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Mobility edge in aperiodic Kronig-Penney potentials with correlated disorder: Perturbative approach

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It is shown that a nonperiodic Kronig-Penney model exhibits mobility edges if the positions of the scatterers are correlated at long distances. An analytical expression for the energy-dependent localization length is derived for weak disorder in terms of the real-space correlators defining the structural disorder in these systems. We also present an algorithm to construct a nonperiodic but correlated sequence exhibiting desired mobility edges. This result could be used to construct window filters in electronic, acoustic, or photonic nonperiodic structures.

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The Kronig-Penney model has been widely used to explore the characteristics of electrons in a periodic potential, as this model provides one with perhaps the simplest instance of Bloch states. This model is also used systematically to provide estimates of the bandwidths in semiconductor superlattices with high reliability.[1] The Kronig-Penney model and its relation with superlattices has also been used in recent times to provide an implementation of the physics of random and quasiperiodic systems,[2] and interesting experiments have been reported on arrangements such as the well-known Fibonacci sequences.[3] It is because of its importance and wide applicability that we focus our attention on the Kronig-Penney model. We will demonstrate that the aperiodic model with constant scattering potential but random spacings yields mobility edges if the disorder has long-range correlations, in sharp contrast to the situation for white noise potentials.

The Kronig-Penney model in this study is given by a one-dimensional (1D) chain of delta-function scatterers with amplitude U_n and centered at points z_n. The Schrödinger equation for a particle moving in this random potential has the form

$$(\hbar^2/2m)\,\psi''(z)+E\,\psi(z)=\sum_{n=-\infty}^{\infty} U_n\psi(z_n)\,\delta(z-z_n). \quad (1)$$

This is equivalent to the discrete equation,

$$\sin\mu_{n-1}\psi_{n+1}+\sin\mu_n\psi_{n-1} =[\sin(\mu_n+\mu_{n-1})+(U_n/q)\sin\mu_{n-1}\sin\mu_n]\psi_n, \quad (2)$$

where $\psi_n\equiv\psi(z_n)$, $\mu_n=q(z_{n+1}-z_n)$, $q=\sqrt{E}$, and the energy is measured in units where $\hbar^2/2m=1$. The linear relation (2) between ψ_{n-1}, ψ_n, and ψ_{n+1}, can be easily arrived at by integrating Eq. (1) in the vicinity of sites $n-1$, n, and $n+1$, and substituting the amplitudes for the various constants in the piecewise zero-potential regions between the scatterers. If the site potential is different from a delta function, a linear relation similar to Eq. (2) can be obtained using a general method described in Ref. 4. Therefore, Eq. (2) can be considered as a rather generic relation for 1D chains with potential scatterers. We focus here on a sequence of scatterers of *equal* amplitude, $U_n\equiv U$, but with varying positions, i.e., the case of ''structural'' or ''positional'' disorder. An obvious experimental realization of this model is a semiconductor superlattice with fluctuating period.

The case of *compositional* disorder, i.e., a periodic arrangement of sites, $z_n=n$, with random amplitude U_n, has been studied intensively during the last decade. The importance of short-range correlations was explored recently,[5] and a ''random dimer'' model was studied as a specific example.[6] Using this model, it was shown that short-range correlations in the infinite random sequence $\{U_n\}$ give rise to a *discrete* number of delocalized states as well as to some anomalies in transport properties.[7] The presence of such anomalies has been recently observed in experiments with GaAs-AlGaAs random-dimer superlattices.[8] Moreover, the nontrivial role of correlations in the formation of mobility edges has been pointed out by the study of localization in pseudorandom and incommensurate potentials.[9] In contrast, only relatively recently the role of long-range correlations in random potentials has received special attention. The interplay of long-range correlations and disorder has been shown to lead to the existence of a *continuum* of extended states in the energy spectrum and to the appearance of mobility edges.[10,11] These edges have been shown to exist in experiments of microwave transmission in a single-mode waveguide with a random array of correlated scatterers,[12] and their possible relevance for metal-insulator transitions in 2D electron systems has been recently explored.[13]

Localization length for weak disorder. To calculate the localization length $l(E)$ in the case of *structural disorder* we use a Hamiltonian approach.[14] In this scheme, the discrete Schrödinger equation is replaced by a classical Hamiltonian map for coordinate x_n and momentum p_n. For the case of Eq. (2), conjugate variables are introduced as, $x_n=\psi_n$ and $p_n=(x_n\cos\mu_{n-1}-x_{n-1})/\sin\mu_{n-1}$. Correspondingly, the discrete-time evolution of x_n and p_n is obtained from

$$p_{n+1}=(p_n+A_nx_n)\cos\mu_n-x_n\sin\mu_n,$$

$$x_{n+1}=(p_n+A_nx_n)\sin\mu_n+x_n\cos\mu_n. \quad (3)$$

This map describes the behavior of a linear rotator subjected to *nonperiodic* delta-kicks with amplitude $A_n = U_n/q$. Free rotation between kicks corresponds to free propagation between scatterers and each kick corresponds to scattering at each δ-function potential. It is easy to check that the first equation in Eq. (3) is equivalent to Eq. (2), while the second is reduced to an identity after p_n substitution.

In what follows we consider the case of weak disorder, assuming that the deviation of the scatterers from their positions in a periodic lattice is small, $|\delta_n| = q|z_n - n| \ll 1$. We can then expand trigonometric functions in Eq. (3) and up to second order in $\lambda_n = q(\delta_{n+1} - \delta_n)$, obtain the approximate map for constant kick amplitude $A = U/q$,

$$\begin{aligned} p_{n+1} &= \cos q\left[p_n\left(1-\frac{\lambda_n^2}{2}\right)+x_n\left(A-\lambda_n-A\frac{\lambda_n^2}{2}\right)\right] \\ &\quad - \sin q\left[p_n\lambda_n + x_n\left(1+A\lambda_n-\frac{\lambda_n^2}{2}\right)\right], \\ x_{n+1} &= \cos q\left[p_n\lambda_n + x_n\left(1+A\lambda_n-\frac{\lambda_n^2}{2}\right)\right] \\ &\quad + \sin q\left[p_n\left(1-\frac{\lambda_n^2}{2}\right)+x_n\left(A-\lambda_n-A\frac{\lambda_n^2}{2}\right)\right]. \end{aligned} \tag{4}$$

Note that since $\lambda_n \propto q = \sqrt{E}$, this expansion is valid only for low energies.

In order to extract the effect that comes only from the positional nonperiodicity, it is convenient to eliminate the mean field associated with the constant amplitude U. This can be done by a canonical transformation of variables,

$$\begin{aligned} p_n &= \alpha^{-1}\cos\phi P_n - \alpha \sin\phi X_n, \\ x_n &= \alpha^{-1}\sin\phi P_n + \alpha\cos\phi X_n. \end{aligned} \tag{5}$$

The parameters of this transformation (α and ϕ) are obtained from the condition that to zeroth order in λ_n the dynamical map for (P_n, X_n) be a simple rotation without kicks, i.e., $P_{n+1}^{(0)} = P_n^{(0)}\cos\gamma - X_n^{(0)}\sin\gamma$, and $X_{n+1}^{(0)} = P_n^{(0)}\sin\gamma + X_n^{(0)}\cos\gamma$. Applying this condition to Eqs. (5) and (4) we get after some algebra

$$\begin{aligned} &\phi = \tfrac{1}{2}q, \quad \cos\gamma = \cos q + (A/2q)\sin q, \\ &\alpha^4 = 1 + 2A/[2\sin q - A(1+\cos q)]. \end{aligned} \tag{6}$$

It is clear that γ plays the role of the Bloch number in the periodic Kronig-Penney model.[1] We can now rewrite the map (4) in terms of variables (P_n, X_n) and angle γ,

$$\begin{aligned} P_{n+1} &= (1-\lambda_n^2/2)(P_n\cos\gamma - X_n\sin\gamma) \\ &\quad - \lambda_n\alpha^2(P_n\sin\gamma + X_n\cos\gamma), \\ X_{n+1} &= (1-\lambda_n^2/2)(P_n\sin\gamma + X_n\cos\gamma) \\ &\quad + \lambda_n\alpha^{-2}(P_n\cos\gamma - X_n\sin\gamma). \end{aligned} \tag{7}$$

Following our previous approach,[11] it is convenient to introduce action-angle variables for map (7),

$$P_n = R_n\sin\theta_n, \quad X_n = R_n\cos\theta_n. \tag{8}$$

The inverse localization length for the original quantum model Eq. (1) [or equivalently, the Lyapunov exponent for the dynamical map in Eq. (3)], can be expressed in terms of the ratio R_{n+1}/R_n (see details in Ref. 14),

$$l^{-1}(E) = \left\langle \ln\frac{\psi_{n+1}}{\psi_n}\right\rangle = \left\langle \ln\frac{X_{n+1}}{X_n}\right\rangle = \frac{1}{2}\left\langle \ln\frac{R_{n+1}^2}{R_n^2}\right\rangle. \tag{9}$$

Here, $\langle \ldots \rangle = \lim_{N\to\infty} 1/N \Sigma_{n=1}^N(\ldots)$ and exponential localization of quantum states is assumed. Using the map (7) we can calculate the ratio R_{n+1}/R_n as

$$\begin{aligned} (R_{n+1}/R_n)^2 &= 1 - U\lambda_n\sin[2(\theta_n-\gamma)]/(q\sin\gamma) \\ &\quad + \lambda_n^2[\alpha^{-4}\sin^2(\theta_n-\gamma) \\ &\quad + \alpha^4\cos^2(\theta_n-\gamma) - 1]. \end{aligned} \tag{10}$$

The fact that the ratio R_{n+1}/R_n is close to unity for small λ_n is what motivated switching from the variables (p_n, x_n) to (P_n, X_n) using Eq. (5). The logarithm in Eq. (9) can be expanded as $\ln(1+x) \approx x - x^2/2$, and, up to second order in λ_n, the average is performed over the unperturbed motion given by the $(P_n^{(0)}, X_n^{(0)})$ variables. Since this motion is a *free* rotation (in the old variables it is a rotation with *periodic kicks*), the angle variable θ_n is clearly distributed uniformly within the interval $[0,2\pi]$. One then obtains that $\langle \sin^2\theta_n\rangle = \langle \cos^2\theta_n\rangle = 1/2$, and

$$l^{-1}(E) = \frac{\langle\lambda_n^2\rangle U^2}{8q^2\sin^2\gamma} - \frac{U}{q\sin\gamma}\langle\lambda_n\sin[2(\theta_n-\gamma)]\rangle. \tag{11}$$

The first term in Eq. (11) gives the inverse localization length in an uncorrelated random potential. In this Born approximation, it is proportional to the variance $\langle\lambda_n^2\rangle$ and to the squared amplitude of the scattering potential, U^2. Since $\langle\lambda_n^2\rangle \propto q^2$, the factor q^2 disappears and the only energy dependence is due to the factor $\sin^2\gamma$ in the denominator. At the edges of the allowed zones $\sin\gamma = 0$, and here the localization length $l(E)$ approaches zero. A similar enhancement of localization in the vicinity of the band edges[15,16] has stimulated the study of photonic-band-gap materials in the last decade.

The second term in Eq. (11) describes the contribution of correlations in the scattering potential. To calculate explicitly the correlator $\langle\lambda_n\sin[2(\theta_n-\gamma)]\rangle$, one needs the recursion relation for the angle variable θ_n. Since this correlator already contains a factor λ_n, only linear terms in the recursion relation are needed from Eqs. (7) and (8), so that $\theta_n = \theta_{n-1} - \gamma - \lambda_{n-1}[\alpha^2 - U\sin^2(\theta_{n-1}-\gamma)/(q\sin\gamma)]$. The correlator $\langle\lambda_n\sin[2(\theta_n-\gamma)]\rangle$ can be written as a Fourier series in Bloch number γ, where the dimensionless correlators $\xi(k)$ are the Fourier coefficients,[11]

$$\langle \lambda_n \sin[2(\theta_n-\gamma)]\rangle = -\frac{Uq\Delta^2}{2\sin\gamma}\sum_{n=1}^{\infty}\xi(n)\cos(2\gamma n). \tag{12}$$

Here $\Delta^2=\langle\Delta_n^2\rangle$, with $\xi(k)=\langle\Delta_{n+k}\Delta_n\rangle/\Delta^2$, and $\Delta_n=\delta_{n+1}-\delta_n$. Note that the localization length is determined by the statistical properties of the sequence of *relative* displacements Δ_n, and not by the displacements δ_n themselves.

Substituting the correlator (12) into Eq. (11) we get the final result for the inverse localization length

$$\frac{1}{l(E)}=\frac{U^2\Delta^2}{8\sin^2\gamma}\varphi(\gamma),\quad \varphi(\gamma)=1+2\sum_{n=1}^{\infty}\xi(n)\cos(2\gamma n). \tag{13}$$

This formula has the same structure as that obtained for a tight-binding (and the corresponding Kronig-Penney) model with random amplitudes U_n, but equidistant sites ($z_n=n$).[11,12] These three different models have a different dependence on energy via the factors q^2 and $\sin^2\gamma$. The present case exhibits the weakest dependence of the localization length on energy within the allowed zone since a factor $q^2=E$ appears in other cases but not here. This property should be favorable for the experimental observation of mobility edges in superlattices with positional disorder.

Correlations and mobility edge. If the sequence of random displacements Δ_n is uncorrelated, $\xi(k)=0$, the localization length is given by the first term in Eq. (13). In the opposite limit of a completely correlated sequence, $\xi(k)=\text{const}$, the displacements are independent on the site number, $\delta_n=\delta_0$, giving a regular sequence with period $1+\delta_0$, and extended states, $l^{-1}=0$, for all energies. A smooth transition between these two limits can be described by an exponential function, $\xi(k)=\exp(-k/k_0)$, where k_0 is a correlation radius. Substituting this form into Eq. (13) one obtains

$$l^{-1}(E)=\frac{U^2\Delta^2}{8\sin^2\gamma}\frac{\sinh(1/k_0)}{\cosh(1/k_0)-\cos(2\gamma)}. \tag{14}$$

For any finite k_0 *all* states are localized. *Only* in a periodic lattice ($k_0=\infty$) does the inverse localization length (14) vanish and the states become delocalized. This localization-delocalization transition occurs simultaneously for all energies, and a mobility edge does not appear in the spectrum. This conclusion is valid for the arbitrary amplitude of the scattering potential U.[17] A discrete number of delocalized states can in fact appear if the binary correlator $\xi(k)$ oscillates with exponentially decaying amplitude.[18] This can be obtained from Eq. (14), if the correlation radius k_0 is allowed to take complex values. On the other hand, a mobility edge may appear if correlations decay not exponentially but according to a power law.[10–12] We show numerically below that sharp mobility edges exist if, e.g., $\xi(k)\propto 1/k$. For correlators decaying faster than $1/k$ the mobility edges also may exist but they become smoother.

Designed mobility edges. In a real (or numerical) experiment one needs to know explicitly the displacements δ_n which provide a desirable dependence $l(E)$. This leads us to the ''inverse problem'' in the theory of localization. The solution would give us in general a random scattering potential $\{U_n,\delta_n\}$ through the dependence $l(E)$. In the present case of positional disorder, $U_n=U$, we need to calculate only the relative displacements. One can explicitly evaluate the correlator $\xi(k)$ as the Fourier coefficient

$$\xi(k)=\frac{2}{\pi}\int_0^{\pi/2}\varphi(\gamma)\cos(2k\gamma)d\gamma, \tag{15}$$

where the energy dependence of $\varphi(\gamma)=8\sin^2\gamma/[U^2\Delta^2 l(E)]$, is assumed to be known. The energy $E=q^2$ is expressed through γ via the dispersion relation in Eq. (6). It is easy to check that the binary correlator of a sequence $(\Delta_n/\Delta)=\Sigma_{k=-\infty}^{\infty}\beta(k)Z_{n+k}$, coincides with $\xi(k)$ if Z_k are random numbers with zero mean and unit variance, and where the function $\beta(k)$ is given by[11,12,19]

$$\beta(k)=\frac{2}{\pi}\int_0^{\pi/2}\sqrt{\varphi(\gamma)}\cos(2k\gamma)d\gamma. \tag{16}$$

Once the relative displacements Δ_n are known, a sequence of absolute displacements can be easily calculated, setting $\delta_0=0$, for example, and then $\delta_1=\Delta_0$, $\delta_2=\Delta_0+\Delta_1, \ldots, \delta_n=\Sigma_{k=0}^{n-1}\Delta_k$. This procedure allows the calculation of displacements δ_n for *any* energy dependence of the localization length $l(E)$, including situations with mobility edges. Appropriately correlated elements may be used for fabrication of effective filters of electrical or optical signals, even if the system is *not* periodic.[20] The bandwidth of a filter can be made arbitrarily wide or narrow depending on the *statistical properties* of the random sequence used [via the function $\beta(k)$].

Numerical examples. In order to examine our predictions, we construct explicit random sequences $\{\delta_n\}$ for which the function $\varphi(\gamma)$ in Eq. (13) has four mobility edges at $\gamma_i=0.2\pi i$, $i=1,\ldots,4$. The positions of the mobility edges are chosen within the interval $0<\gamma<\pi$, symmetrically about $\gamma=\pi/2$. Via relation (6), the position of the mobility edges on the axis q/π are given by 0.326, 0.478, 0.649, and 0.850, for the mean-field amplitude $U=0.7$. In the ideal lattice with the same strength of the potential, the first allowed band lies between $q_l/\pi\approx 0.26$ ($\gamma=0$) and $q_r/\pi\approx 1$ ($\gamma=\pi$). Numerical data are given for two complimentary situations $\varphi_{1,2}(\gamma)$: φ_1 vanishes [i.e., $l(E)=\infty$ and states are delocalized] in the region $\gamma\in(0,\gamma_1)\cup(\gamma_2,\gamma_3)\cup(\gamma_4,\pi)$; while φ_2 vanishes in the complementary region $\gamma\in(\gamma_1,\gamma_2)\cup(\gamma_3,\gamma_4)$. Outside these regions, the function $\varphi_{1,2}(\gamma)$ is a constant defined by the normalization condition $\xi_{1,2}(0)=1$. From Eq. (15), we get that because of the presence of sharp mobility edges the correlators (Fourier components of a discontinuous function) decay slowly:

$$\xi_1(k)=-1.5\xi_2(k)=(5/2\pi k)[\sin(0.8\pi k)-\sin(0.4\pi k)]. \tag{17}$$

We show the corresponding data in Figs. 1 and 2 for $U=0.7$. The analytical dependence (13) for the dimensionless inverse localization length $\Lambda=8/l(E)U^2\Delta^2$ is shown by the full lines for $\Delta=0.05$ in the figures. Numerical data are obtained for a large sample size $N=10^6$, with two amplitudes

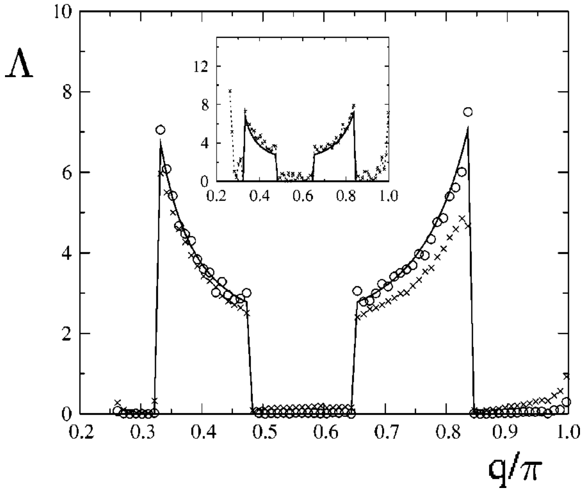

FIG. 1. Inverse localization length for band with four mobility edges, three regions of extended states, and different amplitude of disorder: circles (○), $\Delta=0.05$; crosses (×), $\Delta=0.15$. Solid lines show Eq. (13) for $\Delta=0.05$. Inset shows $N=10^3$ sites averaged over only 100 samplings.

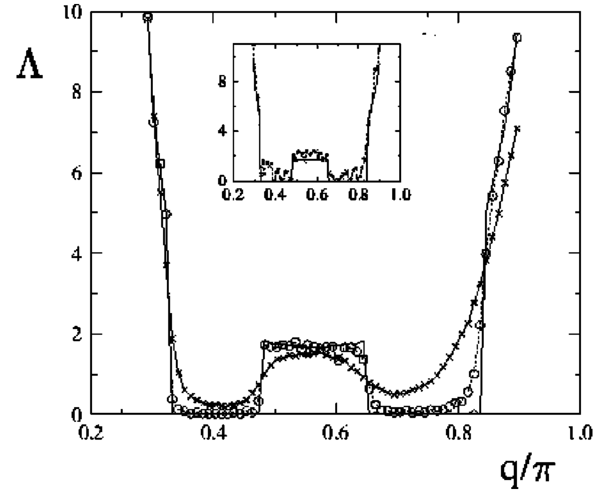

FIG. 2. Results for complementary system to Fig. 1, with four mobility edges but only two regions of extended states. Lines through circles ($\Delta=0.05$) and crosses ($\Delta=0.15$) are guides to the eye.

of disorder, $\Delta=0.05$ (circles) and $\Delta=0.15$ (crosses). The insets show results for a much shorter sample, $N=1000$, with additional average over 100 different realizations of disorder but the same correlations. One can see that for small disorder, $\Delta=0.05$, Eq. (13) describes the numerical results very well, with only minor deviations close to the onset of mobility q_i and band edges, $q_{l,r}$. Notice that Eq. (13) is excellent at giving the mobility edges at the prescribed energies, which proves its usefulness, and breadth of applicability.[21]

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