Energy spectrum, transmittance, and localization in an incommensurate nonanalytic potential

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The energy spectrum, localization properties of eigenstates, and transmittance are calculated for a one-dimensional incommensurate chain with a potential which is the absolute value of the cosine potential used in the Aubry model. This nonanalytical potential, which has cusps, has previously been proposed by Bardeen as a model for the effective pinning potential for the motion of charge-density waves. Results show that, contrary to what happens in the Aubry model, a sharp mobility edge exists for intermediate values of the modulation and separates extended low-energy states from high-energy localized states. The first three terms in the Fourier expansion of the studied potential correspond very closely to the Soukoulis-Economou potential. Compared to that later model, the effect of the nonanalyticity in the Bardeen potential, represented by the infinite rest of the above-mentioned Fourier expansion, is found to be small.

I. INTRODUCTION

An often used and highly idealized one-dimensional model for incommensurate structures is a one-dimensional tight-binding model with constant nearest-neighbor hopping t known as the Aubry[1-3] model, where the site potential is given by $W\cos(Qna)$ where $Q=2\pi/\lambda$ is the modulation wave vector, a is the lattice spacing, λ is the wavelength, and W is the modulation amplitude. Incommensurability is achieved by requiring that a/λ is an irrational number.

More recently there has been evidence that in some problems the effective potential is not such an analytic function.[4] Thus, Bardeen[4,5] has proposed that the potential $-W|\cos(Qna)|$ should be used instead to model the effective incommensurate pinning potential for the motion of charge-density waves (CDW's). Our interest in examining the eigenstates and localization properties of single-electron states in such a potential stems not only from this proposal, but also because the influence of strong nonanalytic properties (here cusps in the potential) can be examined.

It will be found that instead of having a sharp metal-insulator transition at $W=2|t|$ for all energies, as in the Aubry model, a more physically reasonable behavior with a mobility edge is obtained for moderate values of the modulation amplitude. This separates extended low-energy states from localized high-energy states.

The techniques used to study the problem are direct diagonalization by which the energy spectrum and wave functions are examined and also the explicit calculation of the transmission coefficient, through which the Landauer conductance can be inferred.[6] For this later calculation, we make use of the renormalization technique[7-9] for one-dimensional chains. In this calculation the energy must be confined to $|E|<2|t|$ so that there is no simple one-to-one correspondence between the results of diagonalization and transmission coefficient. However, in the energy range where the two can be compared, the results agree quite well. Calculation of transmission through quasiperiodic systems has earlier been studied by several authors, both for electrons[10] and light.[11]

We give results for the eigenspectrum and wave functions in Sec. II and the transmittance results in Sec. III. Results are discussed in Sec. IV.

II. EIGENENERGIES AND EIGENSTATES

The eigenspectrum and eigenstates are first calculated by direct diagonalization for symmetric tridiagonal matrices, the results of solving an eigenproblem of the form

$$\varepsilon(n)c(n)-tc(n+1)-tc(n-1)=Ec(n)\ , \tag{2.1}$$

where $\varepsilon(n)=-W|\cos(Qna)|$, and energies are measured in units of t ($t=1$).

Free boundary conditions were used, and the calculation of the spectrum and wave functions was performed for lengths of up to 2100 atoms. Both the normalized second moment[12] of the wave function and the inverse participation ratio[12,13] were examined.

The modulation wave vector Q is such that $Qa=2\pi q$ where q is now an irrational number. This irrational number is selected here so that it can be expressed as a continued fraction

$$q=q(\mu)=[\mu,\mu,\mu,\ldots]=1/[\mu+q(\mu)]\ , \tag{2.2}$$

where μ is a positive integer. Solving this second-order equation gives

$$q(\mu)=[(\mu^2+4)^{1/2}-\mu]/2\ . \tag{2.3}$$

We will mainly present results concerning the case $\mu=3$, which means $q=(13^{1/2}-3)/2=0.302\,776\ldots$. Results for the eigenspectrum are shown in Fig. 1 for different values of the modulation amplitude W. Compared to the Aubry model, the energy spectrum is shifted towards negative energies. To see the relation between the Bardeen potential and other studied potentials like the Aubry and the Soukoulis-Economou[14] potentials it is useful to make a Fourier expansion:

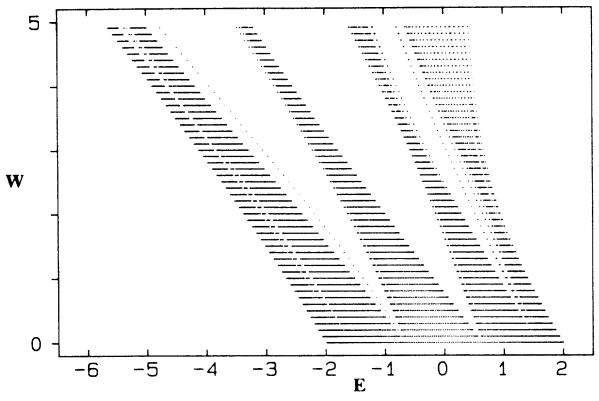

FIG. 1. Energy spectrum for different values of the modulation amplitude W. The length of the chain is 200. On both axes the energies are measured in units of t.

$$-|\cos(Qx)| = (2/\pi)[-1-2/3\cos(2Qx) + 2/15\cos(4Qx) - 2/35\cos(6Qx)+\ldots], \quad (2.4)$$

where the coefficients which multiply the terms $\cos(Qmx)$ are given by $2(-1)^{m/2}/(m^2-1)$ where m is an even integer. The constant, negative, term in this expansion explains the negative shift in the spectrum. The second term is basically the Aubry potential, while the second and the third terms together constitute a potential which is similar to that of Soukoulis and Economou.

The study of the localization properties, in terms of the second moment and the inverse participation ratio, is given in Figs. 2(a) and 2(b), respectively, for the case $W=3t$. It shows a clear mobility edge separating low-energy extended states from high-energy localized states. A rather large value of W of the order of $7t$ is needed to localize all states. The appearance of this large value of W is due to the fact that the absolute value in the Bardeen potential reduces the spread in the bare site energies. The result obtained with a mobility edge whose position is dependent on the amplitude modulation W is consistent with this model being non-self-dual. It still behaves as a rather ideal model in that just one mobility edge appears for the approximate range $7t > W > 2t$. Its low-energy states are extended also for values of $W > 2t$, where the Aubry model $\varepsilon(n) = -W\cos(Qna)$ only has localized states. For chains longer than 400 atoms, the mobility edge already appears to be quite sharp. In order to study the effect of the length of the studied incommensurate chain we show in Figs. 3(a) and 3(b) the logarithm of the inverse participation ratio (R) of all the eigenstates in a system of length 400 and 2101, respectively. It is clear-

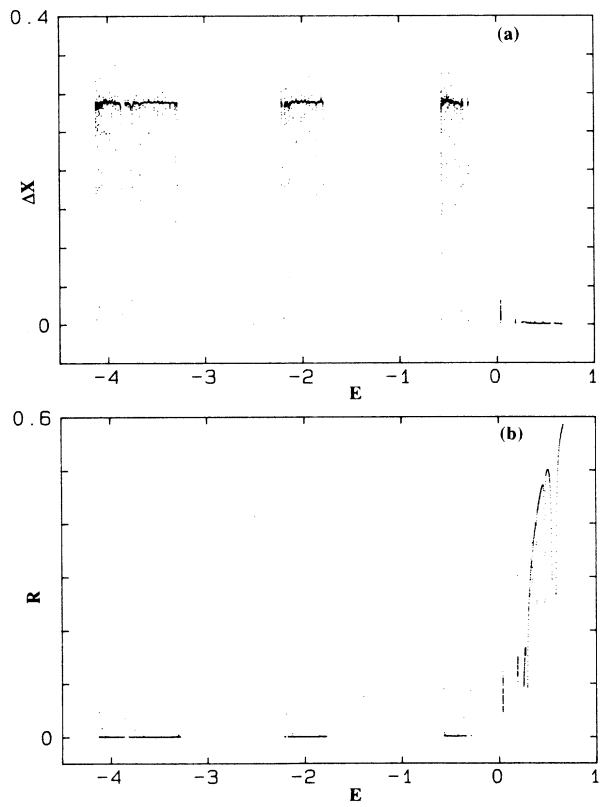

FIG. 2. (a) Normalized second moment Δx of all the wave functions plotted as a function of the eigenenergy E. Values of the order of $12^{-1/2}\approx 0.29$ correspond to extended states. Note that Δx is expressed in units of the lattice constant a. (b) Inverse participation ratio (R) of all the wave functions plotted as a function of the eigenenergy. In both (a) and (b) $W=3t$. Eigenenergies are expressed in units of t.

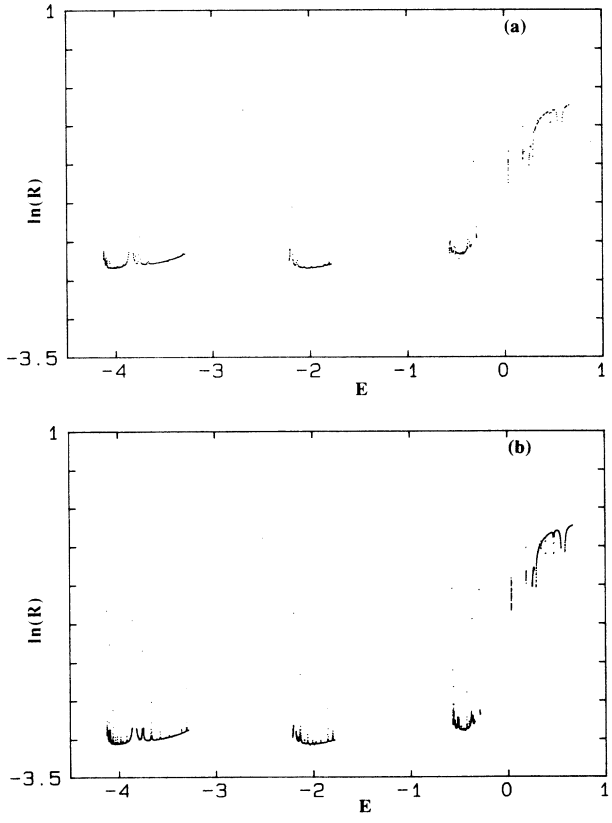

FIG. 3. (a) The natural logarithm of R vs eigenenergy for an incommensurate chain of length 400. (b) The natural logarithm of R vs eigenenergy for a chain of length 2101. Note that only the low-energy part (corresponding to extended states) is drastically changed when compared to (a). $W=3t$ in both (a) and (b). Eigenenergies are expressed in units of t.

ly seen that only the positions of the states with negative energies are different in the two figures. Since R behaves as the inverse of the number of the sites mainly occupied by the specific eigenstate considered,[12] this is consistent with the findings that the eigenstates with positive energies are localized and those with negative energies extended. From Fig. 2(b) it can be seen that R varies in this case between approximately 0.04 and 0.5 for the positive eigenstates for $W=3t$. This means that these eigenstates are located on between 2 and 25 atoms.

The only way a model with the $-W|\cos(Qna)|$ potential can be made self-dual is to retain appropriate matrix elements for the second- fourth-, sixth-, etc. nearest-neighbor interactions. This emerges on making a Fourier transform

$$c(n)=\sum_m b(m)\exp(inmQa) \tag{2.5}$$

so that the Hamiltonian has the same general form in real and reciprocal space.

III. TRANSMISSION COEFFICIENT

The first step in calculating the transmission coefficient is to decimate all intermediate sites of a chain of length N ($i=0,\ldots,N$) which is located between two semi-infinite pure chains representing perfect leads. After this decimation only two effective sites (0 and N) remain, connected by an effective hopping interaction. Both the effective site energies and the effective hopping are then energy dependent. To the left of site 0 and to the right of site N, one still retains the semi-infinite periodic chains with hopping matrix element t and site energies set equal to zero. The decimation procedure can either be used to eliminate every second site at a time or any given site at a time (one-by-one procedure). Here we use the second procedure always eliminating the site immediately to the right of site 0. The relevant iteration equations for the effective hopping and effective site energies, when site n is eliminated, are given by

$$t'(n-1,n+1)=\frac{-t(n-1,n)t(n,n+1)}{[E-\varepsilon(n)]},$$

$$\varepsilon'(n-1)=\frac{\varepsilon(n-1)+t(n-1,n)t(n,n-1)}{[E-\varepsilon(n)]}, \tag{3.1}$$

$$\varepsilon'(n+1)=\frac{\varepsilon(n+1)+t(n+1,n)t(n,n+1)}{[E-\varepsilon(n)]}.$$

In the next step the next surviving site is labeled n and the iteration is repeated until all intermediate sites have been decimated. The "one step at a time" decimation procedure, although slower, has the advantage of allowing one to start from any arbitrary length of chain.

The second step is to match a plane wave $\exp(ikna)$ moving rightwards and a reflected wave $r\exp(-ikna)$ moving leftwards along the semi-infinite portion of the periodic leads to the probability amplitudes $c(0)$ and $c(-1)$ on the left-hand side of the decimated chain. Thus, one has, for example,

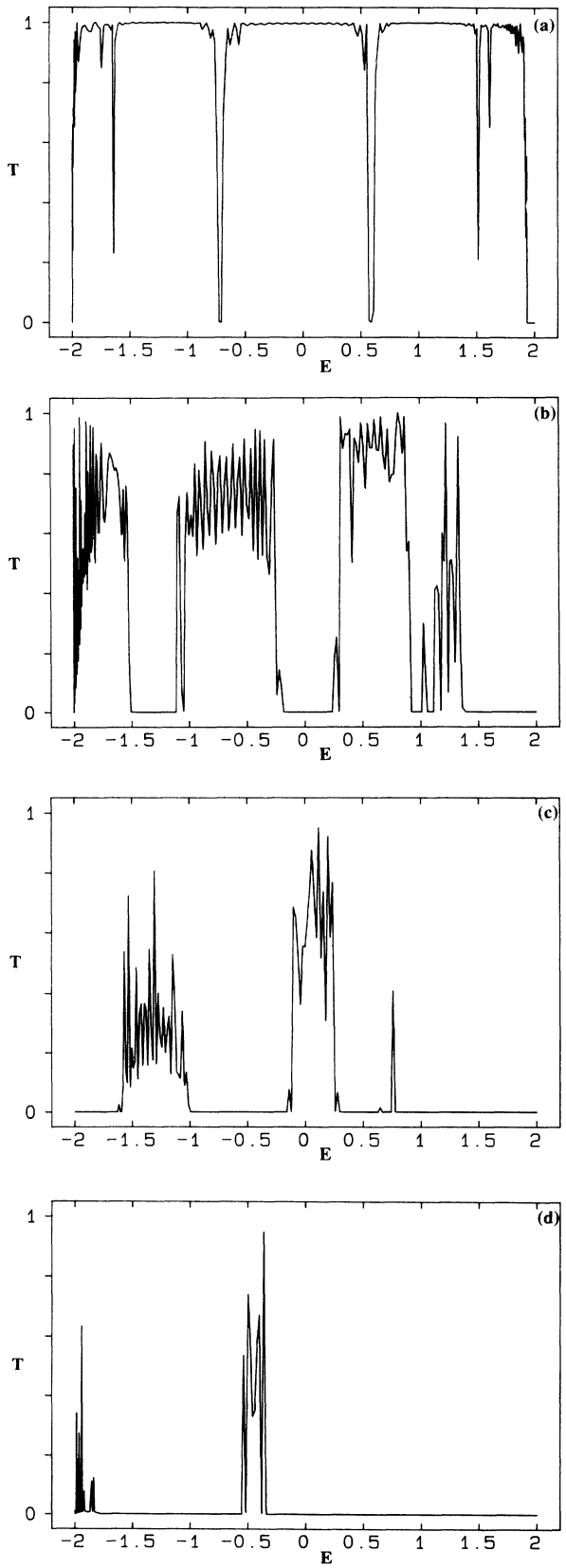

FIG. 4. (a) Transmission coefficient T vs energy E for an incommensurate chain with $N=400$, and the value of the modulation amplitude $W=0.1t$. (b) Same as in (a) but with $W=t$. (c) Same as in (a) but with $W=2t$. (d) Same as in (a) but with $W=3t$. Eigenenergies are expressed in units of t.

$$c(0)=1+r\ ,$$
$$c(-1)=\exp(-ika)+r\exp(ika)\ . \tag{3.2a}$$

Similarly a transmitted wave $t\exp(ikna)$ can be matched to the probability amplitudes $c(N)$ and $c(N+1)$ on the right-hand side of the decimated chain, giving

$$c(N)=t\exp(ikNa)\ ,$$
$$c(N+1)=t\exp[ik(N+1)a]\ . \tag{3.2b}$$

Finally two effective tight-binding equations relate these four amplitudes. Hence, two equations with two unknowns can be solved for r and t, so that the transmission coefficient $T=tt^*$ can be calculated.

Results are shown in Figs 4(a)–4(d) for $N=400$ and for various values of W. Because the plane waves along the ordered sections have energy $E(k)=-2t\cos(ka)$ the energy range is limited to $-2t<E<2t$. This chain is really infinite so that there is no one-to-one correspondence with the finite chain of the previous section.

The results show, however, that in the relevant energy range, the gaps evident in the transmission coefficient coincide quite well with the gaps obtained in the eigenspectrum. Also $T=0$ at the higher range of energies because of the leftmost shift of the spectrum and because of the localizing effect of the modulation on the higher-energy eigenstates.

IV. DISCUSSION

The model is similar to that of Soukoulis and Economou[14] in that the first three terms of the Fourier expansion (2.2) can be considered to be similar to their model, with the rest of the terms dropping off roughly as $1/m^2$. It is definitely not self-dual.

The model localizes at high eigenenergies for $W>2t$, but leads to more extended states, i.e., extended states at low eigenenergies also for $W>2t$, than the Aubry model does. At first it would seem that adding on more $\cos(Qma)$ terms to the Aubry potential would simply provide a greater number of pathways in $|k\rangle$ space, thereby increasing localization in real space. To see why this is not always true, one should consider that propagations through different pathways may interfere with each other. For example, a pathway going from $|0\rangle$ to $|4Q\rangle$ may interfere with another going from $|0\rangle$ to $|2Q\rangle$ and from $|2Q\rangle$ to $|4Q\rangle$. When this happens there is more localization in $|k\rangle$ space and therefore greater extension in real space. Several authors have shown both for quasiperiodic systems[15] and disordered systems[12,16] that adding second-nearest-neighbor interaction in real-space problems sometimes leads to more localized states rather than to more extended ones, presumably through this interference effect.

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