Supplementary material for Chaos-assisted long range hopping for quantum simulation

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In this Supplementary material, we describe the methods used to numerically simulate the dynamic evolutions of the temporally modulated system and of the effective Hamiltonian, whose construction we explain in more details. The code we used is written in Python 3 and uses the Numpy library. It is available at https://framagit.org/mmartinez/dynamics1d. We then describe in detail the derivation of the hopping law.

Numerical methods

Exact dynamics of the periodically modulated lattice

The system, composed of N_c cells of spatial size $\lambda = 2\pi$ is discretized with N_p points per cell; the total basis size is thus $N_t = N_c N_p$. We have used both a spatial $|x\rangle$ and momentum $|p\rangle$ representation. The corresponding grids are centered around $x = 0$ and $p = 0$ with respective size-step:

$$\delta x = \frac{\lambda}{N_p} \quad \text{and} \quad \delta p = \frac{2\pi}{\lambda}\frac{\hbar_{\text{eff}}}{N_c}. \tag{1}$$

For the whole of the study, we took $N_p = 32$ after checking that this discretatization was fine enough to faithfully represent the dynamics of the system: in particular, the total size in the p direction $N_p\hbar_{\text{eff}}$ should be larger than the extension of the chaotic sea in momentum space.

The time propagation of a given state $|\psi\rangle$ is achieved with a symmetrized split-step method:

$$|\psi(t+\delta t)\rangle = U_P F U_X F^{-1} U_P \,|\psi(t)\rangle\,, \tag{2}$$

with

$$U_X = \sum_x \exp\left(-i\frac{V(x,t)\delta t}{\hbar}\right)|x\rangle\langle x|\,,\ U_P = \sum_p \exp\left(-i\frac{p^2\delta t}{4\hbar}\right)|p\rangle\langle p| \tag{3}$$

$$F = \frac{1}{\sqrt{N}}\sum_{x,p}\exp\left(-i\frac{xp}{\hbar}\right)|p\rangle\langle x| \quad \text{(using FFT)}. \tag{4}$$

The time step $\delta t = 4\pi/1000$ was chosen after consistency tests.

Construction of the effective Hamiltonian

The determination of the Floquet-Bloch band is equivalent to the determination of the quasi-energy spectrum of the following Hamiltonian

$$H_\beta(x,t) = \frac{(p-\hbar_{\text{eff}}\beta)^2}{2} - \gamma(1+\varepsilon\cos t)\cos x, \tag{5}$$

on a single cell $N_c = 1$ (with $N_p = 32$, see above), with the quasi-momentum β taking the discrete values $\beta_m = 2\pi m/(N_c\lambda)$, $m = 0,\ldots,N_c-1$. Thus, for a system size N_c, we repeat N_c times the following procedure (for each value of β_m):

- First, we build the matrix (in x reprentation) of the Floquet operator from the propagation of N_p δ-function states $|x\rangle$. To do so, we use the previous split-step method over two periods of modulation $T = 4\pi$ (this choice was made to be consistent with [1], but is of no importance here).

- Second, we diagonalize the Floquet operator and look for the eigenstate having the largest overlap with a Gaussian state centered on the regular island. This eigenstate is associated with a complex eigenvalue α_β that gives the effective energy:

$$\varepsilon_{\text{eff}}^{\text{reg}}(\beta) = -\frac{i\hbar_{\text{eff}}}{T}\log\alpha_\beta. \tag{6}$$

- Once we have obtained the N_c values of $\varepsilon_{\text{eff}}^{\text{reg}}(\beta_m)$, we build explicitly the effective tight-binding Hamiltonian H_{eff}, whose coupling elements $t_n^{\text{eff}} \equiv \langle (m+n)_{\text{reg}}|H_{\text{eff}}|m_{\text{reg}}\rangle$ are computed from the discrete Fourier Transform:

$$t_n^{\text{eff}} = \frac{1}{N}\sum_{\beta_m}\varepsilon_{\text{eff}}^{\text{reg}}(\beta_m)\exp(i\beta_m\lambda n). \tag{7}$$

Dynamic evolution under the effective Hamiltonian

The effective Hamiltonian is a tight-binding model of N_c sites $|n\rangle$, with $n = 0, \dots N_c - 1$. The wavefunction $|\psi\rangle$ is propagated over two periods with effective evolution propagator:

$$|\psi(t+T)\rangle = U_{\text{eff}}\,|\psi(t)\rangle \quad \text{with} \quad U_{\text{eff}} = \exp\left(-i\frac{H_{\text{eff}}T}{\hbar_{\text{eff}}}\right), \tag{8}$$

obtained using a Padé approximation.

Construction of the regular Wannier-states

The Wannier states of the unperturbed lattice (with $\varepsilon = 0$) provide an approximation of the regular modes $|n_{\text{reg}}\rangle$ of the modulated lattice discussed in the letter. To construct them, we thus use a procedure similar to that used for the determination of the effective energy band, but using the unmodulated lattice (with $\varepsilon = 0$): For each value of $\beta_m = 2\pi m/(N_c\lambda)$, $m = 0, \dots N_c - 1$, we diagonalize the evolution operator over two periods $T = 4\pi$ and look for the eigenstate having the largest overlap with a Gaussian state centered on the regular island. The p representation of this eigenstate gives the coefficient of the Wannier state on the partial (uncomplete) grid $p = \hbar_{\text{eff}}\beta + n\delta p$ of size N_p. After repeating N_c times this procedure, we obtain the full p representation of the Wannier state (on the complete momentum basis of size N_pN_c).

Miscellaneous

The classical dynamics is simulated using a RK4 Runge-Kutta algorithm. Husimi phase-space representations are computed using the procedure described e.g. in [2].

Derivation of the hopping law for large system sizes

To derive the hopping law Eq. (3), we first decompose the effective Bloch band as a regular part ε_0 and a sum over all resonance terms:

$$\varepsilon_{\text{reg}}^{\text{eff}}(\beta) = \varepsilon_0(\beta) + \sum_{\text{resonances}}\varepsilon_{\asymp}(\beta - \beta_0, W, \alpha), \tag{9}$$

where each resonance is characterized by three parameters: β_0 the position of the resonance, W the coupling intensity between the chaotic and the regular state and α the slope of the energy of the involved chaotic state with β. Each

resonance can be described by a two-level Hamiltonian of an avoided crossing at $\beta = 0$:

$$\begin{pmatrix} \varepsilon_{\rm reg}(\beta) & W \\ W & \varepsilon_{\rm ch}(\beta) \end{pmatrix} \tag{10}$$

with $\varepsilon_{\rm reg}(\beta) = 0$ (since it is taken into account by ε_0 in Eq. (9)) and $\varepsilon_{\rm ch}(\beta) = \alpha\beta$. The corresponding eigenstates $|\beta_\pm\rangle$ and eigenenergies $\varepsilon_\pm(\beta)$ follow:

$$\varepsilon_\pm(\beta) = \frac{\varepsilon_{\rm reg} + \varepsilon_{\rm ch}}{2} \pm \sqrt{\Delta^2 + W^2} \quad \text{and} \quad |\beta_\pm\rangle = \begin{cases} \cos\theta\,|\beta_{\rm reg}\rangle + \sin\theta\,|\beta_{\rm ch}\rangle \\ -\sin\theta\,|\beta_{\rm reg}\rangle + \cos\theta\,|\beta_{\rm ch}\rangle \end{cases}, \tag{11}$$

with $\Delta = (\varepsilon_{\rm reg} - \varepsilon_{\rm ch})/2$ and $\theta \in [0, \pi/2]$ verifying $\tan 2\theta = |W|/\Delta$. The prescription for the effective spectrum construction is to select the energy associated with the eigenstate having the largest projection on the regular subspace. We thus get:

$$\varepsilon_\asymp(\beta, W, \alpha) = \frac{\alpha}{2}\left(\beta - \mathrm{sgn}(\beta)\sqrt{\beta^2 + \left(\frac{2|W|}{\alpha}\right)^2}\right). \tag{12}$$

Taking the Fourier transform, we then have

$$t_n = t_n^0 + \sum_{\rm resonances} t_n^\asymp(\beta_0, W, \alpha) \quad \text{with} \quad t_n^\asymp(\beta_0, W, \alpha) = \frac{\lambda}{2\pi}\int_{-\pi/\lambda}^{\pi/\lambda} \varepsilon_\asymp(\beta - \beta_0, W, \alpha)\mathrm{e}^{-in\beta\lambda}\,\mathrm{d}\beta\,. \tag{13}$$

We now assume that $\varepsilon_\asymp(\beta - \beta_0, W, \alpha)$ is peaked around β_0 and that β_0 is sufficiently far from the edge of the boundary of the Brillouin zone, so that

$$t_n^\asymp(\beta_0, W, \alpha) \approx \mathrm{e}^{in\beta_0\lambda}\frac{\lambda}{2\pi}\int_{-\pi/\lambda}^{\pi/\lambda} \varepsilon_\asymp(\beta, W, \alpha)\mathrm{e}^{-in\beta\lambda}\,\mathrm{d}\beta\,. \tag{14}$$

The latter expression can be evaluated for large n values. We introduce $x = \beta\lambda$ and $\eta = 2\lambda|W|/\alpha = \lambda\Delta\beta/2$, it reads

$$t_n^\asymp = \frac{\mathrm{e}^{in\beta_0\lambda}\alpha}{4\pi\lambda} \times \underbrace{\int_{-\pi}^{\pi}\left(x - \mathrm{sgn}(x)\sqrt{x^2+\eta^2}\right)\mathrm{e}^{-inx}\,\mathrm{d}x}_{I^*}, \tag{15}$$

we split the integral I (taking complex conjugation) in two parts, the first one gives

$$\int_{-\pi}^{\pi} x\mathrm{e}^{inx}\,\mathrm{d}x = \frac{2i\pi}{n}(-1)^{n+1}. \tag{16}$$

The second part can be rewritten

$$\int_0^{\pi} \mathrm{sgn}(x)\sqrt{x^2+\eta^2}\mathrm{e}^{inx}\,\mathrm{d}x - \text{c.c.}, \tag{17}$$

we then deform the contour of integration $0 \to \pi$ to a complex circuit $0 \to iT \to iT + \pi \to \pi$ with T some large real number. Using Watson's formula, the first part gives (setting $x = iy$)

$$i\int_0^T \sqrt{\eta^2 - y^2}\mathrm{e}^{-ny}\,\mathrm{d}y \sim \frac{i|\eta|}{n}. \tag{18}$$

The second part is negligible for T large enough (setting $x = y + iT$):

$$\mathrm{e}^{-nT}\int_0^{\pi} \sqrt{(y+iT)^2+\eta^2}\mathrm{e}^{-iny}\,\mathrm{d}y \to 0. \tag{19}$$

Using Watson's formula and assuming $\Delta\beta \ll \frac{2\pi}{\lambda}$ so that $(\eta/\lambda)^2 \ll 1$, the third part (setting $x = \pi + iy$) gives:

$$i(-1)^{n+1}\int_0^T \sqrt{(\pi+iy)^2+\eta^2}\mathrm{e}^{-ny}\,\mathrm{d}y \sim \frac{i\pi}{n}(-1)^{n+1}. \tag{20}$$

Putting all terms together (taking care of complex conjugation) we end up with

$$t_n^{\asymp} \approx \frac{\mathrm{e}^{in\beta_0\lambda}\alpha}{4\pi\lambda}\left(\frac{2i\pi}{n}(-1)^{n+1} - \frac{2i\eta}{n} - \frac{2i\pi}{n}(-1)^{n+1}\right)^* = \frac{\mathrm{e}^{in\beta_0\lambda}\alpha}{4\pi\lambda} \times \frac{i4\lambda|W|}{|\alpha|} = \frac{i}{\pi n}\mathrm{sgn}(\alpha)|W|\mathrm{e}^{in\beta_0\lambda}. \tag{21}$$

We finally assume that t_n^0 is negligible for large n values (because it decays exponentially), so that

$$t_n \approx \frac{i}{\pi n}\sum_{\text{resonances}} \mathrm{sgn}(\alpha)|W|\mathrm{e}^{in\beta_0\lambda}. \tag{22}$$

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