\kappa_n$ are real-valued, the emergence of complex values for either hopping rates or site energies being the signature of a non-Hermitian lattice. Our aim is to judiciously engineer the hopping amplitudes $\kappa_n$ and site energies $V_n$ in such a way that the lattice energies $E$ form a set of commensurate numbers, thus ensuring a periodic dynamics of an arbitrary wave packet $\psi(n,t)$ that evolves according to the time-dependent Schrödinger equation $i(\partial\psi/\partial t) = \mathcal{H}\psi$. Examples of such a lattice engineering, corresponding to a set of equally-spaced discrete energy levels, have been previously presented in Refs. [11–13,14]. Here we show that such previous examples belong to a more general class of lattices with commensurate energies, which can be synthesized using the factorization method [15], or the so-called supersymmetric quantum mechanics [16], adapted to ‘discrete’ quantum mechanics and difference equations (see, for instance, [18]). To this aim, let us assume that the hopping amplitudes $\kappa_n$ and site energies $V_n$ can be derived from two functions $F_1(n)$ and $F_2(n)$ according to

$$\kappa_n = \sqrt{F_1(n)F_2(n+1)}, \quad V_n = -[F_1(n) + F_2(n)]. \quad (2)$$

In this case, the Hamiltonian $\mathcal{H}$ can be factorized as $\mathcal{H} = \mathcal{P} \rho \mathcal{P}^\dagger$, with

$$\mathcal{P} = \sum_{n=0}^{N} |n\rangle \langle n+1|, \quad \rho = \sum_{n=0}^{N} |n\rangle \langle n|.$$
where \[ 18 \]
\[
A = \sqrt{F_1(n)} \exp \left( \frac{1}{2} \frac{\partial}{\partial n} \right) - \sqrt{F_2(n)} \exp \left( - \frac{1}{2} \frac{\partial}{\partial n} \right) \]
\[
B = \exp \left( \frac{1}{2} \frac{\partial}{\partial n} \right) \sqrt{F_2(n)} - \exp \left( - \frac{1}{2} \frac{\partial}{\partial n} \right) \sqrt{F_1(n)}. \]  
To realize a finite lattice, with nonvanishing amplitudes \( \psi(n) \) at the \( (N+1) \) lattice sites \([0], [1], ..., [N]\), we require \( F_1(N) = 0 \) and \( F_2(0) = 0 \). For a semi-infinite lattice, we require \( F_2(0) = 0 \) solely. Let us then indicate by \( \psi_0(n) \) the solution to the difference equation \( B\psi_0(n) = 0 \), i.e. \( \sqrt{F_2(n+1)} \psi_0(n+1) = \sqrt{F_1(n)} \psi_0(n) \). It then follows that \( H\psi_0 = 0 \), i.e. \( E = 0 \) is an eigenvalue of \( H \) \[19\]. To find the other eigenvalues of \( H \), let us search for a solution to Eq.(1) in the form \( \psi(n) = \psi_0(n)Q(n) \); it then readily follows that \( Q(n) \) satisfies the second-order difference equation
\[
F_1(n)Q(n+1) + F_2(n)Q(n-1) = [F_1(n)+F_2(n)+E]Q(n). \]  
Assuming for \( F_1(n) \) and \( F_2(n) \) a linear or quadratic functions of \( n \), Eq.(5) can be solved in an exact way by assuming for \( Q(n) \) a polynomial of degree \( M \), i.e. \( Q(n) = \sum_{\rho=0}^{M} a_\rho n^\rho \). Substitution of such an expression of \( Q(n) \) into Eq.(5) yields the following relation
\[
\sum_{\rho=0}^{M-1} \left( \sum_{k=\rho+1}^{M} a_k \left( k \right) F_1(n) + (-1)^{k-\rho} F_2(n) \right) n^\rho = E \sum_{\rho=0}^{M} a_\rho n^\rho \]
which determines the eigenvalues \( E \) and the coefficients \( a_\rho \) of the polynomial \( Q(n) \) after comparison of the terms of the same power \( n^\rho \) on the left- and right-hand-sides in Eq.(6). In particular, the eigenvalue \( E \) is found by comparison of the highest-order power terms \( n^M \). It is worth discussing in a separate way the cases of linear and quadratic forms for \( F_1(n) \) and \( F_2(n) \), which yield a different dependence of the energy eigenvalues on the quantum number \( M \).

**Lattices with equally-spaced energy levels: Bloch oscillations on a finite lattice.** Let us consider a finite lattice comprising the sites \( n = 0, 1, 2, ..., N \) and assume \( F_1(n) = \alpha(n-N) \) and \( F_2(n) = \gamma n \), with \( \alpha \) and \( \gamma \) arbitrary parameters with \( \alpha \neq \gamma \). The hopping amplitudes and site energies of this lattice are thus given by [see Eq.(2)]
\[
\kappa_n = \sqrt{\alpha \gamma (n-N)(n+1)}, \quad V_n = \alpha N - (\alpha + \gamma)n. \]  
Note that the lattice Hamiltonian is Hermitian for \( \alpha \gamma < 0 \), whereas it is not Hermitian for \( \alpha \gamma > 0 \) or for complex values for \( \alpha \) and/or \( \gamma \). Substitution of such expressions of \( F_1(n) \) and \( F_2(n) \) into Eq.(6) and by comparing the coefficient of the highest-degree term \( (n^M) \), yields the following simple expression for the eigenvalues
\[
E = M(\alpha - \gamma), \]
with \( M = 0, 1, 2, ..., N \). Owing to the equal spacing of energy eigenvalues, the lattice model (7) yields a periodic temporal dynamics with period \( T = 2\pi / |\alpha - \gamma| \). Note that, for \( \alpha = -\gamma \) real-valued, this lattice model corresponds to the one previously introduced in Refs. \[11\] \[12\], i.e. to uniform site energies \( V_n \) and to an optimal coupling of adjacent lattice sites. Interestingly, for real values of \( \alpha \) and \( \gamma \) but with \( \alpha \neq -\gamma \) and \( \alpha \gamma < 0 \), a linear gradient of site energies \( V_n \) occurs, and the lattice model (7) thus sustains exact BOs on a finite lattice. Figure 1 shows, as an example, a typical behavior of hopping amplitudes and site energies for such an Hermitian lattice, together with the characteristic BOs behavior for an initial Gaussian wave packet as obtained by numerical simulations of the Schrödinger equation \( i(\partial \psi / \partial t) = H \psi \). To show that exact wave packet reconstruction is insensitive to edge effects, in the example of Fig.1 wave packet excitation was intentionally chosen close to one edge of the lattice, however periodic wave packet reconstruction is observed for any initial wave packet, regardless of its shape or position in the lattice. It should be also noticed that periodic wave packet reconstruction does not mean nor imply shape-invariance of the wave packet evolution. Remarkably, a periodic quantum evolution, associated
FIG. 2: (color online) Bloch oscillations in a non-Hermitian truncated lattice. (a) coupling amplitudes $\kappa_n$, and (b) lattice site energies $V_n$ (real and imaginary parts) as given by Eq.(7) for $N = 15$, $\alpha = 1 + 0.2i$ and $\gamma = -1 + 0.2i$. (c) Numerically-computed temporal evolution of the site occupation probabilities $|\psi(n,t)|^2$ in the $(n,t)$ plane for an input Gaussian wave occupation amplitudes $\psi(0,0) = \exp\left(-\frac{(n-N/4)^2}{4}\right)$. (d) Detailed temporal evolution of the occupation probability $P(t)$ of the left-edge $(n=0)$ lattice site. (e) Behavior of the total occupation probability $P(t) = \sum_n |\psi(n,t)|^2$.

to the existence of equally-spaced real-valued energies, is found even for non-Hermitian lattices by taking $\alpha = \sigma + i\rho$ and $\gamma = -\sigma + i\rho$, where $\rho$ and $\sigma$ are arbitrary real-valued and nonvanishing constants. In this case, according to Eq.(7) the hopping amplitudes $\kappa_n$ turn out to be real-valued $[\kappa_n = \sqrt{(\rho^2 + \sigma^2)(N-n)(n+1)}]$, whereas the site energies $V_n$ are complex-valued and linearly varying with the index $n \left[ V_n = (\sigma + i\rho)N - 2i\rho n \right]$, i.e. the linear gradient of site energies is now imaginary rather than real-valued as in ordinary BO lattice models. Physically, such a new class of non-Hermitian lattices could be realized by a sequence of $(N+1)$ active optical waveguides with a judicious engineering of waveguide spacing (to tune the hopping rates $\kappa_n$) and with a controlled gain/loss coefficient $V_n$ (see, for instance, [20]). In spite of non-Hermiticity, the energy levels are real-valued and equally spaced like in the Hermitian lattice model. However, the kind of periodic wave packet evolution in the such a non-Hermitian lattice is very distinct from ordinary BOs found in Hermitian lattices (see e.g. [3]). In particular, oscillations of the total occupation probability $P(t) = \sum_n |\psi(n,t)|^2$ are found as a result of the non-conservation of the norm, like in other non-Hermitian crystals (see for instance [21]). As an example, Fig.2 shows the behavior of $\kappa_n$ and $V_n$ for a non-Hermitian lattice defined by Eq.(7), together with a typical temporal evolution of an initial Gaussian wave packet, showing a characteristic oscillation of the total occupation probability.

As a final comment, it is worth mentioning that BOs on a semi-infinite Hermitian lattice with linearly-increasing hopping amplitudes, recently predicted in Ref.[14], can be found by assuming $F_1(n) = \alpha(n+1)$ and $F_2(n) = \gamma n$, with $\alpha \gamma > 0$ (to ensure lattice Hermiticity) and $|\alpha| \leq |\gamma|$ (to ensure boundness of $\psi(n)$ as $n \rightarrow +\infty$). In this case one obtains $\kappa_n = J(n+1)$ and $V_n = -fn - \alpha \left( n = 0, 1, 2, 3, ... \right)$, where $J = \sqrt{\alpha\gamma}$ and $f = (\alpha + \gamma)$ are the hopping rate and site energy gradients, respectively. Note that the condition $|f| \geq 2J$ is always satisfied, i.e. the existence of a Wannier-Stark energy level spectrum requires a minimum value of the dc force $|f|$. As discussed in [14], such a minimum value $|f|_m = 2J$ of the dc force corresponds to the existence of a metal-insulator transition in this lattice model.

**Self-imaging in lattices with commensurate energy levels quadratically-varying with the quantum number.** As a second class of lattices showing self-imaging phenomena, let us consider a finite lattice comprising the sites $n = 0, 1, 2, ..., N$ and assume $F_1(n) = (n-N)(n+\alpha)$ and $F_2(n) = n(n+\gamma)$, where $\alpha$ and $\gamma$ are real-valued parameters. The hopping amplitudes and site energies of this lattice are thus given by [see Eq.(2)]

$$\kappa_n = \sqrt{(n+\alpha)(n-N)(n+1)(n+\gamma+1)}$$  \hspace{1cm} (9)

$$V_n = -[2n^2 + (\alpha + \gamma - N)n - \alpha N].$$  \hspace{1cm} (10)
Substitution of such expressions of $F_1(n)$ and $F_2(n)$ into Eq.(6) and by comparing the coefficient of the highest degree term ($\sim n^M$) in the power expansion, one obtains the eigenvalues

$$E = M^2 - M(N + 1 + \gamma - \alpha), \quad M = 0, 1, 2, ..., N,$$  

i.e. the energy eigenvalues are described by a quadratic function of the quantum number $M$. Provided that $(N + 1 + \gamma - \alpha)$ is a rational number, i.e. $(N + 1 + \gamma - \alpha) = r_1/r_2$ with $r_1$ and $r_2$ integer numbers, the energy levels are commensurate numbers and the wave packet dynamics turns out to be periodic. As an example, Figs. 3(a) and (b) show a typical behavior of $\kappa_n$ and $V_n$ in an Hermitian lattice for parameter values $N = 10$, $\alpha = -N$ and $\gamma = 0$, which yield $E = M^2 - 21M$ according to Eq.(11). Periodic quantum evolution is thus expected at the period $T = \pi$. Self-imaging is demonstrated, as an example, in Fig.3(c), where the behavior of the site occupation probability $|\psi(n = 0, t)|^2$ at the lattice edge $n = 0$ versus time $t$ for initial single-site excitation $\psi(n, 0) = \delta_{n,0}$ is depicted.

**Conclusions.** A novel class of truncated tight-binding lattices that sustain a periodic quantum evolution of the wave packet has been presented. In particular, we have shown the existence of Bloch oscillations in Hermitian truncated lattices, Bloch oscillations in non-Hermitian lattices with an imaginary site energy gradient, and discussed self-imaging phenomena in finite lattices with commensurate energy levels that depend quadratically on the quantum number. Photonic waveguide arrays, realized for instance by femtosecond laser writing in fused silica [7], could provide a possible experimental set-up to realize the Hermitian lattice models discussed in this paper (Figs.1 and 3). In such arrayed structures, simultaneous engineering of coupling rates $\kappa_n$ and site energies $V_n$ can be achieved by appropriate design of distances between adjacent waveguides (which determine the values of $\kappa_n$) and choice of waveguide writing speed (which determines the values of $V_n$).

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