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LETTER TO THE EDITOR

Mobility edge in one-dimensional tight-binding models

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Abstract. We introduce a class of one-dimensional tight-binding models with square-well-like potentials, $V_n = \pm V$, which exhibit a mobility edge in the spectrum at the energy $E_c = 2 - V$, provided that $V < 2$. Using the transfer matrix method we are able to find the analytical expression of both the localisation length and the density of states for the whole range of energies E. The transition from extended to localised states is characterised by a singularity in the spectrum as E_c is approached from below.

Recently a great deal of work has been devoted to the study of one-dimensional localisation in the presence of random and pseudorandom potentials (see, e.g., Lee and Ramakrishnan 1987). Perhaps the most simple non-trivial example of one-dimensional disordered systems is the one-dimensional discrete Schrödinger equation with diagonal disorder,

$$\psi_{n+1} + \psi_{n-1} = (E - V_n)\psi_n \tag{1}$$

where ψ_n is the amplitude of the wavefunction on the nth site of a one-dimensional lattice, V_n is the diagonal potential and E is the energy. This model is also referred to as the nearest-neighbour tight-binding model. For random V_n equation (1) is nothing but the one-dimensional Anderson model in the tight-binding approximation (Anderson 1958). There exist rigorous results (Ishii 1973, Kunz and Souillard 1980, Delyou *et al* 1985) proving that for a large class of probability distributions of the random potential V_n, all the states are exponentially localised. For periodic potentials V_n, in contrast, the Bloch theorem ensures that all the states are extended and organised in a band structure. This raises the interesting question of whether there exist potentials such that the behaviour of the system (1) falls, in some sense, in between the two extreme cases of the Anderson model and the Bloch model.

One of such potentials has been found recently by Griniasty and Fishman (1988) by studying the motion of an electron in a one-dimensional lattice with a weak sinusoidal potential whose phase varies as n^ν,

$$V_n = V \cos(\pi \alpha n^\nu) \tag{2}$$

where V, α and ν are positive constants. This potential belongs to a class of pseudorandom and incommensurate potentials (for reviews on incommensurate potentials see, e.g., Simon (1982) and Sokoloff (1985)) lying in between the random Anderson model and the periodic Bloch model. In fact, for α rational and ν integer we get back to the Bloch model, whereas for α irrational and $\nu \geq 2$ it has been shown (Griniasty and Fishman 1988) that the model defined by (1) and (2) is 'equivalent' to the Anderson model.

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For $V<2$ and $\nu<1$, Das Sarma *et al* (1988) have found that the model has both localised and extended states, separated by a mobility edge in the spectrum at the energy $E_c=2-V$. This result was found by solving numerically (1) and (2) by direct diagonalisation of the tight-binding Hamiltonian and by calculating the localisation length using the recursive transfer matrix method. Their discovery of a mobility edge is quite interesting since it was believed that one-dimensional models do not allow for it (Ishii 1973, Thouless 1974). In supporting their results by a heuristic semiclassical theoretical argument, they introduce and solve numerically a simpler model with a square-well-like potential, which captures many features of the original model. In particular they have the same mobility edge and similar shape for the density of states. An interesting property of this model is that it is solvable analytically. In this letter we first calculate the analytical expression of the localisation length and of the density of states for this model, confirming the numerical results of Das Sarma *et al* (1988). Then we show that there is a full class of systems with square-well-like potentials which exhibit a similar behaviour, and in particular a mobility edge at $E_c=2-V$.

The simplified model of Das Sarma *et al* (1988) is defined by (1) with a square-well-like potential V_n ($V_n=\pm V$, $V>0$) with a constant depth ($2V$) and variable well lengths $L_m=q^mL_0$, with $q>1$. At V_0 there can be with equal probability either $+V$ or $-V$.

For one-dimensional systems one has (Thouless 1974, De Callan *et al* 1985),

$$\Lambda=\xi^{-1}(E)+\mathrm{i}\Gamma(E)=\lim_{N_m\to\infty}\frac{1}{N_m}\langle\ln\psi_{N_m}\rangle \tag{3}$$

where ξ^{-1} is the localisation length and Γ is the integrated density of states of (1), i.e. $\Gamma(E)=\int_E^{+\infty}\mathrm{d}E'\,\rho(E')$. The $\langle\ldots\rangle$ means averaging over the realisations of the potential. In our case, since the form of V_n is completely determined once V_0 is given, $\langle\ldots\rangle$ means averaging over the two possible initial states $V_0=\pm V$.

To calculate ψ_{N_m} we will use the transfer matrix method. The first step is to rewrite (1) as

$$\begin{pmatrix}\psi_{n+1}\\ \psi_n\end{pmatrix}=\mathbf{Q}_n\begin{pmatrix}\psi_n\\ \psi_{n-1}\end{pmatrix}\qquad \mathbf{Q}_n=\begin{pmatrix}E-V_n & -1\\ 1 & 0\end{pmatrix} \tag{4}$$

where $\mathbf{Q}_n$ is the transfer matrix from the site n to the site $n+1$. Thus,

$$\begin{pmatrix}\psi_{N_m+1}\\ \psi_{N_m}\end{pmatrix}=\prod_{n=1}^{N_m}\mathbf{Q}_n\begin{pmatrix}\psi_1\\ \psi_0\end{pmatrix}. \tag{5}$$

Equations (4) and (5) hold for any potential V_n. In our case V_n can take only two values, so there will be only two different transfer matrices,

$$\mathbf{A}=\begin{pmatrix}E-V & -1\\ 1 & 0\end{pmatrix}\qquad \mathbf{B}=\begin{pmatrix}E+V & -1\\ 1 & 0\end{pmatrix} \tag{6}$$

corresponding to $V_n=+V$ and $V_n=-V$, respectively. It is well known that the localisation properties of the model (1) depend only on the form of the potential V_n, i.e., in the language of the transfer matrices, on the rule according to which the succession of **A** and **B** in the product (5) is built. For example, if after a matrix **A** (or **B**) there can be with equal probability either a matrix **A** or a matrix **B**, then ξ^{-1} is positive in the band defined by $\rho(E)\neq 0$. All the states are localised. This corresponds to the one-dimensional Anderson model with a $\pm V$ random potential. We note that this result remains valid even if one considers a sequence of matrices **A** and **B** obtained

from a one-step two-state Markov process (Jonston and Kramer 1986, Crisanti *et al* 1989).

On the other hand, a periodic sequence, such as for example **ABAB** ..., leads to $\xi^{-1}=0$ in the regions where $\rho(E)$ is non-zero, so that all the states are extended. We note that in this case, unlike the previous one, the spectrum consists of two bands separated by a gap. This is not surprising since periodic sequences correspond to periodic potentials. Thus this is nothing other than the Bloch theorem. The existence of only two bands is due to the fact that the model is defined on a lattice.

In the model of Das Sarma *et al* the potential has a structure of the form, for example, $V_1=V$, $V_2=V_3=-V$, $V_4=V_5=V_6=V_7=V$, ..., (or the one obtained by exchanging V with $-V$). This particular case corresponds to $q=2$ and $L_0=1$. We will see below that the localisation properties do not depend on q and L_0. Such a potential leads to the product

$$\prod_{n=1}^{N_m} \mathbf{Q}_n = \mathbf{B}^{x_N}\mathbf{A}^{x_{N-1}}\ldots\mathbf{B}^{x_2}\mathbf{A}^{x_1} \tag{7}$$

where $x_1=1$, $x_n=2x_{n-1}$, and $N_m=\Sigma_{n=1}^{N} x_n=2^N-1$. Here we have assumed that N, the number of 'jumps' from **A** to **B** and vice versa, is even. The case of odd N will be discussed below. This ordering is neither random nor periodic, so in general we may expect some new behaviour.

By defininition Det $\mathbf{Q}_n=1$; thus we can write $\mathbf{A}=\mathbf{C}_A^{-1}\tilde{\mathbf{A}}\mathbf{C}_A$ and $\mathbf{B}=\mathbf{C}_B^{-1}\tilde{\mathbf{B}}\mathbf{C}_B$, where

$$\tilde{\mathbf{A}}=\begin{pmatrix} e^{z_a} & 0 \\ 0 & e^{-z_a}\end{pmatrix} \qquad \tilde{\mathbf{B}}=\begin{pmatrix} e^{z_b} & 0 \\ 0 & e^{-z_b}\end{pmatrix} \tag{8}$$

with Re $z_{a,b}\geqslant 0$ and $\mathbf{C}_{A,B}$ constant matrices with determinant one. Defining $\mathbf{C}=\mathbf{C}_B\mathbf{C}_A^{-1}$ one has

$$\prod_{n=1}^{N_m} \mathbf{Q}_n = \mathbf{C}_B^{-1}\tilde{\mathbf{B}}^{x_N}\mathbf{C}\tilde{\mathbf{A}}^{x_{N-1}}\ldots\mathbf{C}^{-1}\tilde{\mathbf{B}}^{x_2}\mathbf{C}\tilde{\mathbf{A}}^{x_1}\mathbf{C}_A. \tag{9}$$

Each matrix $\tilde{\mathbf{A}}^x$ and $\tilde{\mathbf{B}}^x$ is diagonal; thus by using the identity,

$$\begin{pmatrix} a & b \\ c & d\end{pmatrix}\begin{pmatrix} e^{\gamma} & 0 \\ 0 & e^{-\gamma}\end{pmatrix}=\begin{pmatrix} e^{\gamma} & 0 \\ 0 & e^{-\gamma}\end{pmatrix}\begin{pmatrix} a & b\,e^{-2\gamma} \\ c\,e^{2\gamma} & d\end{pmatrix} \tag{10}$$

all the matrices **C** can be moved to the right end of the product. Starting from the rightmost matrix and proceeding to the left we have

$$\prod_{n=1}^{N_m} \mathbf{Q}_n = \tilde{\mathbf{B}}^{x_N}\tilde{\mathbf{A}}^{x_{N-1}}\ldots\tilde{\mathbf{B}}^{x_2}\tilde{\mathbf{A}}^{x_1}\mathbf{G}_N^{(B)}\mathbf{G}_{N-1}^{(1)}\mathbf{G}_{N-2}^{(-1)}\ldots\mathbf{G}_2^{(-1)}\mathbf{G}_1^{(1)}\mathbf{C}_A. \tag{11}$$

The superscripts B, 1, -1 refer to the matrices $\mathbf{C}_B^{-1}$, $\mathbf{C}$, $\mathbf{C}^{-1}$ respectively. All the matrices **G** will be of the form

$$\mathbf{G}_{N-p}=\begin{pmatrix} g_{11} & g_{12}\,e^{-2\gamma_{N-p}} \\ g_{21}\,e^{2\gamma_{N-p}} & g_{22}\end{pmatrix} \tag{12}$$

$$\gamma_{N-p}=z_a\sum_{n\,(\mathrm{odd})}^{1,N-p} x_n + z_b\sum_{n\,(\mathrm{even})}^{1,N-p} x_n \tag{13}$$

with different constants g_{ij}, depending on the superscript. For example, if the superscript is B, then $g_{ij}=[\mathbf{C}_B^{-1}]_{ij}$. To analyse the large-$N_m$ limit of (5) we do not need to know the explicit form of these constants, so we can forget about the superscripts.

Let us see what is the effect of $\Pi \mathbf{Q}_n$ on a vector (ψ_1, ψ_0). The first matrix, $\mathbf{C}_A$, is constant and simply transforms the initial vector into another constant vector. Suppose we have applied $n-1$ matrices $\mathbf{G}$; then the application of $\mathbf{G}_n$ gives a new vector whose components are obtained as follows.

The first new component is given by the sum of the old first component times a constant plus the old second component times a constant times $e^{-2\gamma_n}$.

The second new component is given by the sum of the old second component times a constant plus the old first component times a constant times $e^{2\gamma_n}$.

It is obvious that in the large-N_m limit ψ_{N_m+1} gives the same informations as ψ_{N_m}, so we will concentrate on the first component. Since $\mathrm{Re}\, z_{a,b} \geqslant 0$ then $\mathrm{Re}\, \gamma_n \geqslant \mathrm{Re}\, \gamma_{n'}$ if $n > n'$. As a consequence the leading term in ψ_{N_m+1} is of the form

$$\psi_{N_m+1} = e^{\gamma_N}(pr^N + \ldots) \tag{14}$$

where the exponential comes from the product of $\tilde{\mathbf{A}}$ and $\tilde{\mathbf{B}}$, and p and r are constants. It is easy to realise that this form, with different p, r, is valid also for odd N. Since $N/N_m \to 0$ as $N_m \to \infty$, in the large-N_m limit we can neglect the contribution of $\mathbf{G}$ in (11). The same conclusion is obtained considering ψ_{N_m} instead of ψ_{N_m+1}. Therefore we can write

$$\frac{1}{N_m} \ln \psi_{N_m} = \frac{\gamma_N}{N_m} + f_N \tag{15}$$

where f_N goes to zero as $N_m \to \infty$. We note that (15) is valid for *any* V since it follows from the geometrical form of the potential.

To evaluate the average in (3) we note that exchanging $+V$ with $-V$ is equivalent to exchanging $\mathbf{A}$ with $\mathbf{B}$. Therefore a similar calculation for this sequence leads again to (15), but with exchanged z_a and z_b. By definition $V_0 = +V$ and $V_0 = -V$ have the same probability, so that one has

$$\Lambda = \tfrac{1}{2}(z_a + z_b). \tag{16}$$

Substituting for z_a and z_b their expression in terms of V and E, we finally get for $V < 2$

$$|E| < E_c \quad \begin{cases} \xi^{-1} = 0 \\ \rho = \dfrac{1}{4}\left\{\left[1 - \left(\dfrac{E-V}{2}\right)^2\right]^{-1/2} + \left[1 - \left(\dfrac{E+V}{2}\right)^2\right]^{-1/2}\right\} \end{cases} \tag{17a}$$

$$E_c < |E| < E_b \quad \begin{cases} \xi^{-1} = \dfrac{1}{2} \ln\left\{\dfrac{|E|+V}{2} + \left[\left(\dfrac{|E|+V}{2}\right)^2 - 1\right]^{1/2}\right\} \\ \rho = \dfrac{1}{4}\left[1 - \left(\dfrac{|E|-V}{2}\right)^2\right]^{-1/2} \end{cases} \tag{17b}$$

$$|E| > E_b \quad \begin{cases} \xi^{-1} = \dfrac{1}{2}\left[\ln\left\{\dfrac{E+V}{2} + \left[\left(\dfrac{E+V}{2}\right)^2 - 1\right]^{1/2}\right\} + \ln\left\{\dfrac{E-V}{2} + \left[\left(\dfrac{E-V}{2}\right)^2 - 1\right]^{1/2}\right\}\right] \\ \rho = 0 \end{cases} \tag{17c}$$

where $E_c = 2 - V$, $E_b = 2 + V$ and $\rho(E) = -\mathrm{d}\Gamma(E)/\mathrm{d}E$.

From (17) we see that there is only one band, which ranges from $-E_b$ to E_b, but for $|E| < E_c$ the states are extended, whereas for $E_c < |E| < E_b$ they are localised. The energy E_c is identified as the *mobility edge* of the system. The transition from extended to localised states is characterised by a singularity in the density of states at E_c, $\rho \sim (E_c - E)^{-1/2}$ as $E \to E_c^-$, $\rho \sim O(1)$ as $E \to E_c^+$. The localisation length diverges at E_c^+

as $\xi^{-1} \sim (E - E_c)^{1/2}$. All these results are in agreement with the numerical results of Das Sarma *et al* (1988). In figure 1 we show the density of states for $V = 1$ obtained both from a numerical solution of the model (a) and from our solution (b). We note that in the model defined by (1) and (2) the 'jumps' from $-V$ to $+V$ (and vice versa) are smoother, so we may expect weaker singularities. Indeed the numerical results of Das Sarma *et al* are consistent with a logarithmic singularity of the density of states at E_c.

An important consequence of our solution is that results (16) and (17) can be extended to all models with square-well-like potentials which can be represented by a product of matrices of the form (7) with $\lim_{N\to\infty} N/\Sigma_{n=1}^{N} x_n = 0$. We stress, however, that for these generalised models care must be taken in handling the limit in (3). In fact, depending on the average and on the x_n, the limit may not exist. To be more explicit let us consider the succession $\ln \psi_{N_m} / N_m$ and study its behaviour as $N_m \to \infty$.

Suppose that $x_N / \Sigma_{n=1}^{N-1} x_n$ goes to zero in the limit $N \to \infty$. In this case it can be shown that the succession converges to a well defined limit which, for the product (7), is given by the $N \to \infty$ limit of (15). This in turn implies that the limit (3) is *always* well defined. The explicit form of Λ in general may depend on the probability of

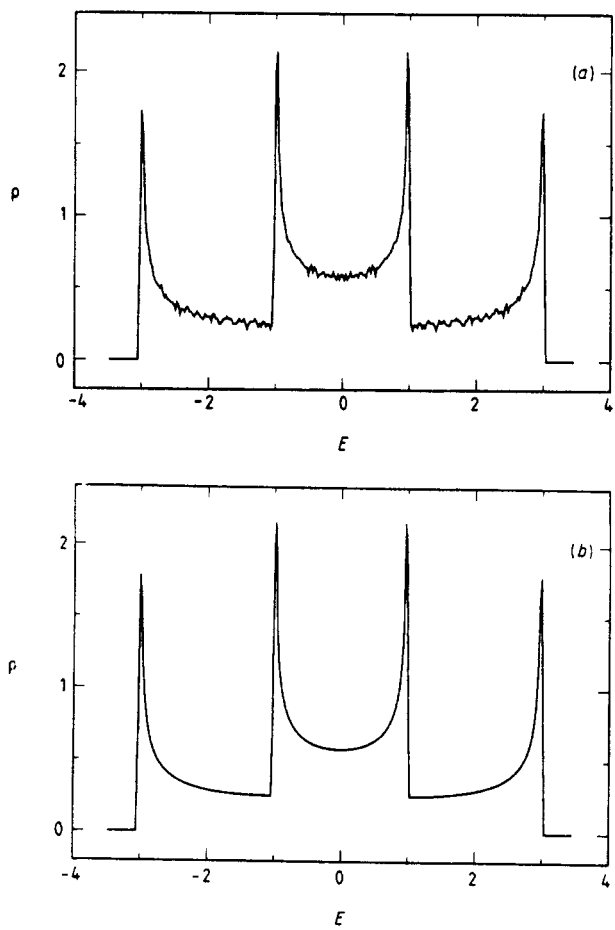

Figure 1. The density of states of the simplified model of Das Sarma *et al* (1988) for $V = 1$. (a) Numerical solution; (b) analytical solution (equation (13)).

having $V_0 = +V$ (or $-V$). For example, if this probability is $\frac{1}{2}$, then Λ is given by (16).

On the other hand, if $x_N / \Sigma_{n=1}^{N-1} x_n$ remains finite in the limit $N \to \infty$, i.e. either it converges to a finite limit or oscillates between two finite values, then the succession $\ln \psi_{N_m} / N_m$ does not have a well defined limit as $N_m \to \infty$, even if it is bounded. Thus, in this case, all we can say is that in general the limit Λ does not exist, but there will be well defined inf lim and sup lim. The existence of the limit Λ, i.e. inf lim = sup lim = Λ, strongly depends on the average $\langle \ldots \rangle$. It can be shown that the only case for which Λ exists is when $V_0 = +V$ and $V_0 = -V$ have the same probability, in which case Λ has the form (16). We note that the model of Das Sarma *et al* (1988) belongs to this second class.

It is easy to realise that all the models for which Λ exist will have similar features. In particular they will exhibit a mobility edge at $E_c = 2 - V$ (for $V < 2$) with the same strength of the singularity in the spectrum. Numerical simulations, not reported here, for different sequences of x_n, are in very good agreement with these theoretical predictions.

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