Localization by electric fields in one-dimensional tight-binding systems

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We show that upon including an electric field within the class of one-dimensional single-orbital, nearest-neighbor, tight-binding models for a general nonperiodic potential, all eigenstates are localized. Irrespective of the details of the potential, the energy eigenstates show factorial localization and the eigenvalue spectrum is discrete, characterizable as a Stark ladder with nonuniform spacing. As an example, all eigenstates of the Aubry model become localized by the electric field, whatever the strength ε_0 of the incommensurate potential, whereas in the field-free case this occurs only if ε_0 exceeds the Aubry critical value. We also present detailed results for the Koster-Slater single-impurity model in an electric field. We indicate briefly some necessary conditions for observing field-enhanced localization.

In recent years several studies[1–4] have been concerned with the influence of constant uniform electric fields on the localization of electrons in the randomly disordered, one-dimensional Kronig-Penney model (KP). In the absence of a field it is generally believed,[5] and there are rigorous theorems,[6] that the eigenstates of one-dimensional systems show exponential localization even for an arbitrarily small degree of disorder. It has been found[1–4] that electric fields destabilize localization to the extent that for weak fields the randomly disordered KP model eigenfunctions show instead only weaker, power-law localization. For large fields the eigenstates are found to be extended. This model is exceptional, for Bentosela *et al.*[7] have shown that if the electron-lattice potential is sufficiently smooth but otherwise arbitrary there are no localized states in the presence of an electric field. On the other hand, it is known that in the case of a single-orbital tight-binding model (TBM) of an electron in a *periodic* potential, the effect of an electric field is to localize eigenstates.[8,9] In particular, the field generates a discrete, uniformly spaced eigenvalue spectrum (Stark ladder, SL) (Refs. 9 and 10) with all eigenfunctions factorially localized [see Eq. (6)]. In this paper we show[11] that in an electric field all eigenstates are localized for *any* non periodic electron potential described by a single orbital TBM. In particular, all eigenstates are factorially localized and the eigenvalue spectrum is necessarily a SL although with nonuniform spacing.

To understand the underlying physics of this general result it is useful to consider the striking special case of the Aubry model[12] which is a single orbital TBM of an electron in an incommensurate potential. In the absence of an electric field, the incommensurate potential splits the unperturbed single band into a complex hierarchy of minibands for potential strengths less than the Aubry critical value. We find that by introducing an electric field all of these extended states are transformed into *factorially* localized states, irrespective of potential strength. At first sight this may appear surprising. One might expect the electric field to induce transitions between the minibands and thereby to further extend the field-free eigenfunctions. In actual fact, the electric field $\mathscr{E}$ destroys the field-free bands in a single-orbital system by removing spatial degeneracies among the lattice sites. The mechanism for generating extended states is the action of the site-hopping matrix element which couples roughly comparable energies of neighboring sites. Introducing an electric field adds an energy disparity $e\mathscr{E}a$ to a pair of adjacent sites, and thus works towards transforming an extended state into a localized state and towards enhancing the localized character of a pre-existing localized state. Indeed, the zero-field localized states of the Aubry model, which occur for potential strengths exceeding criticality, are also transformed by the electric field into factorially localized states. The key point here is that the electric potential drop across large distances completely dominates whatever the form of the site energy ε_n and therefore asymptotically an electron in all cases behaves in the same way, with energy eigenfunctions which turn out to be factorially localized. This underscores the fact that the electric field cannot be treated as a small perturbation to the field-free Hamiltonian. The occurrence of power-law localization in the disordered KP model and the total absence of localization as shown in Ref. 7, can then be traced to electron transitions between the field-shifted site energies for an infinite hierarchy of Wannier basis orbitals. At the end of this article we discuss conditions for which field-enhanced localization might be observed.

After a brief derivation of field-induced factorial localization and the existence of SL spectra for the generic TBM, we present explicit results for the Aubry and Koster-Slater[13] single-impurity models. To the best of our knowledge this is the first investigation of either model in an electric field.

We consider independent electrons in a one-dimensional potential whereby a periodic background potential is sup-

plemented with an arbitrary aperiodic term $V_A(x)$. We restrict our attention to TBM based on a nearest-neighbor tight-binding approximation where the basis states $|n\rangle=\phi(x-na)$, with $\langle n|n'\rangle=\delta_{n,n'}$, utilize a single Wannier orbital. In the absence of an electric field, the site energy is given by $\varepsilon_n=\varepsilon_0\theta_n=\langle n|V_A(x)|n\rangle$. In the Aubry model the quantity $\theta_n=\cos(2\pi nq)$ represents an incommensurate modulation potential for irrational q. In the Koster-Slater model a localized perturbation, corresponding to the introduction of a single impurity, is superimposed upon a periodic potential and $\theta_n=\delta_{n,0}$. Alternatively, θ_n could be taken as a random number as in the Anderson model.[14] Throughout the present work we restrict θ_n to be a bounded function of n, and without loss of generality we suppose that the average of θ_n is zero. The effect of the electric field is to contribute an additional term to ε_n, of the form $e\mathscr{E}an$ where a is the lattice spacing and $\mathscr{E}$ is the magnitude of a uniform electric field directed along the positive direction of the lattice. The time-dependent Schrödinger equation can be written in a convenient dimensionless form as

$$f_{n+1}+f_{n-1}=(2/\beta)[(n+\xi\theta_n)f_n-i\hbar df_n/d\tau] , \quad (1)$$

where $\xi=\varepsilon_0/(e\mathscr{E}a)$, $\beta=2V_1/(e\mathscr{E}a)$, $\tau=\omega_B t$, V_1 is the nearest-neighbor hopping matrix element, and $\omega_B=(e\mathscr{E}a)/\hbar$ is the angular frequency of Bloch oscillations.

The time-independent version of (1) constitutes a three-term recurrence relation among the eigenfunction amplitudes

$$f_{n+1}+f_{n-1}=b_nf_n , \quad (2)$$

where

$$b_n=(2/\beta)(n+\xi\theta_n-W) \quad (3)$$

and the energy eigenvalue E is written as $E/(e\mathscr{E}a)=W$. As shown elsewhere,[15,16] a key quantity for the analysis of the general recurrence relation (2) is an auxiliary function defined by $\Phi=b_0+K_++K_-$. Here $K_\pm$ are the infinite continued fractions

$$K_\pm=-[b_{\pm1}-(b_{\pm2}-\ldots)]^{-1} .$$

If these converge for a given value of W, Eq. (2) possesses solutions f_n^+ and f_n^- which decay to zero[17] for n tending to $+\infty$ and $-\infty$, respectively, and $f_1^+/f_0^+=-K_+$ and $f_{-1}^-/f_0^-=-K_-$. Conversely, if (2) possesses solutions with these properties, Pincherele's theorem[18] insures that K_+, K_-, and Φ exist. A localized eigenfunction exists only if f_n^+ and f_n^- coincide, or equivalently the quantity $\Phi=b_0+K_++K_-$ vanishes for the given choice of parameters of the model, i.e., β,ξ,θ_n,W in the present case. If a band of extended states exists, $K_\pm$ fail to converge for all energies within the band and Φ possesses a branch line along that segment of the real W axis. Testing the convergence of $K_\pm$ and calculating their numerical values are easily performed provided that one is careful to invoke appropriate procedures preventing the occurrence of numerical instabilities, as discussed in detail in Ref. 16.

To obtain the form of the eigenstates of (2) and (3), for positive values of n it is convenient to define a quantity $g_n=b_nf_n/f_{n-1}$, which is seen to satisfy the recurrence relation

$$g_n=[1-g_{n+1}/(b_nb_{n+1})]^{-1} . \quad (4)$$

The solution of (2) can then be formally written as

$$f_n=f_0g_1g_2\ldots g_n/(b_1b_2\ldots b_n) . \quad (5)$$

Now it is easily seen that the denominator of (5) grows as $n!$ for $n\to\infty$ since θ_n is bounded for all n and possesses an average value of zero. Furthermore, the recurrence relation (4) possesses two solutions. It is obvious that for *all* values of W there exists a physically relevant solution of (4) which approaches unity for $n\to\infty$, corresponding to a damped solution $f_n\sim f_{n-1}/n$ of (2), with a correction term of order $1/n^2$ since b_n grows linearly with n. The second solution of (4) is nonphysical since it is easily shown to grow as n^2, corresponding to the growing solution $f_n\sim nf_{n-1}$, and thus, is to be discarded. A similar argument can be made for $n\to-\infty$. It therefore follows that, for all W, (2) and (3) possess decaying solutions $f_n^\pm$. The quantities K_+, K_-, and Φ therefore exist[18] and consequently (2) and (3) fail to possess any extended states. *The physical eigenstates are all localized* and correspond to the energies W which are the roots of $\Phi=0$. In fact, the eigenstates show a generic factorial decay in an electric field since, as we have already remarked, $\Pi_{K=1}^n b_K\sim n!$ and the quantity $\Pi_{K=1}^n g_K$ converges for $n\to\infty$ since $g_n\sim1+O(1/n^2)$. In summary, in the presence of the field, the leading asymptotic behavior of the eigenstates is given by

$$f_n\sim C(\beta/2)^{|n|}/(|n|)! \text{ as } n\to\pm\infty \quad (6)$$

where C is an arbitrary normalization constant. The presence of the electric field in the denominator of (6) [recall $\beta=2V_1/(e\mathscr{E}a)$] confirms what we stated earlier, that these results cannot be obtained by treating $\mathscr{E}$ as a perturbation. Note that the details of θ_n and the choice of eigenvalue W do not appear in the leading term of the asymptotic form of f_n. These formal arguments provide a rigorous framework for the essential physical idea underlying factorial localization which we have presented at the outset. In the following we illustrate the above general arguments by giving explicit results for the Aubry and Koster-Slater models in an electric field.

We have obtained the exact solution of (1) for the Koster-Slater system ($\theta_n=\delta_{n,0}$) subject to the initial condition $f_n(0)=\delta_{n,0}$, corresponding to the injection of the electron at the impurity site. Details of the method of solution will be presented elsewhere.[19] We remark here that (1) is transformed to an equivalent set of equations of the form

$$f_n(\tau)=f_n^{(0)}(\tau)-i\xi\int_0^\tau d\tau' f_0(\tau-\tau')f_n^{(0)}(\tau') , \quad (7)$$

where the quantity $f_n^{(0)}(\tau)$, given by[8]

$$f_n^{(0)}(\tau)=(-1)^n\exp(-in\tau/2)J_n(2\beta\sin(\tau/2)) , \quad (8)$$

is the site probability amplitude in the *absence* of the impurity but in the *presence* of the field and satisfies the same initial condition as does the full solution f_n, and J_n is the Bessel function of the first kind. Note that (7) is an

integral equation of the Volterra convolution form for $f_0(\tau)$ and can therefore be solved using Laplace transform methods. Once f_0 is determined, (7) and (8) provide an expression for f_n for all other sites. The general solution of (7) and (8) can be written in the standard Fourier series representation of an almost-periodic function,[20]

$$f_n(\tau)=\sum_{l=-\infty}^{\infty} r_{n,l}\exp(-iW_l\tau)\ . \tag{9}$$

We have obtained analytic expressions for the expansion coefficients $r_{n,l}$ but these will be presented elsewhere.[19] The infinite set of real quantities W_l are the roots of the eigenvalue equation $\Phi=0$ which in the present problem is equivalent to

$$\sin(\pi W)=\pi\xi J_W(\beta)J_{-W}(\beta)\ . \tag{10}$$

Recall that $\{E_l=W_l\hbar\omega_B\}$ are the energy eigenvalues of the system. The roots of (10) are distributed such that there is one and only one root in every unit interval along the entire real W axis. Moreover, for given values of ξ and β the roots W_l very rapidly approach integer values as $|l|$ is increased. In short, the eigenvalue spectrum consists of discrete energy levels extending over the entire real number system $(-\infty,\infty)$ having an *almost*-uniform spacing $e\mathscr{E}a$. This is a generalization of the equally spaced Stark ladder (SL) scheme proposed by Wannier[9,10] for periodic crystals in an electric field. The deviation from a uniformly spaced SL in the present case is of course due to the impurity which destroys perfect translational periodicity. Setting $\xi=0$ (no impurity), the roots of (10) are the set of all integers and one recovers the original Wannier SL. We mention without further elaboration that as a manifestation of the SL spectrum, for strong electric fields resonant hopping between the impurity and distant sites is possible when the field is tuned to a sequence of ultranarrow, almost-uniformly spaced intervals. This will be discussed in a forthcoming publication.[19]

Introduction of the electric field has a dramatic effect upon the solution of the full time-dependent problem defined by (1). With $\mathscr{E}$ set equal to zero the probability of finding the electron at a given site n in the long-time limit has the asymptotic form[19]

$$|f_n(t)|^2\to\zeta^2(\zeta^2+1)^{-1}[\zeta+(\zeta^2+1)^{1/2}]^{-2|n|}+O(t^{-1/2})\ \text{ as } t\to\infty\ , \tag{11}$$

where $\zeta=\varepsilon_0/(2V_1)$. At first glance (11) describes a localized electron, by virtue of the exponential decay with n. However, note carefully that if we retain only the first term of (11) we obtain

$$P(\infty)=\sum_{n=-\infty}^{\infty}|f_n(\infty)|^2=\zeta(1+\zeta^2)^{-1/2}\ ,$$

which is manifestly less than unity, despite the initial condition $f_n(0)=\delta_{n,0}$. This seeming discrepancy is easily resolved since one can show[19] that the remaining probability, $1-P(\infty)$, is associated with diffusive hopping of the electron to infinity. We have found that with the introduction of the electric field, $|f_n(\tau)|^2$ for all values of τ is a very rapidly decreasing function of n with a very rich time dependence. At all times the electron is wholly confined within a finite interval straddling the impurity site.[19] That is, the electric field completely precludes diffusive hopping; this is the hallmark of localization.[14]

To study the effects of the electric field in the Aubry model we substitute $\theta_n=\cos(2\pi nq)$ in (2). As in the Koster-Slater model, the effect of the electric field in the Aubry model is to create a SL of energy eigenvalues with nonuniform spacing. In Table I we list a selection of successive energy eigenvalues for two different sets of parameters defined as the roots of $\Phi=0$. In Fig. 1 we display a semilog plot of the values of $|f_n|^2$ for two of these energies. For the choice of parameters $\varepsilon_0=0.6V_1$, $e\mathscr{E}a=2V_1$, and $q=0.7/(2\pi)$ which corresponds to $\beta=1$, $\xi=0.3$, the existence of factorially localized eigenstates is in striking contrast to the results in the field-free case for $\varepsilon_0=0.6V_1$. In the latter case all physically admissible eigenstates of the Aubry model are extended. Likewise, if $\varepsilon_0=2.4V_1$, $e\mathscr{E}a=2V_1$, corresponding to $\beta=1$, $\xi=1.2$, the site probability has decreased to less than 10^{-10} of its peak value within *six* sites of the peak. By contrast in the field-free case there exist localized eigenstates when $\varepsilon_0=2.4V_1$, but these decay to zero at a far slower rate. For example, for this case we find an eigenstate for the energy $E/(2V_1)=0.714\,169\,943\,87$, but the site probabilities decrease to below 10^{-10} of the peak value after only approximately 100 sites. Note also that in the field-free case it has been shown (see Ref. 15, footnote 12) that physically admissible eigenstates can occur in the Aubry model only for energies in the range $|E|<\varepsilon_0+2V_1$ whereas the effect of the electric field is to create an infinite Stark ladder of allowed energies.

To test the effectiveness of the numerical algorithm developed by one of us[16] for constructing localized eigenstates of the general TBM of the form (2), we have compared the numerical results for f_n with the asymptotic analytic expression (6). In particular we have utilized the numerical algorithm to calculate the quantity

TABLE I. Selection of successive energy eigenvalues (in units of $e\mathscr{E}a$) belonging to the Stark ladder generated by an electric field in the Aubry model for $q=0.7/(2\pi)$, and $\beta=1.0$, corresponding to $e\mathscr{E}a=2V_1$. (a) $\xi=0.3$, i.e., $\varepsilon_0=0.6V_1$; (b) $\xi=1.2$, i.e., $\varepsilon_0=2.4V_1$.

(a)	(b)
−5.244 365 212 42	−5.855 956 144 48
−4.253 675 907 53	−5.039 042 053 21
−3.138 408 593 72	−3.579 471 095 94
−1.953 233 407 12	−1.803 906 544 58
−0.791 771 254 50	−0.132 678 001 31
0.265 480 325 71	1.038 476 184 61
1.196 279 235 83	1.594 323 184 59
2.042 653 578 10	2.111 345 790 49
2.872 239 638 76	2.652 886 004 43
3.753 924 410 11	3.132 311 819 80
4.747 722 755 98	3.965 368 016 92
5.865 556 049 43	5.437 054 993 61

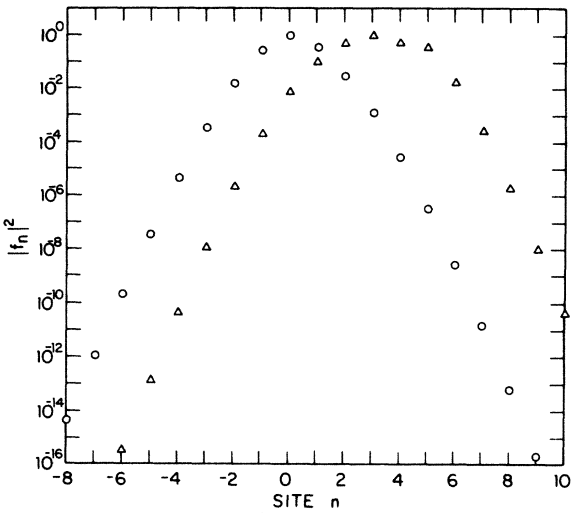

FIG. 1. Site probabilities for two eigenfunctions of the Aubry model in the presence of an electric field. Points labeled ○ and △ correspond to $\beta=1.0$, $Q=0.7$, $\xi=0.3$, $E=0.265\,480\,325\,71(e\mathscr{E}a)$, and $\beta=1.0$, $Q=0.7$, $\xi=1.2$, $E=3.132\,311\,819\,8(e\mathscr{E}a)$, respectively.

$$c_n=-\ln(|f_n|)/\ln(n!)$$

for values of n up to 2×10^4. According to (6) this quantity is asymptotically given by

$$c_n\sim1-\ln(\beta/2)/\ln(n/e)+O(1/n)\ .$$

For all of the energies listed in Table I, the computed values of c_n agree to high precision with this asymptotic analytic form. This provides ample confirmation of the effectiveness of the numerical algorithm

Finally, we believe that the enhancement of localization by an electric field can occur in certain systems even if one drops the restriction of TBM based on a single Wannier orbital. An exact representation of the Hamiltonian can always be given in terms of an infinite set of Wannier basis orbitals, labeled by an index $l=1,2,3,\ldots$. For any given lattice site n there corresponds an infinite hierarchy of site energies of the form $\varepsilon_{n,l}+ne\mathscr{E}a$. Now consider some segment S of the lattice which includes N lattice sites. Suppose that in the absence of the field there is a minimal separation energy $E_G(l)$ between the site energies associated with orbital l and those for any other orbital for the sites in S. A factorially localized (approximate) eigenstate based on orbital l can occur in segment S as long as the energy difference $Ne\mathscr{E}a$ is small compared to $E_G(l)$. Using (6) it is easily seen that for this requirement to be met it is necessary for V_1 to be very small compared to E_G. Rare-gas solids and various ionic crystals are some examples of systems where this condition could be met. By contrast, for potentials of the type considered in Ref. 7 as well as for the disordered KP model one has $V_1\gtrsim E_G$. That is, for the latter systems the condition for the approximate validity of a single orbital TBM cannot be met and, as to be expected, the electric field destabilizes localization.

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