Mobility Edge in a Model One-Dimensional Potential

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We show that a one-dimensional tight-binding electron moving in a slowly varying potential, $V_n=\lambda\cos(an^\nu)$, where n is the site index and $0<\nu<1$, has a mobility edge in its spectrum provided that 2λ is smaller than the total unperturbed bandwidth of the system. We study the nature of the localized and extended eigenstates of this system as a function of λ and ν.

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The motion of an electron in a one-dimensional lattice as described by the nearest-neighbor tight-binding equation

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

is a paradigm in condensed-matter physics. In Eq. (1), u_n is the amplitude of the wave function at the nth site, V_n is the on-site diagonal potential, and E is the energy. For periodic V_n Bloch's theorem gives extended band states. Specifically for $V_n=0$, Eq. (1) is trivially solved with $u_n=u_0e^{in\theta}$, giving rise to the one-dimensional tight-binding energy band $E=2\cos\theta$ with $0\le\theta\le\pi$. For random V_n, Eq. (1) is the Anderson model[1] with localized states as the only allowed solutions. It is well known[2] that in one-dimensional systems with any diagonal randomness all states are localized and there is no mobility edge separating localized and extended states. There is a class of pseudorandom and incommensurate potentials lying in between the random Anderson model and the periodic Bloch model which have attracted a lot of recent attention.[3-10] A very simple model to study such potentials is given by[7,8]

$$V_n=\lambda\cos(\pi an^\nu)\,, \tag{2}$$

where λ, a, and ν are positive numbers which completely define the tight-binding problem. For a rational and ν an integer, we get back the periodic Bloch model, whereas it has been shown[7] that for a irrational and $\nu\ge 2$, the pseudorandom tight-binding model defined by Eqs. (1) and (2) becomes equivalent to a corresponding random Anderson model with all the states localized and the localization length equal to that of the corresponding random model. For $\nu=1$ and a irrational, Eqs. (1) and (2) define Harper's equation with an incommensurate potential which has been studied extensively in the last few years.[3,4] For this situation ($\nu=1$, a irrational) the model has either all extended or all localized states depending on whether λ is smaller or larger than 2, the $\lambda=2$ case being the self-dual point discovered by Aubry[3,4] where all the states are critical.

We have studied the model defined by Eqs. (1) and (2) for arbitrary values of ν in the range $0<\nu<2$ and for arbitrary irrational a. In particular, we find that for $0<\nu<1$ there exists a mobility edge in this one-dimensional problem provided that $\lambda<2$. Thus for $0<\nu<1$ (and for $\lambda<2$) we find extended states in the middle of the band ($|E|<2-\lambda$) and localized states at the band edge ($2+\lambda>|E|>2-\lambda$), with the mobility edge at $E_c=\pm(2-\lambda)$. For $\lambda>2$ all states are found to be localized. For $\nu>1$ our results are consistent with Thouless's recent finding[8] that all states away from the exact band center are localized even though the localization length could be very large at the band center; in particular, Thouless showed that the Lyapunov exponent approaches zero extremely slowly at the band center, $E=0$. We differ with the recent perturbative conclusion[7] of Griniasty and Fishman (for $\nu<1$) who studied only the band-center states, found them to be extended, and concluded that *all* states are extended for $\nu<1$ at least within the perturbation theory. As we show in this paper, for $\nu<1$ there are localized states near the band edge, separated from the extended states near the band center ($E=0$) by a mobility edge. We emphasize that our conclusions, in contrast to the results obtained in Ref. 7, are based on exact numerical calculations on small systems and *not* perturbation theory (we also provide a semiclassical theoretical argument in support of our numerical results).

Our discovery of a mobility edge in this one-dimensional problem is quite interesting because the popular wisdom has been that one-dimensional models, particularly in the gapless spectrum of a one-dimensional Schrödinger operator, do not allow for the existence of a mobility edge.[2] It is all the more surprising that a mobility edge exists (for $\nu<1$ and $\lambda<2$) in a model as simple as the one defined by Eqs. (1) and (2). In this Letter we will report our results for the mobility edge in the $0<\nu<1$ regime. Details of the localization phase diagram with results for other values of ν will be given in a forthcoming longer publication. Our numerical results have been obtained by direct diagonalization of the tight-binding Hamiltonian up to a system size of 20000 sites. In addition, we have verified a number of our results by calculating the localization length using the recursive transfer matrix technique for systems of up to 10^6 sites. We believe that our numerical evidence in

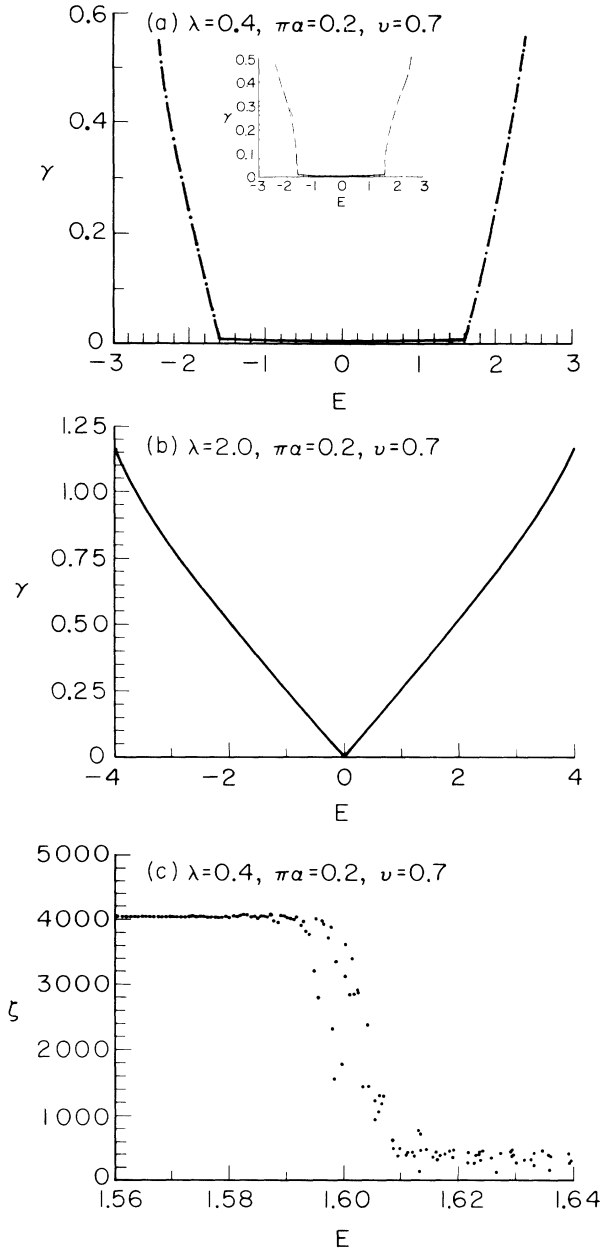

FIG. 1. (a),(b) The "inverse localization length" γ defined by $\gamma(E_\alpha)=(N-1)^{-1}\sum_{\beta\neq\alpha}\ln|E_\beta-E_\alpha|$ as a function of eigenenergy $E\equiv E_\alpha$ for the cosine model (N = total number of sites). Inset of (a): γ for the square-well model. (c) The correlation length ξ defined in the text as a function of E for the cosine model.

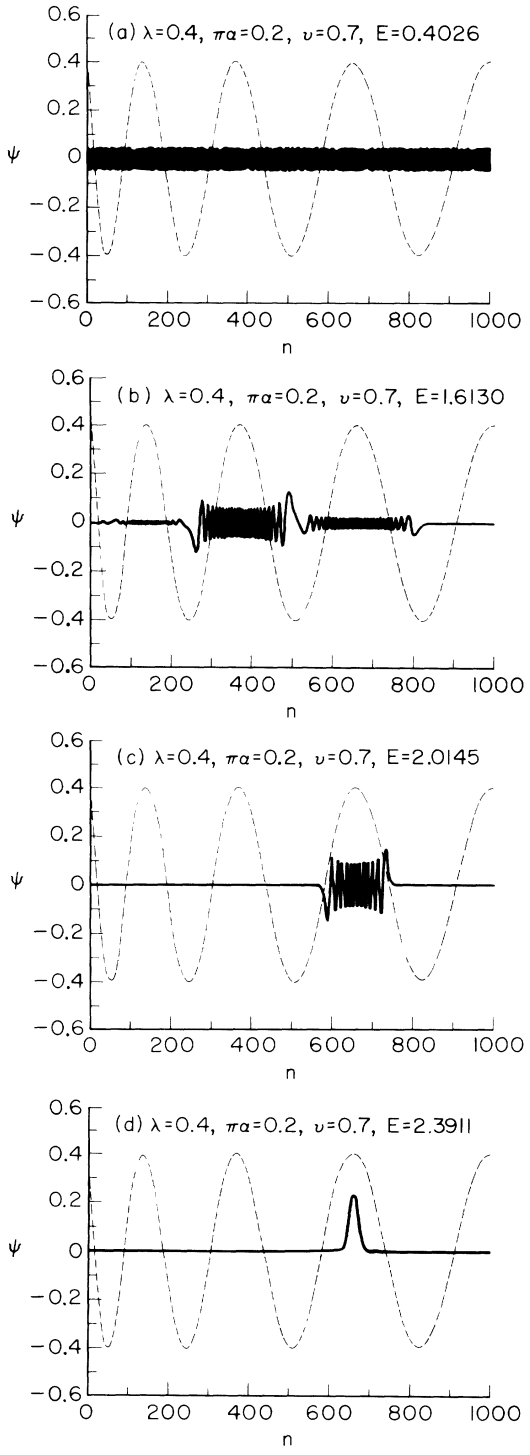

FIG. 2. Some typical (a) extended and (b)–(d) localized eigenstates for the cosine potential, which itself is shown as the dashed line.

support of the existence of a mobility edge for this model potential is quite compelling.

In Figs. 1(a) and 1(b) we show our calculated *inverse* localization length γ as a function of the electron energy E for $\pi\alpha=0.2$, $\nu=0.7$, and $\lambda=0.4$ and 2.0, respectively. The mobility edges for the two cases are clearly at $E_c=\pm 1.6$ and 0, respectively. For all values of $0<\lambda<2$ we find the mobility edge to be located at $|E_c|=2-\lambda$, whereas for $\lambda>2$ we find all states to be localized. The dependence of γ on E for other values of α, ν, and λ is very similar to that shown in Fig. 1(a). In Fig. 1(c) we show the localization correlation length ξ which is defined as

$\int_{-\xi/2}^{\xi/2} |u(x-x_0)|^2 = P$, where x_0 is the center (*the peak*) of the wave function and P is a preassigned number very close to unity. We choose $P=0.99$ for this figure (we have varied P systematically between 0.95 and 0.99 to check our results). For extended states, ξ will span the whole system whereas for localized states ξ will typically be the size of the localization length. We see the existence of a mobility edge around $E_c = 2-\lambda$ in the ξ-E plot. This is again a typical result for $\xi(E)$ as long as $\lambda < 2$ and $\nu < 1$.

In Figs. 2(a)–2(d) we show some typical localized and extended eigenstates for the model. As one would expect, a state just above E_c is less localized than a state near the band edge $(2+\lambda)$. The extended state at an energy $E < E_c$ is clearly extended over the whole system.

We can understand the behavior shown in Figs. 1 and 2 on the basis of the following simple argument. We emphasize that our arguments are of rather heuristic nature. For large n, V_n defined by (2) is very slowly varying and can be regarded as a constant *locally*. Then the tight-binding Eq. (1) becomes $u_{n+1}+u_{n-1} = (E - V_n)u_n \equiv C_n u_n$, where $C_n \approx C$ is locally a constant. The condition for a complex solution (i.e., locally extended) to this equation is that $|C_n| < 2$, whereas for $|C_n| > 2$ the local solution is real (exponentially decaying or growing). Since $|V_n|^{\max} = \lambda$, it follows that $|E| > 2-\lambda$ or $< 2-\lambda$ produces, respectively, a locally (exponentially) localized or extended (i.e., a trigonometric solution) eigenstate. These locally extended or localized states are, in fact, globally localized (as is clearly seen in our numerical work) because of the incommensurate nature of the potential. Alternatively, if we construct the continuum version of the equation defined by (1) and (2), it is easy to see that for large n states with $|E| < 2-\lambda$ are all extended and with $|E| > 2-\lambda$ are all localized. We believe that the states for $|E| > 2-\lambda$ remain localized globally because the incommensurate nature of the very slowly varying potential defined by Eq. (2) ensures that no energy degeneracy exists in the problem—in fact, the wave-function overlap decays exponentially whereas the energy spacings between neighboring wells decrease algebraically ruling out the possibility of any resonance. It is easy to show that the wave-function overlap between neighboring localized states goes down as $\exp(-\gamma N^{1-\nu})$ (where N is the total number of sites) whereas the energy spacings decrease as a power law of N. Thus, locally localized states remain globally localized in the large-N limit. We, therefore, conclude that there is a mobility edge at $|E| = E_c = 2-\lambda$, consistent with our numerical results. Note that our argument applies only for $\nu < 1$ (so that for large n, the potential is locally a constant). From the same argument it also follows that for $\lambda > 2$ all states are localized for this system. We also note that there are no eigenstates for the model with $|E| > 2+\lambda$. We have numerically calculated the localization exponent β defined by

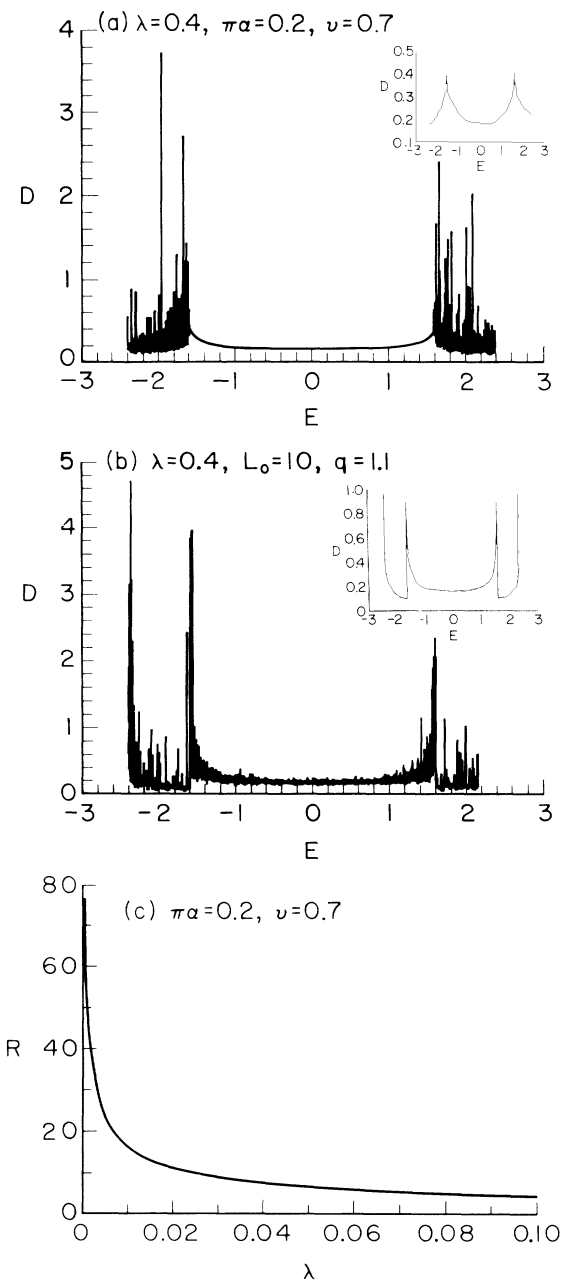

FIG. 3. (a) The density of states (DOS) for the cosine model. Inset: The average DOS which is obtained by averaging over the nonrelevant parameter α. A logarithmic divergence is observed at $E = E_c$. (b) The DOS for the square-well model. In the inset, we show the average DOS (by averaging over q). A square-root divergence at the mobility edge is found in this case. (c) The ratio of the number of extended states to the number of localized states as a function of λ in the cosine model. A square-root divergence is found at $\lambda = 0$.

$\gamma \sim |E - E_c|^{\beta}$ and our numerical value of β for Fig. 1 is 1.0 ± 0.1.

To check the above analytic ideas we calculate the localization exponent for a system where the potential bar-

riers are square-well-like. We choose a model potential which is piecewise constant (locally square-well-like) and with a constant depth 2λ, but with variable well widths L_n defined by $L_n = q^n L_0$, where $L_0 = 10$, $q = 1.1$. The variable well width ensures that no exact energy degeneracy exists and, clearly, the same considerations as above apply to this model as well except that the assumption of locally constant potential is a better approximation for this model even for small n. For this model, the above simple considerations show that $\beta = \frac{1}{2}$. In the inset of Fig. 1(a) we show our calculated inverse localization length γ for this model and our numerically calculated value of the localization exponent is $\beta = 0.5 \pm 0.05$ in agreement with the theoretical consideration. The eigenstates for this square-well model look very similar to those shown in Fig. 2 with the mobility edge at $E_c = 2 - \lambda$.

In Fig. 3 we show our calculated density of states for the cosine and the square-well potentials, respectively. As insets we also show the average density of states for the two cases. Finally, in Fig. 3(c) we show, as a function of λ, the ratio of the number of extended to localized states—we have verified that this result is independent of the system size. Clearly, a mobility edge exists for $0 < \lambda < 2$. It is interesting to point out that the average density of states seems to have a singularity at $E = E_c$ in this model (unlike the random Anderson model where the density of states is thought to be smooth through E_c). Our numerical results indicate that the average density of states diverges at E_c as $(E - E_c)^{-1/2}$ or $\ln|E - E_c|$ for the square-well-like and the cosine potentials, respectively.

Before concluding, we point out that the model potential defined by Eq. (2) (or, its square-well counterpart) is inhomogeneous in space which makes it different from most other localization problems studied in the literature. A rigorous understanding of the localization length and of the structure of the mobility edge in the thermodynamic limit for such an inhomogeneous problem requires subtle mathematical considerations which are lacking at the present time. What we hope to have established in this paper is that the model defined by Eqs. (1) and (2) is a class of one-dimensional problems which allow for the existence of a mobility edge. We find this interesting and hope that this paper will motivate further work on this model, particularly along the line of obtaining rigorous results.

We conclude by pointing out that it is, in fact, feasible to construct a *finite* experimental system very closely corresponding to the model of Eqs. (1) and (2)—this would be the plasmon spectrum in artifically constructed semiconductor superlattices[10] where suitable doping can mimic the potential of Eq. (2). In the plasmon problem,[10] the hopping is of longer range; however, we have explicitly verified that adding a next-nearest-neighbor hopping term to Eq. (1) does not change our results. Thus, the mobility edge predicted in this paper should be observable via Raman scattering experiments in suitably constructed semiconductor superlattices. We will report details of our numerical work in a longer publication.

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