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Localization and multifractal wave functions in a one-dimensional incommensurate system under an electric field

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Abstract. We study the Kronig–Penney model with incommensurate potentials in the presence of an electric field. Both localization and delocalization by electric fields are observed, which are results intermediate between those obtained in periodic and disordered systems under electric fields. By performing a multifractal analysis, we show that the wave functions for large fields are multifractal.

1. Introduction

There has been much interest in periodic and disordered systems with a uniform electric field (Cota *et al* 1985, 1987). In the presence of an electric field, periodic systems are known to have Wannier–Stark ladders (WSL) (Wannier 1960, 1962) and exponentially localized eigenfunctions when interband transitions are absent. As the interband transitions become appreciable, the discrete energy levels convert into resonances in the continuum, resulting ultimately in an absolutely continuous spectrum. Recent experiments on periodic superlattices showed that large electric fields lead to delocalization if the system contains several WSLs, as well as the field-induced localization (Voisin *et al* 1988, Schneider *et al* 1990).

In the disordered chain of length N with δ-function potentials under an electric field, the electronic states are power-law localized for $X > 1$, where X is the ratio of the electrostatic energy FN to the incident energy E (Soukoulis *et al* 1983). It was proved that there exists a transition from power-law localized states to extended ones for large fields (Delyon *et al* 1984).

On the other hand, little has been reported for either periodic or disordered systems (Kim 1991, Oh *et al* 1992). One-dimensional (1D) incommensurate systems which are intermediate between periodic and disordered systems can have extended, localized or critical eigenstates (Sokoloff 1985). Luban and Luscombe (1986) studied a 1D single-orbital tight-binding (TB) model with incommensurate potentials under an electric field and found that all the eigenstates are factorially localized and the spectrum is a WSL with non-uniform spacing. Weisz and Slutzky (1986) and Weisz (1988) examined the effect of a weak electric field on the localized states in a 1D TB model with incommensurate potentials, in order to explain non-linear conduction effects for the low-temperature semiconducting phase of crystals containing charge-density waves. Note that interband transitions were not considered in the models. It is

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the purpose of this paper to examine the localization properties of the electronic states and the characteristics of the field-induced extended states in a 1D incommensurate system under an electric field, by considering interband transitions.

2. The model and the methods

We consider the Kronig–Penney (KP) model

$$H\psi(x) = \left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sum_{n=1}^{N} V_n \delta(x-n) - Fx \right] \psi(x) = E\psi(x) \tag{1}$$

where $\hbar^2/2m = 1$, $e = 1$, F is the electric field strength, $V_n = V_1 + V_2 \cos(2\pi\beta n)$ with irrational β, and the lattice constant is taken to be 1. The irrationality of β makes the field-free potential incommensurate with the underlying lattice. We take $\beta = \sqrt{5} - 2$, as used by Azbel and Rubinstein (1983). In the absence of an electric field, localized states can be found more easily in an array of potential wells (Ryu 1988) than in that of potential barriers (Azbel and Rubinstein 1983). We choose $V_1 = -5$ and $V_2 = 3$.

When a wave is incident from the right with $E < 0$, the wave is completely reflected and the transmission coefficient, which is the quantity of experimental interest, goes to zero (Cota *et al* 1987). We consider an electron incident from the left with positive energy. The electron can tunnel from one band to another in KP models for sufficiently long lengths or sufficiently strong electric fields. We use the ladder approximation that replaces the ramp potential by a step function. Taking the cell solutions as plane waves instead of Airy functions, equation (1) can be exactly mapped to the second-order difference equation (Soukoulis *et al* 1983)

$$X_n \psi_{n+1} + X_{n-1}\psi_{n-1} - E_n \psi_n = 0 \tag{2}$$

where $\psi_n = \psi(x = n)$ and $E_n = V_n + X_{n-1}Y_{n-1} + X_n Y_n$. And here $X_n = k_n / \sin k_n$, $Y_n = \cos k_n$ and $k_n = [E + F(n + 0.5)]^{1/2}$. Equation (2) has a similar form to the familiar TB model but has all the band-structure information contained in equation (1). We note that E_n and X_n are non-linear functions of E.

To examine the localization properties, we study the transmission coefficient T, wave functions and the density of states (DOS). We calculate T by using the recursion relations (Stone *et al* 1981) obtained from the transfer matrix of equation (2), wave functions using periodic boundary conditions, and the DOS using the negative-eigenvalue theorem (Dean 1972) or node-counting method (Lambert 1984).

To study the fluctuations of the wave functions, we use multifractal analysis (MFA) (Halsey *et al* 1986). Recently, MFA has been used to investigate the multifractalities in the fluctuating regimes of localized wave functions in disordered systems (Mato and Caro 1987, Pietronero *et al* 1987) and those of wave functions in quasiperiodic systems (Evangelou 1987, Roman 1987, Hiramoto and Kohmoto 1989). It has also been used to examine the characteristics of the wave function at the mobility edge in three-dimensional disordered systems (Evangelou 1990, Schreiber and Grussbach 1991). We compute $\tau(q)$ which obeys

$$\tau(q) = \lim_{l \to 0} \ln Z(q, l) / \ln l \tag{3}$$

where $Z(q,l) = \sum_{i=1}^{N/L} P_i^q$ and $l = L/N$. The lattice is covered with consecutive boxes of size L and P_i is the probability of finding the electron within the ith box. We use the normalized wave functions and find $\tau(q)$ by plotting $\ln Z(q,l)$ against $\ln L$ for a fixed q. Using the relations

$$\mathrm{d}\tau(q)/\mathrm{d}q = \alpha \qquad f(\alpha) = q\alpha - \tau(q) \tag{4}$$

we can obtain the multifractal spectrum characterized by a continuous set of scaling indices α and the fractal dimensions $f(\alpha)$.

For an extended wave function, one can obtain a single point $f = \alpha = 1$, which means the absence of multifractal features in the wave function. When a wave function is localized, if L is larger than the localization length, the $f(\alpha)$ spectrum consists of two points, one being $f(0) = 0$ and the other $f(\infty) = 1$. For a critical (self-similar or chaotic) wave function, one gets a continuous $f(\alpha)$ spectrum. But a chaotic wave function shows quite different shapes in each scale and does not yield an $f(\alpha)$ spectrum independent of L (Tokihiro 1989). Thus, the multifractality of a wave function is confirmed by the L-independent $f(\alpha)$ spectrum.

3. Results and discussion

Figure 1(a) shows the DOS and $-\ln(T)/N$ for the first and the second main bands. In the absence of an electric field, $-\ln(T)/N$ is equal to the inverse localization length. When $F = 0$, the first band is localized and the second one consisting of five subbands is extended. As one can see from Zener's tilted band picture, the states lying near band edges are most easily influenced by electric fields. As F increases, discrete levels occur near band (main bands and subbands) edges and the band widths increase by FN, as shown in figure 1(b). But the interband tunnellings between the subbands make it difficult to see a WSL in each main band. For large fields, there are no clear gaps or discrete levels, but resonances in the continuum as shown in figure 1(c). The positions of resonances correspond exactly to those of the peaks of T.

Figure 2(a) shows that the localized states in the first band are more strongly localized by electric fields when interband tunnellings are negligible. Luban and Luscombe (1986) showed that this field-enhanced localization is the factorial one. The field-enhanced localization is also found in a disordered system with δ-function potentials. When the interband transitions become appreciable, T shows a power-law decay as shown in figure 2(b). For large fields, the states become extended. Next, we examine the influence of electric fields on the extended states in the second band. For small fields, the states become power-law localized for large N as shown in figure 3. The noticeable jumps seen in figure 3 are due to interband tunnellings. The plateaus and the slopes correspond exactly to bands and gaps that the electron moves through, respectively. This shows that Zener's tilted band picture is a good guide to understanding the transport properties of the electrified chains. For large fields, the states also become extended.

We have performed an MFA to study the characteristics of the extended wave functions for large fields. Figure 4 shows the log–log plots of $Z(q,l)$ against the box size L. It is a very good straight-line fit to the plot for a positive but not large q. This procedure is not so accurate for negative q as for positive q, since the smallest part

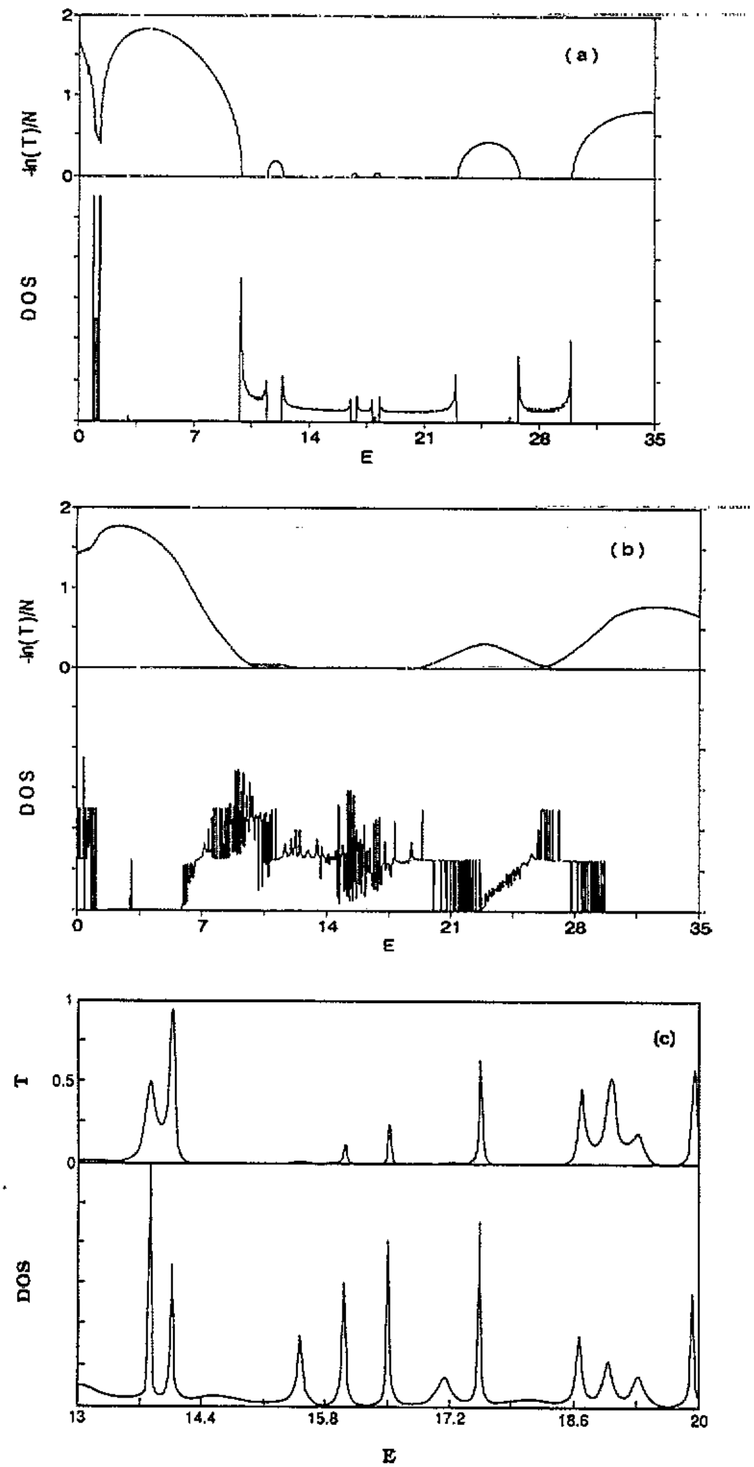

Figure 1. The DOS and $-\ln(T)/N$ for $N = 400$ and (a) $F = 0$, (b) $F = 0.01$. In (b), the subband gaps are almost washed out. (c) The DOS and T for $N = 400$ and $F = 10$. The scale of the DOS is arbitrary.

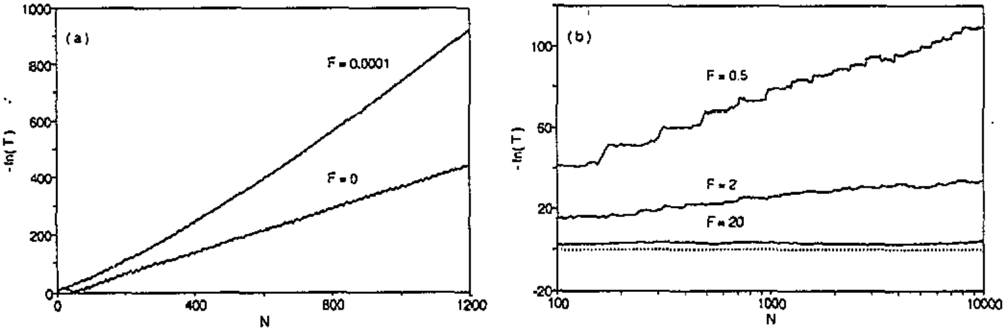

Figure 2. (a) The plots of $-\ln(T)$ against N for different electric fields at $E = 1.250\,121\,725\,6$. (b) The log–log plots of T and N for power-law localized states ($F = 0.5, 2$) and an extended state ($F = 20$) at the same energy.

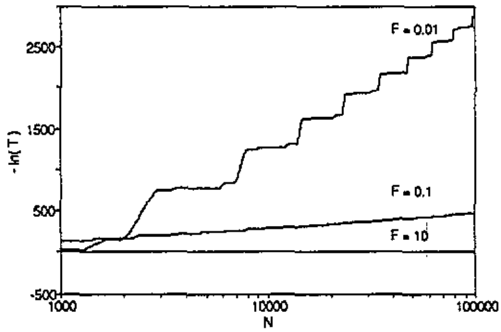

Figure 3. The log–log plots of T and N for different electric fields at $k = \sqrt{E} = 3.231\,11$. The state is extended for $F = 10$.

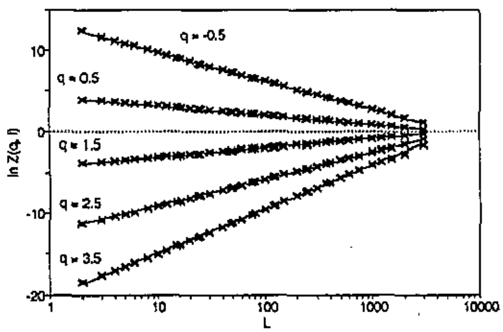

Figure 4. The log–log plots of $Z(q, l)$ against L. The slopes give $\tau(q)$.

of the amplitudes of the wave function makes the largest contribution to $Z(q, l)$ for negative values of q. The good fit of the straight line for all values of L considered means that $\tau(q)$, the slope of the line, is independent of L. The L-independence of $\tau(q)$ confirms that of the $f(\alpha)$ spectrum, which means that the wave function shows multifractal properties at all length scales. One may find continuous $f(\alpha)$ spectra for certain extended states (Siebesma and Pietronero 1987, Johansson and Riklund 1990). But the spectra are maintained only up to critical lengths. In such cases, the slopes of plots change significantly at the critical lengths.

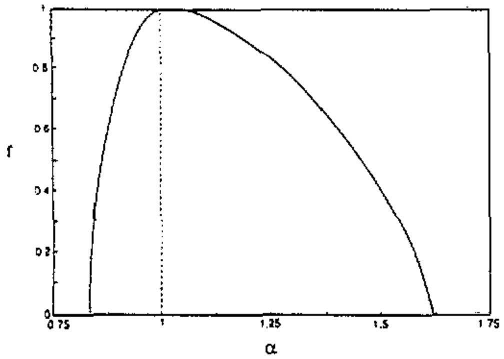

Figure 5. The $f(\alpha)$ spectrum for a field-induced extended wave function. We have $k = 3.231\,11$, $F = 10$ and $N = 6000$.

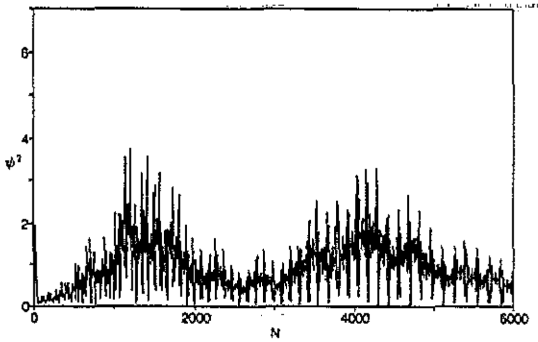

Figure 6. The amplitudes squared of the wave function at $k = 3.231\,11$ and $F = 10$. The amplitudes squared of smaller subpatterns are averaged and the wave function is not normalized.

In figure 5, the continuous $f(\alpha)$ spectrum proves the multifractality of the field-induced extended wave function shown in figure 6. At $q = 0$, we obtain the Hausdorff dimension $f(\alpha(q = 0)) = 1$, the dimension of the support of the measure. From these results, we conclude that the field-induced extended states are not the extended ones in the usual sense. We have obtained a single point $f = \alpha = 1$ for the wave function at the incident momentum $k = 3.231\,11$ in the absence of an electric field. We have performed an MFA on a field-induced extended wave function in a periodic system under an electric field and obtained a similar curve to that in figure 5. These indicate that this multifractality is not due to the incommensurability of the system but due to electric fields.

Finally, we discuss the effect of the ladder approximation on the multifractal feature of the field-induced extended wave function. The ladder approximation has been used successfully in studying the localization properties in electrified chains with periodic and disordered potentials (Nagai and Kondo 1980, Cota *et al* 1985) and is expected to affect mainly the short-range behaviour of the wave function (Soukoulis *et al* 1983). Thus it may affect the multifractality at small length scales. But as one can see from the L-independence of the $f(\alpha)$ spectrum, the multifractality is maintained at all length scales. Therefore, the multifractality is not an unexpected result, in view of the approximation used, and the approximation is considered not to yield any significant change in our results.

4. Summary

In conclusion, we have studied the influence of an electric field on the electronic states in a 1D incommensurate system. We found both localization and delocalization by electric fields. Note that the former has been found in periodic systems and the latter in disordered systems. As F increases, exponentially localized states in the first band change into power-law localized ones via the field-enhanced localized ones. The states become extended for large fields. The field-free extended states in the second band become power-law localized for small fields and extended for large fields. We have shown that the field-induced extended wave functions are multifractal. We have also obtained similar results for the field-induced extended wave functions in a 1D hierarchical system under an electric field (Oh *et al* 1992). Kim (1991) has studied the TB model, which is asymptotically equivalent to equation (1) for large N, with quasiperiodic potentials and found that critical and extended states coexist. We have not found extended states in the usual sense under large fields.

We need to study the electronic spectrum further. Delyon *et al* (1984) did not decide whether the continuous spectrum, which corresponds to extended states for large fields in a disordered system, is absolutely continuous or singular continuous. Taking into consideration our results for an MFA on the wave functions, it seems that the spectrum for large fields is not absolutely continuous but is singular continuous.

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