Localization by Pseudorandom Potentials in One Dimension

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Localization in one dimension in the presence of a pseudorandom potential is investigated. The localization length of the tight-binding model $V_n u_n + u_{n+1} + u_{n-1} = E u_n$ with $V_n = \lambda \cos \pi \alpha |n|^\nu$ is calculated numerically and in perturbation theory for $\lambda \ll 1$, for generic values of α and ν. The similarity between the potential V_n and random potentials increases with ν. It is found that for $\nu \geq 2$ all the states are localized and the localization length is equal to that of the corresponding random model while for $0 < \nu \leq 1$ there are extended states. The intermediate regime $1 < \nu < 2$ is discussed as well.

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It is well known that in one dimension, in the presence of a random potential, all the states are localized.[1,2] This localization is a quantum mechanical phenomenon and takes place for arbitrarily weak random potentials, if the hopping is of a sufficiently short range. In this Letter localization in the presence of pseudorandom potentials will be studied. These are well-defined potentials that exhibit some properties of random ones. Such properties are, in particular, ergodicity and the absence of correlations between the potential at various sites. Ergodicity does not imply localization as is well known from the studies of Harper's equation with an incommensurate potential.[3,4] We will see that the correlations between the values of the potential at various sites determine its localization properties.

Pseudorandom potentials were encountered in the analysis of the quantal behavior of the kicked rotor,[5,6] which is the simplest driven quantum mechanical system that is chaotic in the classical limit.[7,8] Therefore it is representative of a family of problems of experimental relevance, such as molecular[9] and atomic[10] beam experiments as well as the behavior of mesoscopic systems.[11] Superlattices with various periods can be fabricated and their electronic localization properties are expected to be related to those of random systems.[12]

In what follows we will study the nearest-neighbor tight-binding model

$$V_n u_n + u_{n+1} + u_{n-1} = E u_n, \tag{1}$$

where u_n is the amplitude of the wave function on the nth site of a one-dimensional chain, V_n is the diagonal potential, and E is the energy. It will be assumed that the diagonal potential is

$$V_n = \lambda \cos \phi_n, \tag{2}$$

with

$$\phi_n = \pi \alpha |n|^\nu. \tag{3}$$

For $\nu = 1$ it is just Harper's equation. It represents the crystalline solid if α is rational, and an incommensurate potential if it is irrational.[4] Therefore, for $\nu = 1$ and α irrational, the states are extended for $\lambda < 2$ and localized for $\lambda > 2$, as was found by Aubry and Andre,[3] Sokoloff,[4] and Simon.[4] If $\{\phi_n\}$ is truly random, then (1) is the one-dimensional Anderson model for localization where all the states are localized.[2] It was shown that a model like (1) where V_n is replaced by $\bar{V}_n = \tan(\pi \alpha n^2 - \omega)$ (ω is a phase) and $E = 0$ corresponds to a kicked rotor.[6] It was argued that $\{\bar{V}_n\}$ is effectively random leading to Anderson localization, and the argument was verified by numerical calculations.[5,6] One may suspect that for this model the localization results from the fact that the tangent is unbounded rather than from typical interference effects.[13] In particular, it will be shown that for the model (1)–(3) with $\nu = 2$ all the states are localized. This result supports the assumption that Anderson localization takes place for the kicked rotor as well. It is reasonable to expect that for an irrational α the pseudorandomness of the sequence $\{V_n\}$ will increase with ν. The reason is that the rate of growth of ϕ_n with n increases with ν (for $\nu > 1$). The potentials V_n depend only on $\phi_n \bmod 2\pi$, that are small fractions of large numbers with rapidly growing differences among them. In what follows these arguments will be stated in more quantitative terms. Consequently, for the model that is defined by (1)–(3), the degree of pseudorandomness is controlled by the parameter ν. This model will be analyzed for irrational α in the regime $\lambda \ll 1$ in the framework of perturbation theory[14,15] in λ. Some subtleties encountered in random systems[16] may be found also in our model, but such refined questions will not be addressed in this work. Since the diagonal potential tends to localize the states, it is reasonable that if states are localized for small λ, localization persists for larger values of λ as well. The full "phase diagram" in the (λ, ν) space will be published elsewhere.[17]

To the second order in the strength of the diagonal potential the localization length ξ satisfies

$$\gamma = \lim_{N \to \infty} \frac{\lambda^2}{8 \sin^2 \theta} \frac{1}{N} |S_N|^2, \tag{4}$$

where $\gamma=1/\xi$ and $S_N=\frac{1}{2}(S_N^+ + S_N^-)$ with

$$S_N^{\pm}=\sum_{n=0}^{N} e^{\pm i\phi_n+2in\theta}. \tag{5}$$

The energy of the unperturbed problem, that is defined by (1) with $\lambda=0$, is $E=2\cos\theta$. The approximation (4) should hold for a weak potential and for energies that are sufficiently far from the band edges $\theta=0$ and $\theta=\pi$. It can be derived following the derivation that was used by Thouless for the Schrödinger equation in the differential form. The only difference is that the unperturbed Green's function is $G_{nr}^0=\frac{1}{2}i\exp(i\,|n-r\,|\,\theta)/\sin\theta$, rather than (11) of Ref. 14. The equation corresponding to (4) was derived by Thouless[14,15] for a random potential V_n, but randomness is not required for the derivation. For large N, the randomness of $\{V_n\}$ implies $|S_N|^2\sim N$ and consequently the localization length is finite. For the potential V_n of (2) with $\nu=1$ and α irrational, S_N is bounded and consequently γ vanishes and the states are extended in agreement with well-known results.[3,4] Within the leading order in perturbation theory, Eq. (4) implies that the "random walk" property of S_N, namely $|S_N|^2\sim N$, for large N implies exponential localization. This is a property of random potentials but it may be shared by a much wider class of pseudorandom potentials.

The asymptotic behavior of S_N (and $S_N^{\pm}$) for $\nu=2$ and irrational α was analyzed in detail by Hardy and Littlewood.[18,19] They proved that $S_N\sim\sqrt{N}$ for large N, namely

$$S_N=O(\sqrt{N}) \quad \left[\lim_{N\to\infty} S_N/\sqrt{N}=\text{const}\right].$$

For integer values of $\nu>2$ a result that is mathematically weaker but is similar for our purposes, namely $S_N=o(N^{1/2+\epsilon})$, with ϵ arbitarily small, was established

$$\left[\lim_{N\to\infty} S_N N^{-1/2-\epsilon}=0\right].$$

Since the pseudorandomness of the terms in the sum S_N increases with ν, it is reasonable to assume that $S_N\sim\sqrt{N}$ for all $\nu\geq 2$ (for generic ν and α). Moreover, if the phases $[\phi_n\pm 2n\theta]\mathrm{mod}2\pi$ can be considered random, one finds

$$|S_N|^2=\tfrac{1}{2}\,|S_N^{\pm}|^2=\tfrac{1}{2}N+o(N). \tag{6}$$

In order to estimate S_N^+ (or S_N^-) for $1<\nu<2$ it can be rewritten with the help of the Poisson summation formula in the form

$$S_N^+=\sum_{m=-\infty}^{\infty}\int_0^N dn\exp[i\pi\alpha n^{\nu}-2i\pi mn+2in\theta]. \tag{7}$$

Since we are interested in the large-N behavior, the integrals can be estimated by the method of stationary phase. The resulting estimate is

$$S_N^+=A\sum_{m=0}^{M} m^{\beta/2}\exp[i\pi\alpha' m^{\nu'}], \tag{8}$$

with $\nu'=\nu/(\nu-1)$ and $\beta=(2-\nu)/(\nu-1)$, while $\alpha'=\alpha B^{\nu'}-2B^{1/(\nu-1)}$, and $M=N^{\nu-1}/B$ with $B=2/\alpha\nu$. The proportionality constant is $A=B^{\beta/2}[\alpha\nu(\nu-1)]^{-1/2}(1+i)$. Since we are interested in the asymptotic behavior of the sum, θ was neglected relative to m in (8). Note that $\nu'>2$ for $1<\nu<2$; therefore, following our assumptions, the phase of the exponential of (8) can be considered random if α' is a generic irrational number. Therefore, to the leading order in N it is found that

$$|S_N|^2=\tfrac{1}{4}\,|S_N^+ + S_N^-\,|^2=\tfrac{1}{2}\,|A\,|^2\sum_{m=0}^{M} m^{\beta}=\frac{N}{2}. \tag{9}$$

Therefore for $\nu>1$, for nearly all values of α the asymptotic form (6) holds. For $0<\nu<1$, following the derivation of (8) one can show that the sums $S_\infty^{\pm}$ are bounded, away from the band edges $\theta=0$ and $\theta=\pi$. We conclude that in the framework of the second-order perturbation theory,

$$\gamma=\tfrac{1}{16}\lambda^2/\sin^2\theta\equiv\tilde{\gamma} \text{ for } \nu>1,$$
$$\gamma=0 \text{ for } 0<\nu\leq 1. \tag{10}$$

The states are localized for $\nu>1$ and extended for $0<\nu\leq 1$. The value of γ for $\nu>1$ is identical to the one that is found if ϕ_n is random and uniformly distributed in the interval $[0,2\pi]$.

We turn now to characterize the potential V_n in terms of its pair correlations. For this purpose (4) is rewritten in the form

$$\gamma=\lim_{N\to\infty}\frac{\lambda^2}{8\sin^2\theta}\left[C_0^N+2\sum_{r=1}^{N} C_r^N\cos 2r\theta\right], \tag{11}$$

where

$$C_r^N=\frac{1}{N}\sum_{n=0}^{N-r}\cos\phi_{n+r}\cos\phi_n. \tag{12}$$

In the limit $N\to\infty$, the C_r^N approach the pair correlation function

$$C_r=\lim_{N\to\infty}\frac{1}{2N}\left[\sum_{n=0}^{N}\cos(\phi_{n+r}-\phi_n)+\sum_{n=0}^{N}\cos(\phi_{n+r}+\phi_n)\right]. \tag{13}$$

The terms in this equation are averages over sequences of N terms. If the phase of the cosine is ergodic these averages can be replaced by the average of the cosine with respect to its phase. For $\nu>0$ the second term is always ergodic and

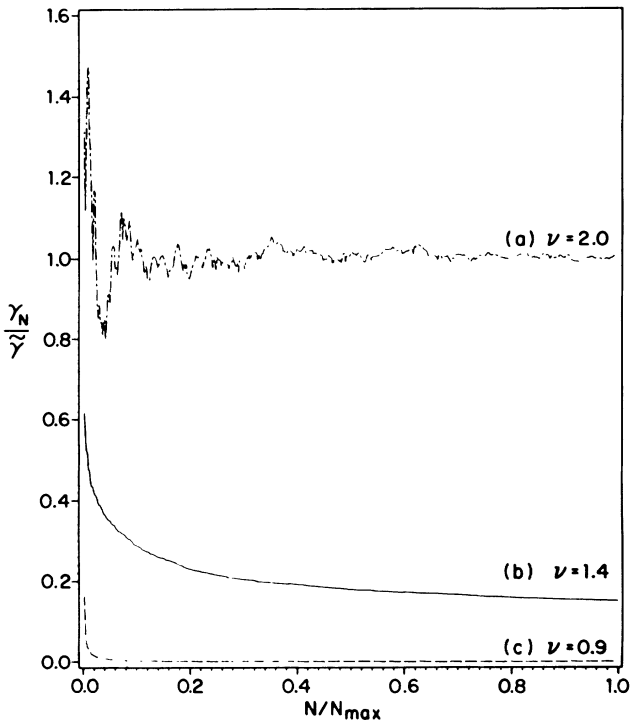

FIG. 1. The numerical value of the inverse localization length γ_N as function of the number of iterations N for $\lambda=0.1$, $\pi a=3.5$, $E=0$, and (curve a) $\nu=2.0$, $N_{\max}=10^7$; (curve b) $\nu=1.4$, $N_{\max}=10^8$; (curve c) $\nu=0.9$, $N_{\max}=10^7$. $\tilde{\gamma}$ is the theoretical value (10).

therefore its contribution vanishes. The first term is ergodic for $\nu>1$ while for $\nu<1$ its phase tends to zero, namely

$$\lim_{n\to\infty}[\phi_{n+r}-\phi_n]=0.$$

Therefore the pair correlation function is $C_r=\frac{1}{2}\delta_{0r}$ for $\nu>1$ and $C_r=\frac{1}{2}$ for $\nu<1$, while $C_r=\frac{1}{2}\cos\pi a r$ for $\nu=1$. Substitution in (11) leads to the result (10). For $\nu<1$ this result is found with the help of the Poisson summation formula. For $\nu<1$ it holds except for an energy for which $2\theta=\pi a$. This calculation of the localization length which required the interchange of the order of summation is allowed only if the sums are absolutely convergent. The results agree, however, with those obtained by direct estimation of the sums (6)–(9).

In order to test the analytic predictions of the perturbative calculation, the localization length was calculated numerically. For this purpose $z_n=u_{n+1}/u_n$ were found iteratively from (1) with some arbitrary initial conditions u_0 and u_1. The approximation of the inverse localization length is

$$\gamma_N=\frac{1}{N}\sum_{n=1}^{N}\ln|z_n|.$$

The typical dependence of γ_N on N is depicted in Fig. 1.

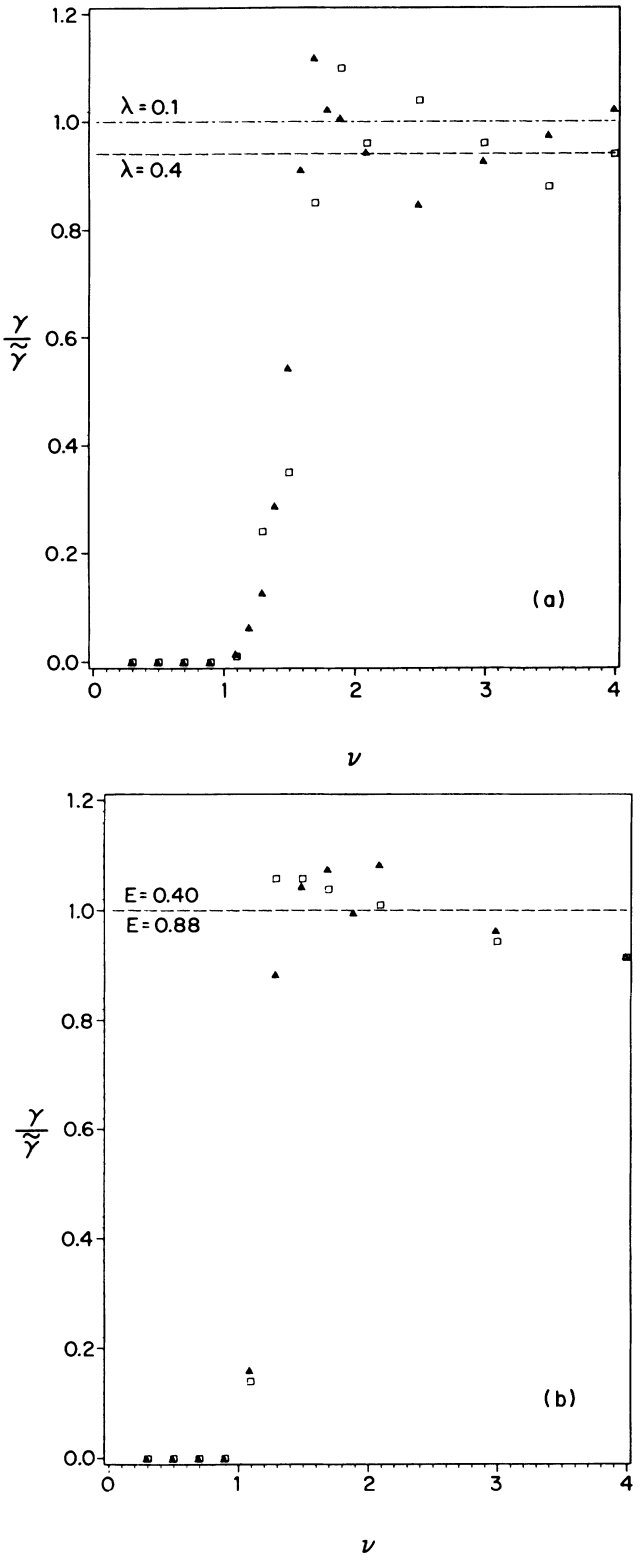

FIG. 2. The inverse localization length γ as a function of ν for (a) $E=0$, $\lambda=0.1$ (triangles) and $\lambda=0.4$ (squares); as well as for (b) $\lambda=0.4$, $E=0.4$ (squares) and $E=0.88$ (triangles). The dashed lines show the value of $\gamma/\tilde{\gamma}$ for the corresponding model where $\{\phi_n\}$ of (2) is random.

The number of iterations N_{max} in each calculation is such that γ_N converges to a constant that approximates the inverse localization length γ. The line a is typical for $\nu > 1.7$ and $E = 0$ where γ converges rapidly to finite values, while c is typical for $\nu < 1$ where rapid convergence to zero takes place. For $1 < \nu \leq 1.7$, γ seems to approach a finite value extremely slowly as demonstrated by b where $N_{max} = 10^8$. We cannot rule out from our numerical results the possibility that γ vanishes for these values of ν. The dependence of γ on ν is presented in Fig. 2. It is demonstrated that for $\nu > 1.7$ and $E = 0$ the value of $\gamma/\tilde{\gamma}$ is in good agreement with the analytical result of (10), namely $\gamma/\tilde{\gamma} = 1$. It is also in agreement with the values that are found for the corresponding model, where $\{\phi_n\}$ is random. For $\nu < 1$ it is found that $\gamma = 0$ in agreement with perturbation theory. In the intermediate regime $1 < \nu \leq 1.7$, the numerical results disagree with the prediction of perturbation theory (10). For $E \neq 0$ the behavior is qualitatively similar to the one that is found for $E = 0$. But the behavior is similar to that of a random system for $\nu > 1.3$ (rather than $\nu > 1.7$ for $E = 0$).[20]

For $\nu \leq 1$, correlations of long range are present and the states are extended. For $\nu \geq 2$, the pair correlations, as well as correlations of higher order, are short ranged and all the states are localized with a localization length that is equal to that of the corresponding random model. For a weak diagonal potential it can be calculated from a perturbation expansion that is similar to the one that is applicable to random systems. In both regimes, $\nu \leq 1$ and $\nu \geq 2$, the numerical results are in agreement with those that are obtained from perturbation theory. In the intermediate regime there is a clear disagreement between the numerical and the perturbative results. In this regime the pair correlations are short ranged, but fourth-order correlations of long range are present.[17]

For $1 < \nu < 2$ there is a clear discrepancy between Eq. (10) and the numerical results, in particular for $E = 0$. It is possible that the perturbative calculation fails because terms of order λ^4 are affected by the fourth-order correlations, that are of long range for $\nu < 2$. This disagreement may result also from the fact that S_N, and consequently γ, are dominated by sparse, narrow regions [see Eq. (8)] with separations, that exceed the localization length. It is possible that accumulation of errors in the numerical calculations, when it is combined with this sparsity, makes them inaccurate.[20] Further investigation of these problems is required.

We believe that the localization properties that are reported in this Letter are quite general for models of the form (1), and are relevant also for potentials that are not of the specific form (2) and (3).

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[20]David Thouless derived Eq. (10) for $1 < \nu < 2$ and $E \neq 0$ [under assumptions leading to Eq. (9)] in a different way. He alerts us to the possibility that its disagreement with the numerical results is due to accumulation of numerical errors.