Localization in an Almost Periodically Modulated Array of Potential Barriers

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It is argued that an array of potential barriers modulated in position and strength in a manner incommensurate with the barrier spacing can be replaced by a δ-function Kronig-Penny model. With this equivalence it is shown, with use of renormalization-group arguments as well as known results from other calculations, that this model possesses both localized and extended states separated by mobility edges.

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Recently there has been a good deal of interest in the problem of the nature of electronic states in an almost periodic potential (APP). This interest is due in part to the connection with the problem of two-dimensional electronic systems in a magnetic field[1] and to that of electrons in a random potential.[2] It is well known that a two-dimensional (2D) solid in a magnetic field can be mapped to a one-dimensional tight-binding model for an electron in a sinusoidal potential with period which can be incommensurate with that of the lattice.[3] Since the wave vector of the sinusoidal potential is proportional to the number of magnetic flux quanta through a unit cell of the 2D system, it is usually extremely small, for the values of the fields easily obtainable in the laboratory. It is known, however, that for a two-dimensional metallic system, a strong magnetic field can aid in the formation of a Wigner lattice or charge-density wave and the unit cell of the Wigner lattice can be large enough to contain a sufficiently large magnetic flux to make the effects observable.[4] Furthermore, regarding the relationship to the random-potential problem, APP are potentials that lack translational invariance; yet they are not disordered in the usual sense because there can be distances over which the potential almost repeats.[2] In fact work by several authors, including one of the present authors, has indeed shown that an APP represents a case intermediate between random and periodic.[2,3] It is well known that in a 1D disordered system almost all states are localized.[5] In a periodic potential there are regions in energy for which the states are completely extended. In an APP, however, there can be both extended and localized states, with the possibility of a metal-insulator transition at a critical value of the potential strength. This would seem to indicate that if there is a lower critical dimensionality in the APP problem it should be smaller than 1. Although there can be extended states in an APP,[2,3] the spectrum is not the usual band structure that occurs in the periodic case. Rather, as proven by Avron and Simon for Aubry's tight-binding *one-band* model, the spectrum is singular continuous.[6] Intuitively we can understand this from the fact that a gap can occur at one half of any reciprocal lattice vector, and for an APP every possible linear combination of the periods of these potentials with integer coefficients is a reciprocal lattice vector. Since the periods are incommensurate, by taking linear combinations with appropriate integer coefficients, we can construct a reciprocal lattice vector arbitrarily close to any value, and hence a band gap can occur arbitrarily close to any wave vector. In Ref. 2b it has been argued that while the spectrum can be Cantor-set like in the region of extended states, most of the gaps are negligible, making the band structure appear like that of an ordinary periodic system.

Hogg and Huberman have recently extended work by Romerio which claims to prove that all states in an APP are extended.[7] The model considered in Ref. 7 is that of a *continuous* Schrödinger equation with an APP. Since most of the studies to date on APP systems, which give localized states, have been on either one-band approximation or δ-function potential models, the possibility always exists that the localization found is specific to these models. Without arguing about the correctness of the mathematical proof given in Ref. 7, we show that for a fairly general almost periodic array of noninfinite potential barriers, localized and extended states exist.

Let us start by considering APP's which consist of a chain of arbitrary potential barriers of finite height. We assume that between adjacent barriers there is some point or line on which the potential is zero. This class of potentials represents a case of high physical interest. We shall restrict our discussion initially to potential

barriers symmetric about their maxima but will argue later on that this restriction is not essential. Let us first consider equally spaced potential barriers with lattice constant a and with the strength of the potential at a point x proportional to a periodic function $f(na)$ of period λ. Here na is the location of the maximum of the nth potential barrier (which we take to be the barrier on which x falls) and λ is a period incommensurate with the lattice of potential barriers (i.e., a/λ is an irrational number). Since our potential barriers are symmetrical, the transmission and reflection amplitudes for waves incident on the right and the left are equal. Hence the transfer matrix for a single barrier has the form

$$\begin{pmatrix} 1/t^* & r/t \\ r^*/t^* & 1/t \end{pmatrix}, \tag{1}$$

where r and t are the reflection and transmission amplitudes, respectively. Following an argument given by Borland, the symmetric potential barrier can be replaced by a δ-function placed at the barrier's center with the strength chosen to give the above transmission matrix.[8] According to Borland, the strength of the nth δ-function potential must be chosen to be equal to $\beta_n = 2k|r_n|/|t_n|$, where $k = [2mE/\hbar^2]^{1/2}$. Here m and E are the mass and energy of the electron, respectively. Then our model is equivalent to the following δ-function Kronig-Penny (KP) model:

$$\left\{ -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \sum \beta_n \delta(x-na) \right\} \Psi(x) = E\Psi(x), \tag{2}$$

where β_n, from the above arguments, must be a periodic function of na with period λ. We can now use the techniques of dynamical systems theory used by Bellissard *et al.*[9] to construct the Poincaré map associated with Eq. (2), obtaining

$$\Psi_{n+1} + \Psi_{n-1} + \beta_n (\sin K/K)\Psi_n = 2\cos K \Psi_n, \tag{3}$$

in which $K = ka$ and $\Psi_n = \Psi(x^+ = na)$. We stress the fact that nothing has been lost when passing from Eq. (2) to Eq. (3). For instance in the periodic case with $\beta_n = \beta_0$, the whole band structure of the usual KP model is recovered. This mapping has also been used by one of us to prove localization in a general random one-dimensional alloy problem.[10]

We recognize that the form of Eq. (3) is similar to that of Aubry's model[2] if we taken $\beta_n = V_0 \cos Qna$, with Qa an irrational multiple of π. The difference is the occurrence of K-dependent coefficients. The study of this model can proceed by means of any of the methods used to study the Aubry model. In that model the existence of extended states was established for $V_0 < 2$ and localized states when $V_0 > 2$. In the model given by Eq. (3) this condition translates to

$$V_0 > 2K/\sin K. \tag{4}$$

It is clear from this condition that the occurrence of localized states is more likely in the lowest bands of the energy spectrum. From the definition of β_n we see that it also depends on energy. For example, if we take for our potential barriers the potential

$$U_n(x) = V_0 f(na)/\cosh^2\alpha(x-na), \tag{5}$$

where $f(x)$ is the previously introduced periodic function of x and na is the nearest potential maximum, it is easily shown that[11]

$$\beta_n = 2K \frac{\cosh\{\frac{1}{2}\pi[8mV_0 f(na)/\hbar^2\alpha^2 + 1]^{1/2}\}}{\sinh(\hbar K/\alpha)}. \tag{6}$$

For sufficiently low energies, β_n is independent of energy, and we recover the model of Bellissard *et al.*[9] Such behavior is also found for several other simple potential barriers. Notice that we can always make β_n as large as we wish by increasing V_0. Thus, according to Eq. (4), there will always exist localized states for sufficient potential strength. Also we can generally expect that the localized states are separated from the extended states by mobility edges. The use of other periodic forms for β_n does not seem to change our conclusions.[2a,2e]

Another case that can be considered is the one in which the strengths of the potential barriers are identical, but the spacing between the barriers is modulated with a period incommensurate with the lattice spacing. Again using Borland's arguments[8] we find that this model is equivalent to a δ-function KP model with modulated δ-function spacings. This model has been studied by Azbel',[2d] and by deLange and Janssen.[12] In fact deLange and Janssen have shown recently by direct calculations of the wave functions and spectra that there exist both localized and extended states in this model. This implies that the potential barrier model described above also has this type of energy spectrum.

Let us now consider a more general case in which both the positions and strengths of the bar-

riers vary in an almost periodic way. Also we consider the asymmetry associated with each potential barrier, which by symmetry varies also in an almost periodic way. This model maps into a δ-function Kronig-Penny model but now both the strength β_n and the locations of the δ's vary almost periodically. If we follow a similar route to the one that leads from Eq. (2) to Eq. (3), the Poincaré-mapped Schrödinger equation reads

$$\Psi_n = \cos k(x_n - x_{n-1})\Psi_{n-1} + \frac{\sin k(x_n - x_{n-1})}{k}\Psi_{n-1}', \tag{7a}$$

$$\Psi_n' = -k \sin k(x_n - x_{n-1})\Psi_{n-1} + \cos k(x_n - x_{n-1})\Psi_{n-1}' - \beta_n \Psi_n. \tag{7b}$$

Here the prime on Ψ_n means derivative with respect to x, at $x = x_n^+$, x_n is the location of the δ-function potential, and β_n is the strength of the potential. Eliminating Ψ' we have

$$t_{n+1,n}\Psi_{n+1} + t_{n,n-1}\Psi_{n-1} + (\beta_n/K)\Psi_n = \epsilon_n \Psi_n, \tag{8}$$

where

$$t_{n,n+1}^{-1} = \sin k(x_{n+1} - x_n) \tag{9}$$

and

$$\epsilon_n = t_{n+1,n}\, t_{n,n-1} \sin k(x_{n+1} - x_{n-1}). \tag{10}$$

We have studied the question of localization in this model using a renormalization-group (RG) decimation technique designed explicitly for models of this type in a previous publication.[10] This RG method consists of eliminating the wave-function amplitude on every other lattice site in Eq. (8). After each elimination the resulting equation of motion is of exactly the same type as in Eq. (8), but with different coefficients. From the exact analytic recursion formulas given in Ref. 10, appropriately modified to treat this problem, we have studied the existence of localized states. The advantage of using this method is that after r iterations of the RG procedure the lattice spacing increases exponentially with r (as 2^r). Taking $\beta_n = V_0 \cos(Qan)$ and different values of Q and K the amplitudes are studied as a function of r. Specifically, we find indeed that there are both localized and extended states in this model for specific values of K, V_0, and Q. The identification of localized states is evident by the tendency of the t's to go to zero as r increases while β_n and ϵ_n remain finite. This intuitive criterion was also checked and compared positively with the known results of Ref. 2 for the Aubry model and also with those of de-Lange and Janssen.[12]

There appears to be a contradiction between our results and Romerio's proof of a Bloch theorem for a Schrödinger equation with an APP[7] (see Dinaburg and Sinai[3]). DeLange and Janssen in fact consider essentially the same transformation of the system to higher dimensions as is used in Romerio's proof (see also Ref. 14). They conclude that if there are localized states, the wave function must be nonanalytic in this higher-dimensional space, because it is in fact a non-analytic function of the phase of the incommensurate periodic potentials relative to each other. In fact, they present numerical calculations of the wave function based on this model, as a function of position and phase for high-order commensurate systems. As the system becomes higher-order commensurate the localized wave functions become rapidly varying functions of the phase. We have performed similar calculations on the Aubry model which show that, although when the phase is shifted by $2\pi/N$, where N is the order of commensurability, the energy spectrum does not change, each localized state becomes localized around a new lattice site which is generally quite far from the location of the original site around which the state was localized. This implies that when N becomes infinite (the incommensurate limit), the wave function will be a nonanalytic function of the phase. The physical reason for expecting such nonanalyticity can be understood as follows: Consider a pair of incommensurate sinusoidal potentials chosen so that their minima coincide at one point; call it the origin. An infinitesimal phase shift will make the potentials coincide at another point which is in general far from the original origin. If we shift the origin to this new point we recover the original problem, but clearly a state localized at a point in the crystal which is a given distance away from the old origin will be shifted to a point which is the same distance from the new origin. Such nonanalyticity actually signifies a translational symmetry break.[12,14] Since Romerio's proof depends crucially on the assumption that the wave function is analytic in the phase, the above observation may be the source of the discrepancy.

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Localization and Spectral Singularities in Random Chains

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This paper reports consideration of the Hamiltonian for tight binding in one dimension with off-diagonal disorder of two forms, corresponding to Dyson's types I and II. The density of states and localization function at the center of the band are found by perturbation theory and a scaling argument. The distinction between the two types of disorder is clearly drawn, and new singularities in the Green's function pertinent to the problem of random classical diffusion are predicted.

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The dynamic properties of random chains have been of interest since Dyson[1] calculated the density of states for a model of phonons in a disordered chain. More recently there has been extensive work on the mathematically related problem of classical diffusion in a random chain.[2] Of particular interest is the fact that disorder leads to singularities in the density of states different from those of homogeneous systems. Dyson found such singularities for a soluble class of models with a form of disorder he dubbed "type I." Quite different singularities have recently been found by Alexander *et al.*[2] for a form of disorder (type II) superficially similar. Hitherto the reasons for such different behaviors have remained relatively obscure. I shall show how the singular behaviors found follow quite simply once the localization properties of the excitations are considered. In one dimension localization and spectral densities are closely related: Thouless[3] showed that the localization function $\lambda(E)$ and the integrated density of states are essentially real and imaginary parts of the same complex K vector. As well as illuminating the