# Discontinuous behavior of the localization properties in a finite-length incommensurate potential with weak applied electric fields

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Model calculations are performed for a tight-binding model with an incommensurate potential of finite length, in a weak electric field $\mathcal{E}$, with site energies given by $E_n = W\cos(2n) - ea\mathcal{E}n$ $(n = 1,2,\ldots,N)$. It is found that there is a discontinuous delocalizing behavior in that localization properties and the position of the localized wave function have sudden discontinuities as a function of the electric field, where the calculations are performed for values of $W > W_C$, where $W_C$ is the value of $W$ above which the states are localized in the absence of an external electric field. As $W$ decreases, the discontinuities become more frequent, resulting in a "noisy" behavior near threshold.

In a previous publication[1] the behavior of finite incommensurate potentials was examined in the presence of a weak electric field in a tight-binding model with a finite bandwidth. Conditions were such that the length of the system was shorter than the band length $L_B$ $(L < L_B)$, where $L_B = B/ea\mathcal{E}$, $B$ is the total bandwidth, $\mathcal{E}$ is the electric field and $a$ is the lattice space. Additionally, the potential $W$ is made strong enough so that the localization length is shorter than $L$. Hence the strongly localized wave functions turn out to have almost all their weight on a single site. The numerical calculation of $\gamma$, the inverse of the convergence length of a self-energy expansion at the zeroth site, which was identified with the inverse localization length, showed resonances and a delocalizing behavior for weak fields under these conditions, in which exponential localization was assumed.

Over limited length scales $(L < L_B)$ interband mixing effects would be negligible in Kronig-Penny models, so that our model is relevant for short lengths in which the single-band effects are relevant. On the other hand the electrons are always able to tunnel from one band to another in Kronig-Penney models for long enough lengths or strong enough electric fields, so that delocalizing behavior is then seen for long length scales.[2]

On the other hand, for models with limited bandwidth, over larger lengths $L > L_B$, or for larger electric fields, it is clear that the band will be tilted enough so that the states will be increasingly localized by the electric field, even if $W = 0$. This was the result of Luban and Luscombe[3] who performed their calculations by actually finding the eigenstates. On the other hand, calculations in Ref. 1 were performed by sweeping across the band horizontally with an arbitrary energy ($E = 0$ for $n = 0$), whereby the calculation sees a mixture of the degenerate zero-field states for lengths shorter than the band length, and delocalization rather than increasing localization is found.

The purpose of the present work is to examine the eigenstates for the finite system (of total length $N = 100$) by explicit diagonalization using a $QL$ diagonalizing routine for tridiagonal symmetric matrices. Free-end boundary conditions are applied.

The symmetric tridiagonal matrix which was diagonalized had diagonal matrix elements $E_n = W\cos(2n) - ea\mathcal{E}n$, where $ea\mathcal{E} > 0$, and a constant nearest-neighbor hopping parameter $V = 1$ was taken to fill the main subdiagonals.

The quantity which was computed was the participation ratio $P$ for the $n = 50$ eigenstate, corresponding to an eigenvalue near the band center, at the edge of an interior gap. $P$ is defined as

$$P = \frac{\left[\sum_i (C_i^2)\right]^2}{\sum_i C_i^4},$$

where the $c_i$'s are the amplitudes of the eigenstate. For a

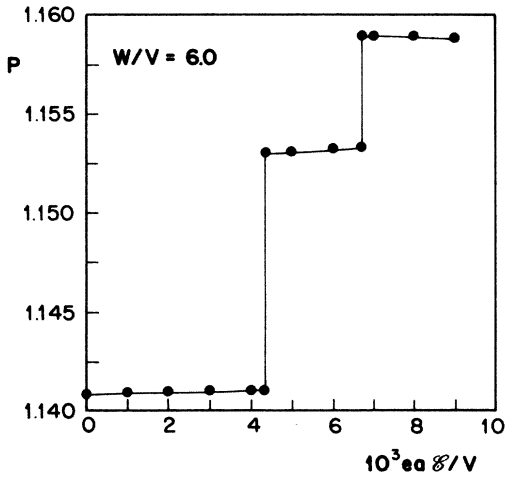


FIG. 1. This figure shows the participation ratio $P$ plotted as a function of the electric field strength $ea\mathcal{E}/V$ for $W/V = 6.0$.

 

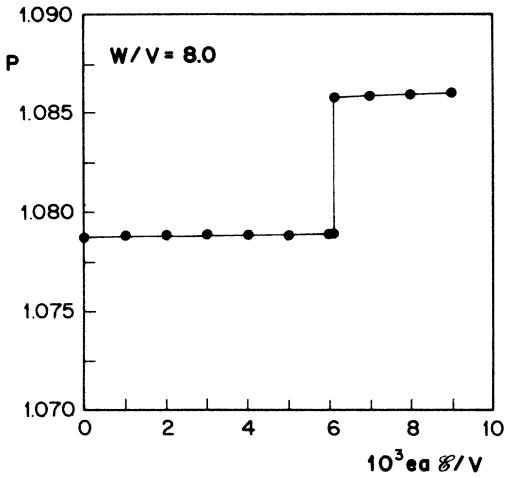


FIG. 2. This figure shows the participation ratio $P$ as a function of the electric field strength $ea\mathcal{E}/V$ for $W/V=8.0$.

completely extended state $P$ is of the order of the size of the system, but for a strongly localized state it approaches the value of 1. This later situation was the case in these calculations. The spectrum and total bandwidth was simultaneously monitored. The behavior of the eigenvalues (spectrum) was continuous with the electric field, but not so the eigenvectors. The results are shown in Figs. 1–4.

Previous results showing a delocalizing effect for these weak fields are confirmed. $P$ has sudden delocalizing discontinuities which become more frequent as $W$ decreases (Figs. 1–3). These discontinuities are associated with a sudden change in the site about which the wave function is most strongly localized. The values of $P$ are close to 1, indicating strong localization. $P$ increases as $W$ decreases, as expected.

The total bandwidth with no externally applied electric field increases with increasing $W/V$ (see Fig. 4). This

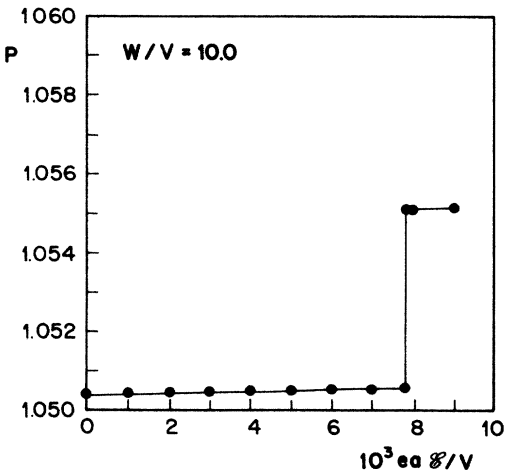


FIG. 3. This figure shows the participation ratio $P$ as a function of the electric field strength $ea\mathcal{E}/V$ for $W/V=10.0$.

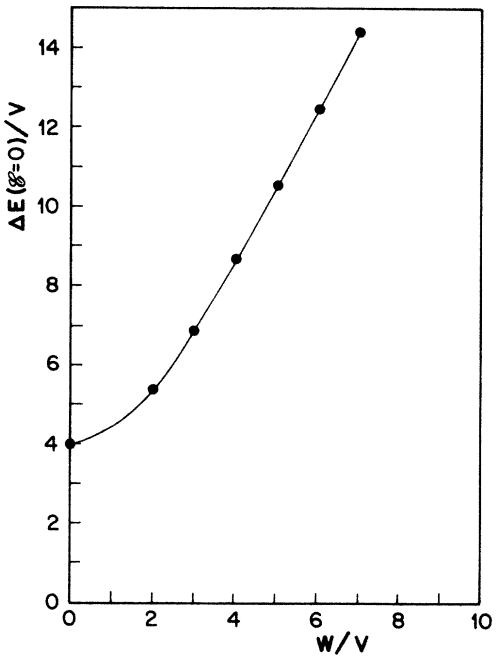


FIG. 4. This figure shows the zero field total bandwidth $\Delta E(\mathcal{E}=0)/V$ as a function of the incommensurate potential $W/V$.

shows that the conditions of the calculation improve when stronger potentials are used. For finite values of electric field, the total bandwidth also increased with $ea\mathcal{E}/V$ and interior gaps become slightly larger. (The spectrum is of course discrete).

The tendency for the discontinuities to become more frequent as $W/V$ decreases continues down to values of $W/V$ just above $W_C/V$. The behavior just above $W_C$ is in fact extremely discontinuous or "noisy," indicating that in this region the discontinuities become dense as a function of $ea\mathcal{E}/V$.

For the values of $W/V$ shown in the figures, the site about which the wave function is strongly localized was simple to identify. For $W/V=10.0$ the wave function shifted from site number 84 to site number 18 at the discontinuity. For $W/V=8.0$ it also shifted from site 84 to site 18. Finally the discontinuities for $W/V=6.0$ involve shifts from site 84 to site 18 and then from site 18 to site 4.

Even though the information contained in $P$ differs from the previously defined $\gamma$, a delocalizing and resonant behavior with electric field strength is still apparent. The observed features are analogous to the noisy behavior near the threshold of charge-density-wave (CDW) motion.[4] It can also be pointed out that there is evidence for resonant behavior (dips with negative differential resistance) in some samples measured by Monceau, Richard, and Renard.[5]

Two clarifications should be made about the results. Firstly, since there is no level crossing in one dimension the results are not due to this effect. The second is that the value of $P$ may both increase or decrease when the electron is localized about the new site, and the position

of maximum localization can move both with or against the externally applied field. The effect can be thought of as arising from a balance between kinetic energy (which is larger in a more localized state) and the change in potential energy.

To summarize, what happens here is an instantaneous shift in the site about which the wave function has its greatest weight at certain critical values of $ea\mathcal{E}/V$. This can be associated with tunneling in the finite band, at certain sharply defined values of electric field and with no apparent discontinuities in the corresponding eigenvalues.

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