Multiscaling, Ergodicity and Localization in Quasiperiodic Chains

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We report results of numerical simulations of wave-packet dynamics in a class of chains consisting of two types of weakly coupled clusters arranged in a quasiperiodic sequence. Properties of eigenstates are investigated using perturbation theory of degenerate levels in the coupling strength \( v \) and by numerical diagonalization. Results show that wave packets anomalously diffuse \textit{via} a two-step process of rapid and slow expansions, which persist for any \( v > 0 \). An elementary analysis of the degenerate perturbation expansion reveals that non-localized states may appear only in a sufficiently high order of perturbation theory, which is simply related to the combinatorial properties of the sequences. Numerical diagonalization furthermore shows that eigenstates ergodically spread across the entire chain for \( v > 0 \), while in the limit as \( v \to 0 \) ergodicity is broken and eigenstates spread only across clusters of the same type, in contradistinction with trivial localization at \( v = 0 \). An investigation of the effects of a single-site perturbation on wave-packet dynamics shows that, by changing the position or strength of such an impurity, it is possible to control the long-time wave-packet dynamics. By adding a single impurity it is possible to induce wave-packet localization on individual subchains as well as on the whole chain.

Understanding the relation between spectral properties of a given Hamiltonian and the dynamics of wavepackets governed by it remains one of the elementary questions of quantum mechanics that still poses significant challenges, further emphasized by the discovery of quasicrystals \cite{1, 2}. While spectra of many Hamiltonians decompose into a point part and an absolute continuous part with, respectively, bound (localized) and unbound (delocalized or extended) eigenstates, there is a large variety of Hamiltonians whose spectra, for certain values of the parameters, are neither pure point nor absolute continuous nor a combination of both. In this case the spectrum contains a singular continuous part, with multifractal eigenstates and/or Cantor-set spectra. Examples are Harper’s model of an electron in magnetic field \cite{4}, the kicked rotator \cite{5}, as well as the Anderson model of an electron in disordered medium \cite{6}. In the case of an electron in a quasiperiodic system, as studied in this Letter, many examples lead to spectra which are purely singular continuous \cite{10}.

It is known that a particle’s return probability decays with the same powerlaw as the scaling of the local density of states \cite{12}, and that the spreading of the wave-packet width \( d(t) \) (defined below) exhibits anomalous diffusion, \( d(t) \sim t^\beta \), with \( 0 < \beta < 1 \) (\( \beta = 0 \) corresponds to the absence of diffusion, \( \beta = 1/2 \) to classical diffusion and \( \beta = 1 \) to ballistic spreading) \cite{8}. In addition, the wave-packet dynamics exhibits multiscaling, where different moments of the wave-packet scale with different, non-trivially related exponents \( \beta \) \cite{14, 16, 21, 22}. While wave-packet localization implies a pure-point spectrum, the converse is not true, and the more refined notion of semi-uniform localization is necessary \cite{20}. The exact relations between particle dynamics and singular or absolute continuous spectra, on the other hand, is less well understood. As a rule, systems with singular continuous spectra exhibit anomalous diffusion, while absolute continuous spectra may lead to either anomalously diffusive or ballistic dynamics \cite{11}.

In this Letter, we study eigenstate and wave-packet properties of an electron moving in a one-dimensional quasiperiodic system described by the tight-binding Hamiltonian \( H = \sum_{<ij>} t_{ij} \epsilon_i^c \epsilon_j^c + \text{H.c.} \). Here \( \epsilon_j \) is the annihilation (creation) operator of an electron at site \( j \), and the nearest-neighbors-only hopping integrals \( t_{ij} \) take values 1 or 0 \( \leq v \leq 1 \) for, respectively, letters \( l \) or \( s \) (“large” and “small” hoppings) of a quasiperiodic sequence of letters obtained by the inflation rules \{ \( s \to l, l \to ls^{-1} \) \} iterated \( m \) times, starting with the letter \( s \). Denoting the length of the \( m \)-th iterant by \( N_m \), these sequences have the property that \( N_m/N_{m+1} \to \delta_\alpha \) as \( m \to \infty \), where \( \delta_\alpha \) is an irrational number with continuous fraction representation \[ n, n, n, \ldots \]. The quantities of interest are the solutions of the eigenproblem \( \hat{H} \psi_k (j) = E_k \psi_k (j), \ k = 1, \ldots N_m + 1 \), as well as the width \( d(t) \) of a wave-packet \( \Psi(j, t) \),

\[
\frac{d^2(t)}{\sum_{j=1}^{N_m+1} |j - j_0|^2 |\Psi(j, t)|^2},
\]

which is initially localized at a site \( j_0 \), so \( \Psi(j, t = 0) = \delta_{j, j_0} \).

Figure 1 shows the change of the wave-packet width with time for the silver-mean \((n = 2)\) model. While the asymptotic behavior can be characterized as anomalous diffusion \( d(t) \sim t^\beta, \beta \approx 0.2 \), there are also “flat” parts in the regime of strong quasiperiodic modulation (small \( v \)). As demonstrated by the insets in Fig. 1, these can be characterized by the existence of time intervals, exponentially growing at a constant rate for a given \( v \), during which \( d(t) \) strongly oscillates in a self-similar manner reflecting the hierarchical structure of system,
Eigensstates delocalize, in contradistinction to (trivial) low-energy levels at \( t \) as a result of the perturbation theory of degenerate rather than hierarchical [18] properties. By an elementary eigenstate analysis of the secular problem in first order and numerical simulations, it was argued that an eigenstate spreading in the semiclassical approximation reveals that breathing modes are responsible for the oscillations, while the wave-packet spreading itself is limited to low-amplitude "leaking" out of the region in which it is confined. Eventually, the wave-packet expands fast to reach the next level (this spreading can be described as \( d(t) \propto t^{\beta'} \) with \( \beta' \approx 0.79 \)), and the whole process repeats.

Such a behavior is in agreement with results of Ref. [10], where, based on a qualitative model of the wave-packet spreading in the semiclassical approximation and numerical simulations, it was argued that an hierarchical splitting of the spectrum into constant-width bands leads to a step-like behavior with \( \beta' = 1 \), which then is smoothed out due to the (broad) distribution of band widths. The here observed value \( \beta' < 1 \) for small \( v \) suggests that there is a dispersion of band widths even in the limit as \( v \to 0 \) (when band widths go to 0 [13]), and that the self-similar spreading of the wave-packet is only an approximate description of a more general multiscale dynamics. This self-similarity can be used, e.g., for calculating \( \beta' \) by \( \beta' \approx \delta \ln d/\delta \ln t \), where \( \delta \ln d \) and \( \delta \ln t \) are the horizontal and vertical displacements between each of the two steps in Fig. 1, respectively, giving in the case studied \( \beta' \approx 0.20 \) for \( v = 0.025 \).

The self-similarity of quasiperiodic sequences was previously used in a renormalization-group perturbative expansion that provided a great deal of insight into the eigenstate properties [17], and showed multiscaling of wave-packet dynamics. Here we focus on ergodic rather than hierarchical properties. By an elementary analysis of the perturbation theory of degenerate levels at \( v = 0 \) for small \( v \) we show that (a) for any \( v > 0 \) eigenstates delocalize, in contradistinction to (trivial) localization at \( v = 0 \); and (b) in the limit as \( v \to 0 \) eigenstates delocalize across only one set of clusters containing the same number of atoms (subcluster localization due to ergodicity breaking).

Raleigh-Schrödinger theory allows the recursive construction of matrices in subspaces of a given degenerate eigenenergy to a given order \( p \), whose diagonalizations (the "secular problem") yield corrections to the unperturbed eigenenergies, hopefully accurate up to \( O(v^{p+1}) \). In the case of an unperturbed chain \( (t_{ij'} = t) \), for instance, the solution of the secular problem in first order in \( t \) is equal to the exact solution of the problem.

For the quasiperiodic sequences considered here, however, such perturbation expansions yield two qualitatively different types of solutions, depending on the values of \( p \) and \( n \). To that end we first notice that approximants for a given \( n \) consist of two types of words, \( l^{n-1} \) and \( l^n \), separated by the letter \( s \), corresponding to clusters with \( n \) and \( n + 1 \) atoms, respectively, coupled via hopping of strength \( v \) which is treated as a perturbation. The unperturbed system then has \( 2n + 3 \) degenerate levels with all eigenstates localized on individual clusters. In higher orders of perturbation theory, these localized states spread as the coupling among the clusters of the same type is taken into consideration, and, for a sufficiently high order, delocalize across the whole chain. Since the maximal number of letters \( s \) between two consecutive clusters of length \( k \) is also \( k \), the eigenstates of the clusters \( l^{n-1} \) and \( l^n \) delocalize only in the \( n \) and \( n + 1 \) order of the perturbation theory, respectively. More precisely, the dimension of the secular problem for each cluster of length \( q = n, n + 1 \) changes from at most \( O(n^2) \) for \( p < q \) to \( O(N_m) \) for \( p \geq q \). Only the latter case allows for multifractal and/or extended states.

As an example we analyze the case \( n = 2 \). There are 7 unperturbed levels, with \( E_{il}^{(0)} = \pm(\sqrt{5} \pm 1)/2 \) and \( E_{ll}^{(0)} = \pm \sqrt{2}, 0 \). In first order, the only correction are 6 bands in \( v \), splitting off the three \( E_{il}^{(0)} \) bands, because \( llllls \) is the only possibility where two clusters of the same type are connected by a single \( s \) bond. For \( p = 2 \), all \( ll \) clusters become connected while \( lll \) states are still not extended due to the existence of \( llllllslslslls \) sequences in the chain. For \( p = 3 \), states belonging to \( lll \) bands delocalize as well.

To investigate further the issue of convergence, we notice that, even when calculated to all orders of \( v \), the secular problems for the two types of clusters give solutions that are inevitably localized on the clusters of the given type and with zero component on the cluster of the other type. For various values of \( v \), we check by numerical diagonalization whether this is confirmed. Fig. 2 shows \( p_{ll}(E_k) \equiv \sum_{j \in ll} | \psi_k(j) |^2 \), the total probability that the particle in an eigenstate \( \psi_k \) with an energy \( E_k \) will be on the cluster \( lll \). The result implies that \( p_{ll} \) strongly depends on the energy band of the given eigenstate for small \( v \), being large for the states belonging to the \( lll \) bands, and vanishing for the states from \( ll \) bands in the

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**FIG. 1:** Evolution of the width \( d(t) \) of a wave-packet initially localized in the middle of the silver-mean chain for \( m = 9 \), for several small values of \( v \). The insets show two magnified "steps" for \( v = 0.025 \).
limit $v \to 0$. While Fig. 2 shows results for $m = 9$, we have also checked $p_{ll}$ for the iterants $m = 10, 11, 12$ to see whether there is any systematic deviation from the values shown in Fig. 2. We found that, while there are many more states for larger $m$’s, the values of $p_{ll}$ do not shift systematically for almost all of the states. Instead, the additional points cluster in the same way as in Fig. 2.

This supports the possibility that eigenstates remain ergodic (i.e., spread over both types of clusters) even for very small values of $v$, and that, in turn, the Schrödinger-Raleigh perturbation expansion of degenerate levels has zero radius of convergence but, nevertheless, might still be accurate in the limit as $v \to 0$ since $p_{ll}(v \to 0) \to 0$ or 1 (which is, however, only a necessary but not a sufficient condition). On the other hand, the nearly non-ergodic behavior of wave-packets for small $v$ has interesting consequences when a single impurity is added, as we show next.

An impurity $H' = u_{c_i}c_i^\dagger c_i$ added at a site $i$ will, for large $u$ (e.g., $u \gg 1$), act as a barrier, effectively cutting the chain into two halves. The consequence of ergodicity in this limit is that the wave-packet reflects off the impurity independently of its initial site, even if $v$ is small. For $u \to 0$, on the other hand, the unperturbed wave-packet propagation of the case $u = 0$ is restored. Understanding the wave-packet propagation in the regime of intermediate $u$ values, however, still poses significant challenges and surprising results [20]. We performed several numerical experiments for various initial positions of impurities and wave-packets for intermediate values of $u$, and one common situation is shown in Fig. 3. The evolution of an initially localized wave-packet exhibits high sensitivity on the position of the impurity, approaching two quite different stationary states. In particular, while in Fig. 3(a) the final state is just slightly perturbed from a final state for $u = 0$, in Fig. 3(b) certain parts of the wave packet get reflected, with a small-amplitude “leak” reminiscent of the similar process mentioned above. This kind of wave-packet dynamics is a consequence of the nearly non-ergodic properties of eigenstates discussed above (cp. Figure 2).

Finally, we address the influence of an impurity at the initial site of the wave-packet on its dynamics, by studying the dependence of the final wave-packet width on the value of $u$. Fig. 4 shows the maximum value of $d(t)$ attained in the course of the evolution of a wave-packet, which was initially localized at the site $j_0 = N_m/2$, in the presence of an impurity located at the same site. The $m = 7$ iterant of the silver-mean model has unperturbed wave-packets exhibiting one full step from Fig. 1, reaching the final stationary state after beginning of the second step.

Fig. 4 shows that, apart from the strongly localized final wave-packets for large $u$ and unperturbed final stationary wave-packets for small $u$, there is a wide range of values of $u$ for which the final width of the wave-packet is significantly reduced even for $u \ll v$, signaling (dynamical) localization. There are nevertheless several well defined peaks about some values of $u$ where the maximum wave-packet width is significant enhanced compared with the case for slightly smaller and slightly larger values of $u$. We additionally checked whether such peaks persist when the system size is increased, by performing the same calculation for the $n = 9$ iterant. Fig. 4 shows that there is again a peak structure, with both small and large peaks. The relation of the values of $u$ where these peaks appear and the spectrum of $H$ remains unclear. Repeating similar numerical experiments for various values of $v$, we find that the peak structure persists as long as the band widths are smaller than the band gaps ($v \lesssim 0.4$ in the silver-mean case). These results, however, show that in quasiperiodically modulated quantum wires one can strongly influence the electronic transport by inducing local perturbations that act as sort of control gates for long-range quantum interference effects in electronic transport.

FIG. 2: Probability that a particle in an eigenstate with the given energy is on the $ll$ sublattice, for $v = 0.1, 0.2, \ldots 0.9$ (going from top to bottom in the central part of the plot). The line connecting points for $v = 0.5$ is for guidance only. Only states $E < 0$ are shown due to the symmetry about the band center.
unperturbed final state
“quasilocalized” state

FIG. 3: Snapshots of the evolution of two wave-packets, both starting as \( \delta \)-functions in a local environment \( \ldots \psi(x) \delta \ldots \) at the same initial site \((x)\), in the presence of an impurity. In the two panels (a) and (b), the impurity is located in a local environment \( \ldots \psi(x) \delta \ldots \) at the position marked by (a) and (b), respectively, as indicated in each panel by a vertical line. For easier comparison, the vertical dashed line in each panel marks the position of the impurity in the other panel. The long-time wave-packet dynamics exhibit high sensitivity on whether the impurity is located or not on the cluster of the same type as the one where the wave-packet was localized initially. The remaining parameters are \( n = 2, m = 8, v = u = 0.1 \).

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