One-Dimensional Schrödinger Equation with an Almost Periodic Potential

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Recent theories of scaling in quasiperiodic dynamical systems are applied to the behavior of a particle in an almost periodic potential. A special tight-binding model is solved exactly by a renormalization group whose fixed points determine the scaling properties of both the energy spectrum and certain features of the eigenstates. Similar results are found empirically for Harper's equation. In addition to ordinary extended and localized states, "critical" states are found which are neither extended nor localized according to conventional criteria.

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This article describes extensions of renormalization-group work[1-4] on circle maps and invariant curves of area-preserving maps[5] to the behavior of the Schrödinger equation with a quasiperiodic potential. These models display interesting spectra because a quasiperiodic potential is intermediate between a truly random potential which causes localization in one-dimensional (1D) systems and periodic potentials which lead to energy bands and extended states. The weak-coupling limit of this problem shares a common mathematical foundation with the small-divisor perturbation theory of Kolmogorov, Arnold, and Moser (KAM)[6] and it is not surprising that certain of the recent nonperturbative[1-4] approaches to dynamical systems can be used in the present problem as well.

Although the models we consider explicitly are defined by a tight-binding Hamiltonian, KAM and renormalization-group theory suggest that the scaling results may be generally applicable to the continuous Schrödinger equation as well. The Hamiltonian H that we consider is defined by

$$H=\sum_{n=1}^{\infty}\{-[c_{n+1}{}^{\dagger}c_n-2c_n{}^{\dagger}c_n+c_n{}^{\dagger}c_{n+1}] + V(n\sigma)\,c_n{}^{\dagger}c_n\}, \qquad (1)$$

where $V(x)=V(x+1)$ and σ is a "good" irrational number.[1] The operators $c_n{}^{\dagger}$ and c_n are the usual creation and destruction operators. Our most detailed results are obtained for $V(x)$ defined by

$$V(x)=\tfrac{1}{2}\epsilon\times\begin{cases}1, & -\sigma\leq x\leq 0,\\ -1, & 0<x<\sigma^2,\end{cases} \qquad (2)$$

with $\sigma=(\sqrt{5}-1)/2$. We have also studied Harper's potential $V(x)=V_0\cos[2\pi(x-\varphi_0)]$ as an example of an analytic potential. The equations for Harper's potential have many convenient symmetries[7,8] which can be exploited to guide the numerical analysis.

We now summarize our results. In addition to confirming a localization transition at $V_0=2$ for Harper's potential, we find the following new results:

(1) *Scaling.*—We implement numerically an empirical scaling analysis in which the quasiperiodic system is approximated by a sequence of periodic systems with progressively larger unit cells of size q_k defined by the optimal rational approximants to σ, $\sigma_k=p_k/q_k$. The spectra and wave functions of both models satisfy scaling relations (defined below) in the immediate vicinity of gap edges and at other special points in the spectrum. The potential (2) is always "critical" in the sense that exponents are nontrivial and the wave func-

tions are neither localized nor extended. Harper's potential is critical in the same sense only for $V_0=2$, while all exponents are trivial for $V_0<2$.

(2) *Renormalization group.*—A renormalization transformation is constructed for model (2) which confirms the scaling found numerically. For Harper's potential we infer the structure of the renormalization group from our numerical results as was done in previous problems.[1,4] There is a trivial fixed point for extended states and a critical fixed point which governs the localization transition. If there are no other relevant parameters present, we expect the same fixed points and exponents for any quasiperiodic operator of the form (1) with V analytic (e.g., Harper's potential). In our study it is necessary to control the rotation number of the wave function and we see no way to obtain results of comparable generality for quantities averaged over the spectrum.[9]

To proceed further we need several definitions. All our calculations are done for $\sigma=(\sqrt{5}-1)/2 \equiv \sigma_G$, though we believe that here, as in related problems,[1-3] similar results hold for any irrational σ which is the root of a quadratic equation with integer coefficients.

For $\sigma=\sigma_G$, $\sigma_k=q_{k-1}/q_k$, where q_k are the Fibonacci integers defined by $q_{k-1}+q_k=q_{k+1}$, $q_0=1$, and $q_1=2$. The spectrum for σ_k has q_k-1 gaps which may be labeled by the Bloch index $\kappa_s=\frac{1}{2}(s\sigma_k \bmod 1)$, where $|s|\leq[\frac{1}{2}(q_k+1)]$ and the square brackets denote the integer part. (We have divided the Bloch index in an extended zone scheme by $2\pi q_k$.) The size of the gaps decreases roughly with increasing s.[7,8] In the quasiperiodic limit the Bloch index becomes the rotation number κ which continues to exist for all energies[10,11] and is a convenient way to label the states. There are now a dense set of gaps at $\kappa_s=\frac{1}{2}(s\sigma \bmod 1)$.

To characterize how the spectrum scales, we define factors $\delta(\kappa)$ and $\gamma(\kappa)$ in terms of $E_k(\kappa)$, the energy of the state with rotation number κ for $\sigma=\sigma_k$. Note that κ is a monotone (nondecreasing) function of E. Let

$$\delta(\kappa)=\lim_{k\to\infty}\frac{E_k(\kappa)-E_{k+1}(\kappa)}{E_{k+p}(\kappa)-E_{k+p+1}(\kappa)}, \tag{3}$$

where p implicitly depends on κ and is the smallest integer (if any) such that the limit exists. Given that p is finite, we define the p different scale-invariant band structures near $E_\infty(\kappa)$ by

$$\tilde{E}_j(\rho,\kappa)=\lim_{k\to\infty}\gamma^k(\kappa)[E_{pk+j}(\kappa+\rho\sigma^{pk+j})-E_\infty(\kappa)], \tag{4}$$

where $\gamma(\kappa)$ is defined to make the limit exist and $0\leq j<p$.

Characterizing the states which exist at various energies in the spectrum is more subtle. In a periodic system, there are a pair of extended states at each energy in the band, and a single extended state at the gap edge. For quasiperiodic potentials, in the limit where KAM theory applies, one expects to find the generalized Bloch form:

$$\Psi(n)=e^{2\pi i n\kappa}\chi(n\sigma), \tag{5}$$

where $\chi(x)$ is smooth and periodic.[6,10,11] In addition to these extended states, we can expect[8] to find states which are square summable for other values of energy and potential strength. When the potential is nonanalytic and of the form (2) and when $V_0=2$ for Harper's potential we find that the solutions to the discrete Schrödinger equation do not fall into either of these categories.[12] These states, which we will term critical, have a maximum at a site N_k for $\sigma=\sigma_k$ and a series of subsidiary maxima at sites $\tilde{N}_k$ which do not decay to zero. For certain k, the amplitude obeys $|\psi(N_k)/\psi(\tilde{N}_k)|\to\tau$ if $1\ll|N_k-\tilde{N}_k|\ll q_k$ and a scaled version of the structure about N_k occurs around the site $\tilde{N}_k$.

The degree of localization around the central site N_k is measured by the exponent β defined by

$$\frac{1}{p\ln\sigma}\ln\left(\frac{L_m}{L_{m+p}}\right)\to\beta(\kappa) \tag{6}$$

when $1\ll m\ll k$, where the norm L_m is defined by

$$L_m=\left[q_m^{-1}\sum_{n=0}^{q_m}|\Psi(n+N_k)|^2\right]. \tag{7}$$

An ordinary extended state has $\beta=0$ while a localized state has $\beta=-1$. When β exists for a state Ψ it follows that the Liapunov exponent (defined below) l is 0, while if $l>0$, β does not exist. Our critical states are characterized by $-1<\beta<0$.

The quantities defined in Eqs. (3)–(5) are readily found numerically. For any rational approximation to σ, the bands consist of those energies for which

$$\left|\mathrm{tr}\prod_{n=1}^{q_k}M(n\sigma_k)\right|\leq 2,$$

where $M(x)$ is the matrix with elements $M_{11}=2-E-V(x)$, $M_{12}=-1$, $M_{21}=1$, and $M_{22}=0$. A similar matrix product with σ replacing σ_k relates $[\Psi(n-1),\Psi(n)]$ to $[\Psi(0),\Psi(1)]$ in a quasiperiodic system.

The renormalization procedure of Ref. 1 applied to $M(x)$ induces a renormalization operation on the matrix string. For the potential in Eq. (2)

and $\sigma=\sigma_G$ the matrix string assumes the particularly simple form ... *BABAABAABABAABA*, where A and B correspond to $V(x)=\epsilon/2$ and $-\epsilon/2$, respectively. Our renormalization group is then identical to the irrational decimation discussed by Feigenbaum and Hasslacher[4] where it is observed that the string is invariant under $T[A,B]=[BA,A]$. Denoting the original matrices $[A_0,B_0]$, we define $T^k[A_0,B_0]\equiv[A_k,B_k]$.[13] A fixed point or limit cycle can only exist for energies in the spectrum where $\lim_{k\to\infty}\kappa q_k \bmod 1$ converges to a limit cycle. In general, therefore, we expect that the renormalization transformation behaves ergodically on some set which is universal but whose elements are not self-similar (cf. Ref. 1, Sec. 7). For energies in a gap, we expect the sequence of matrix products $\prod_{n=1}^{N} M(\sigma n)$ to grow as e^{Nl}, where $l>0$ in accord with the usual definition of the Liapunov exponent l.

We now turn to a presentation of specific results. For the discontinuous potential (2) the transformation T acts on a six-dimensional space consisting of pairs of unimodular matrices. There are, however, many invariants I_{CD} of T^2 defined by two matrices C and D: $I_{CD}=\det[CAB-DBA]$. Only four of these are independent: $I_1=\det[AB-BA]=-\epsilon^2$, $I_2=I_{m^{11}m^{21}}=[\epsilon^3+4\epsilon(4E-E^2-3)]/4$, $I_3=I_{m^{11}m^{22}}=-[\epsilon^2+(4-2E)\epsilon+2]/2$, and $I_4=I_{m^{12}m^{22}}=-\epsilon$, where the matrices $(m^{ij})_{kl}=\delta_{ik}\delta_{jl}$.

At a gap edge at $\frac{1}{2}(s\sigma \bmod 1)$, the matrices $[A_k, B_k]$ are conveniently parametrized by $x_0,\ldots,x_5$ implicitly defined by

$$(-1)^{Q_k(s)}A_k=\tilde{A}_k=\begin{bmatrix} x_0 & (x_0+x_0^{-1}+x_1)/x_2 \\ -x_2x_0 & -(x_1+x_0)\end{bmatrix}, \tag{8a}$$

$$(-1)^{Q_{k-1}(s)}B_k=\tilde{B}_k=\begin{bmatrix} x_3x_0 & \dfrac{x_3x_0+(x_3x_0)^{-1}+x_4}{x_2[1+x_5(x_3x_0)^{-1}]} \\ -x_2(1+x_5/x_3x_0)x_3x_0 & -(x_4+x_3x_0)\end{bmatrix}, \tag{8b}$$

where $x_1,\ldots,x_5$ are finite and $x_0\sim\alpha^k$ with $|\alpha|\geqslant 1$. Each *entry* in the matrix A and B tends to ∞ although the Liapunov exponent is zero. {The function Q is defined by $Q_k(s)=sq_{k-1}+q_k[s\sigma]$ and $Q_k=q_k$ when $\kappa=\frac{1}{2}$.} The transformation T in the limit $x_0=\infty$ induces a transformation $\tilde{T}$ on $x_1,\ldots,x_5$ which is independent of x_0.

At a gap edge, we find a fixed point of $\tilde{T}^2$ with one relevant, two marginal, and two irrelevant directions. The relevant eigenvalue $\lambda=\delta=\gamma$ as it must at a fixed point with only one relevant direction. One marginal direction is perpendicular to a surface of constant $-\epsilon^2=I_1$. The other marginal direction is associated with the variable x_2 which turns out to be redundant in the limit $x_0=\infty$. This explains the observed fact that all eigenvalues are equal at all gap edges. The other invariants I_2, I_3, and I_4 are not differentiable in the limit $x_0=\infty$ and do not determine any eigenvectors.

The characterization of the gap-edge states is subtle. There is clearly a preferred initial vector $[\Psi(0),\Psi(1)]=[1,-x_2]$ so that the amplitude at sites which are a Fibonacci number away from the origin remains finite. This would seem to be the analog of the single extended gap-edge states in a periodic system. However, we have found numerically that the hull function χ in Eq. (5) is discontinuous and the states are critical. For other initial vectors we find that the envelope of $\Psi(n)$ grows as $n^{|\ln(\alpha)/\ln(\sigma_G)|}$. For $\epsilon=2$, $p=2$ we find from the fixed point $\gamma=\delta=\lambda=8.282\,386\,08\pm10^{-7}$ and $\alpha=3.408\,147\,60\pm10^{-7}$, while a calculation of ψ yields $\beta=-0.257\pm0.01$ and $\tau=1.051\pm0.01$.

Although we have not made a systematic study of states away from the gap edges, we have examined the case $\kappa=\frac{1}{4}$ in some detail to illustrate the type of scaling behavior we can expect at values of κ which do not correspond to a gap edge. We find that T^6 has a fixed point $[A^*,B^*]$ with all matrix entries finite. There is one relevant eigenvector at the fixed point, four marginal directions corresponding to each of the invariants I_m, and one irrelevant direction. Using $p=3$ and $\epsilon=2$ in Eq. (3), we verified that the relevant eigenvalue λ of T^6 satisfies $\lambda^{1/2}=8.123\,105\,627\pm10^{-7}$ and is equal to δ and γ. (This reflects the fact that the scaling of the spectrum corresponds to a subcycle of the scaling of the matrices themselves, analogous to the situation at the gap edges.) The two solutions to the Schrödinger equation at this energy are critical and at $\epsilon=2$, $\beta=-0.770\,495\pm10^{-6}$ and $2\tau=\epsilon+(\epsilon^2+4)^{1/2}$ to twelve figures.

The natural parameter space for Harper's equation consists of E, V_0, and a free phase φ_0. By use of duality, Aubry and Andre[8] have argued that a typical state will be extended for $V_0 < 2$ and exponentially localized above this critical value. In the vicinity of a gap edge for $V_0 < 2$ the spectrum scales according to Eqs. (3) and (4) with the trivial exponent $\delta = -\gamma = -\sigma_G^{-2}$ and $p = 1$ for all φ_0. At the gap edge itself the product matrix $S(q_k) = \prod_{n=1}^{q_k} M(n\sigma)$ is again conveniently expressed in the form (8a) up to a finite similarity transformation. The quantities x_0/q_k, x_1, and x_2 converge to smooth periodic functions of φ_0 (within a finite cycle) in the limit $k \to \infty$. There is a single extended state of the form in Eq. (5) with χ smooth.

Although convergence is poor, precisely at $V_0 = 2$, we find that γ assumes a nontrivial value of approximately 3.1 with $p = 1$. This value is independent of φ_0. However, the limit in Eq. (3) no longer appears to exist unless we choose the phase $\varphi_0 = \varphi^*$. The phase φ^* can be determined by duality to within integer multiples of σ_G for a given κ. There are clearly two relevant operators for gap-edge states at $V_0 = 2$ corresponding to changing φ_0 and E. We find that for any rational approximation to σ_G, $\Psi(n)$ has one or two similar maxima at sites N_k whose phase $N_k \sigma_G \bmod 1$ converges to φ^*. The scale-invariant structure of the Ψ appears to be governed by the relations described previously for critical states. For $\kappa = \frac{1}{2}$, $\beta = -0.89 \pm 0.02$ and $\tau = 4.73 \pm 0.02$. The function χ in Eq. (5) is discontinuous but bounded. For $V_0 > 2$, these states become exponentially localized.

We have also examined a variety of states in the quasiperiodic limit that are not at gap edges. For $V_0 < 2$ (weak coupling) the matrices $S(q_k)$ remain bounded and their trace approaches $2\cos(2 \times \pi \kappa q_k)$. There are two independent extended eigenstates (5) with χ smooth. Localization again occurs for $V_0 > 2$. In the weak-coupling regime, and with κ suitably far removed from a gap, we believe that $S(q_k)$ will tend to a set which is isomorphic to the simple rotations.

A number of recent papers have considered special quasiperiodic operators which are exactly solvable or have employed uncontrolled approximations.[14] By contrast, the renormalization group discussed here and extensions thereof permit one to establish the universal features associated with typical or generic potentials since the relevance or irrelevance of perturbations about the fixed points can be analyzed.

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[13]For analytic potentials *with* $\sigma = \sigma_G$, take a reference phase $\varphi_0{}^*$ and let T act on the matrices

$$A_k(x) = \prod_{n=1}^{q_k} M[n\sigma + (-\sigma)^{k+1} x],\quad B_k(x) = \prod_{n=1}^{q_{k-1}} M[n\sigma + (-\sigma)^{k+1} x].$$

Using the property that $q_k \sigma - q_{k-1} = -(-\sigma)^{k+2}$ it can be shown that

$$[A_{k+1}(x), B_{k+1}(x)] = T[A_k(x), B_k(x)] \equiv [B_k(-\sigma(x-1))A_k(-\sigma x),\ A_k(-\sigma x)].$$

The variable x is constrained to the interval $-\sigma < x < 1$. This renormalization group and the extension to arbitrary σ has been studied in detail by S. Ostlund and R. Pandit, unpublished.

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