Conditions for Dynamic Localization in Generalized ac Electric Fields

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We examine the conditions for dynamic localization of electrons in a periodic potential due to an applied ac electric field. Using a general one-band model, we establish the surprising result that only electric fields that are discontinuous at all changes of sign can lead to exact dynamic localization. We also develop a general procedure for constructing ac fields that yield dynamic localization and derive an "area condition" for such fields. We confirm this result numerically in a multiband simulation.

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Over the past decades, the behavior of an electron in a periodic potential in the presence of an applied electric field has attracted much attention. The behavior in a dc field was discussed many years ago by Bloch [1] and Wannier [2], and the predictions of localized stationary states—the Wannier-Stark ladder (WSL)—and their dynamic analog, Bloch oscillations (BO), were observed in semiconductor superlattices by Mendez *et al.* [3] and Feldmann *et al.* [4], respectively. More recently, equivalent phenomena were observed in trapped atomic systems [5] and using light propagating in fiber Bragg gratings [6] and coupled optical waveguides [7].

The recent development of strong, tunable THz radiation sources has spurred interest in the dynamics in ac fields. In combined ac and dc fields, one can observe multiphoton absorption [8], absolute negative conductance [9], and fractional WSLs [10]. It was further predicted [11–15] that, for a purely sinusoidal ac field in the nearest-neighbor tight binding (NNTB) approximation, *dynamic localization* (DL) can be achieved for particular field amplitudes. DL is the phenomenon whereby an applied *ac field* results in the continued localization of an initially localized wave packet. However, if one goes beyond the NNTB approximation, DL disappears for a sinusoidal field [14], but can be attained for a square-wave field with the correct amplitude [16,17]. We refer to this type of DL, which occurs for arbitrary band structures and not just in the NNTB approximation, as *exact dynamic localization* (EDL). Here we address the general question as to what types of ac fields lead to EDL. We show that *the only purely ac fields, $E(t)$, that can yield exact dynamic localization are never zero, and hence are discontinuous at all changes in the sign of the field.* In fact, many fields that yield EDL may have additional discontinuities where the field does not change sign. We show that for ac fields that do not contain any such nonessential discontinuities: *If EDL is to be attained, then the total area under the $E(t)$ curve between discontinuities must be an integral multiple of $2\pi\hbar/ed$*, where d is the period of the potential.

Although most DL work refers to electronic systems, many of the phenomena are generic and also occur for atomic [5] and optical [6,7] waves. Though the arguments below apply to all three wave types, we use the electronic terminology for consistency with most of the existing literature. Throughout, we ignore the effects of dephasing; this is justified for optical systems and is a common approximation in the electronic literature [11–15].

The dynamics of a wave packet in a periodic potential, in an arbitrary external time-dependent electric field, has not been solved analytically. However, within a one-band approximation, exact closed form solutions are known. Expanding the electron state, $|\psi(t)\rangle$, in the basis of single-band Wannier functions, $|a_n\rangle$ [16], we obtain

$$|\psi(t)\rangle = \sum_n B_n(t)\,|a_n\rangle\,, \tag{1}$$

where n labels the localization site of the Wannier function $|a_n\rangle$. Substitution into the Schrödinger equation, and assuming lattice inversion symmetry, we obtain

$$i\hbar\dot{B}_n = \sum_m \varepsilon_{n-m}B_m + nedE(t)B_n\,, \tag{2}$$

where the ε_p are the Fourier components of the band's energy dispersion, $\epsilon(k)$. One can show via direct substitution that the solution to Eq. (2) is

$$B_n(t) = e^{-i[\varepsilon_0 t/\hbar + n\gamma(t)]}\sum_m A_{n-m}(t)B_m(0)\,, \tag{3}$$

where

$$\gamma(t) = \frac{ed}{\hbar}\int_0^t E(t')\,dt', \tag{4}$$

is the dimensionless area associated with $E(t)$, and

$$A_m(t) \equiv \int_{-\pi}^{\pi}\frac{dx}{2\pi}\,\exp\left\{imx - i\sum_{p\neq 0}\frac{\varepsilon_{-p}}{\hbar}\,\beta_p(t)e^{ipx}\right\}, \tag{5}$$

where $\beta_p(t) \equiv \int_0^t e^{-ip\gamma(t')}\,dt'$. This result was earlier reported by Zhu, Zhao, and Niu [16]; it holds for arbitrary band dispersion beyond the NNTB approximation.

An electron is considered to be dynamically localized in a field of period τ if it returns to its original state at times $t = \tau, 2\tau, 3\tau, \ldots$. From Eq. (3), this can occur only if $A_m(\tau) = \delta_{m,0}$. Using this, multiplying Eq. (5) by $\exp(-imx')$, and summing over m on both sides, we obtain the condition $\varepsilon_p \beta_p(\tau) = 0$. For this to be true for any band structure, we must have $\beta_p(\tau) = 0$. Thus, EDL occurs only if $\beta_p(\tau) = 0$ for all $p \neq 0$.

Because $\beta_p(\tau)$ is the key to EDL, we now examine the related dimensionless quantity

$$S_p \equiv \beta_p(\tau)/\tau = \frac{1}{\tau}\int_0^\tau e^{-ip\gamma(t)}\,dt\,. \qquad (6)$$

We consider *purely ac fields* without a dc component, so that $\gamma(0) = \gamma(\tau) = 0$. The most studied ac field in DL is sinusoidal: $E(t) = E_1 \sin(\omega t)$, where $\omega \equiv 2\pi/\tau$. For this field, we find $S_p = J_0(p\Omega/\omega)$, where $\Omega = edE_1/\hbar$. For EDL to occur, this must vanish for all p, which is not possible for any Ω/ω. For a NNTB band structure, however, only $S_1 = 0$ is required, which reduces to the usual condition for dynamic localization in a sinusoidal field [11]. Thus, a sinusoidal field yields only DL in the NNTB approximation [14,15].

Until now, the only purely ac field known to exhibit EDL is the square wave which alternates between $\pm E_n$, where $E_n \equiv 4\pi\hbar n/(ed\tau)$ [16,17] and n is a positive integer; indeed, for this field $S_p = 0$ for all $p > 0$. This can be simply understood: The field is constant over time intervals during which n complete dc BO occur. At the end of each interval, the electron returns exactly to its initial state, and thus remains localized. Therefore, although a number of different fields have been reported for which DL or EDL occur [11–16,18], *the general requirements of electric fields that lead to EDL have not been examined; this is the question that we address here.*

Though the infinite set of conditions, $S_p = 0$, required for EDL are straightforward to evaluate for a given field, they are ill-suited to the inverse problem of constructing fields for which EDL occurs. To this end, we define

$$f(x) \equiv \sum_{p=-\infty}^{\infty} S_p e^{ipx}, \qquad \text{where } -\pi < x < \pi\,, \qquad (7)$$

and $S_0 \equiv 1$. Thus, if $S_p = 0$ for $p \neq 0$, then $f(x) = 1$ for $-\pi < x < \pi$. Inserting (6) for S_p we obtain

$$f(x) = \frac{2\pi}{\tau}\int_0^\tau \sum_{m=-\infty}^{\infty} \delta[x - \gamma(t) - 2\pi m]\,dt\,. \qquad (8)$$

We restrict ourselves for now to fields for which $\dot\gamma(t) \neq 0$. This is equivalent to requiring that $E(t) \neq 0$ for all times, and therefore limits us to electric fields that are discontinuous when crossing the horizontal axis. As we show below, this is in fact the only type of field for which EDL occurs. With this condition on $\dot\gamma(t)$, we may write

$$f(x) = \frac{2\pi}{\tau}\sum_{m,j} |\dot\gamma(t_{jm})|^{-1}, \qquad (9)$$

where the t_{jm} follow from $\gamma(t_{jm}) = x - 2\pi m$, where $0 < t_{jm} < \tau$. According to Eq. (9), electric fields that yield EDL can be identified as follows. (i) Consider the functions $\Gamma_m(t) \equiv \gamma(t) + 2\pi m$, with m an integer. (ii) For each x, solve $\Gamma_m(t) = x$ for $0 < t < \tau$. (iii) For each solution, determine $1/|\dot\gamma(t)|$. (iv) For each x, add these values for all solutions. (v) If this sum is independent of x, then the field associated with $\gamma(t)$ leads to EDL.

It is easy to see that Eq. (9) can be satisfied by a square wave. Then γ is triangular, and so the slope at all intersections has the same magnitude. The only remaining requirement is then that the same number of intersections occur for every x. This is guaranteed for γ's with a peak-to-peak amplitude of $2\pi, 4\pi, \ldots$. More general square-wave-type solutions can easily be constructed: We require $x = \gamma(t)$ to be a piecewise linear function, with $\dot\gamma \neq 0$ at all times, and with slope changes only when x is an integer multiple of 2π. This is a simple extension of the dc BO discussed earlier: An integer number of BO occurs in each segment.

Returning to general ac fields, we now show that EDL cannot occur if $\dot\gamma(t) = 0$ at any time. Consider a *continuous* function, $\gamma(t)$, which, since it is also periodic, has at least one minimum and one maximum per period. At the extremum (or inflection point) at, say, $t = t_0$, $\gamma(t)$ can be Taylor expanded as $\gamma(t) = \gamma(t_0) + B(t - t_0)^{q+1} + \ldots$, where B is a constant, and q is a positive integer. Now for x near $\gamma(t_0)$, the integral in Eq. (8) diverges as $[x - \gamma(t_0)]^{-q/(q+1)}$. Since $f(x)$ evidently becomes arbitrarily large near each extremum, and is finite elsewhere, it is not constant. EDL thus does not occur when γ has minima or maxima, i.e., for fields that cross the horizontal axis: *EDL does not occur for continuous ac electric fields.* We refer to discontinuities that occur when the field changes sign as *essential discontinuities.* We can place limits on these essential discontinuities as follows. Consider an ac field and denote the minimum value of $|E|$ by E_0. Then $|d\gamma/dt| = edE_0/\hbar$, and so $\sum |\dot\gamma_i|^{-1} \geq \hbar/edE_0$. Thus, from (9), and since $f(x) = 1$, we find $\tau \geq 2\pi\hbar/edE_0$. Similarly, it follows that if an ac field has an essential discontinuity of magnitude ΔE, then $\tau \geq 8\pi\hbar/ed\Delta E$. Thus, one can only reduce the magnitude of the essential discontinuities by allowing a long ac period.

Having established some general properties of ac fields that yield EDL, we now show how to construct the most important type: those with only essential discontinuities and no others. Note first that, if an essential discontinuity occurs when $\gamma(t) \neq 2\pi n$ (with n an integer), this requires at least one *nonessential* discontinuity to occur. Thus, we consider only fields with essential discontinuities when $\gamma(t) = 2\pi n$. Now condition (9) is more easily implemented as a function of x, in terms of which, however, γ is multivalued. We therefore write it as a sum of invertible segments, denoting times where $\gamma(t) = 2\pi n$ by t_i. We divide γ into N segments, such that $\gamma(t) = \gamma_i(t)$ for $t_{i-1} < t < t_i$, where $i = 1, \ldots, N$. For each segment, $\dot\gamma_i(t) \neq 0$ and is continuous, and, hence, each $\gamma_i(t)$ is invertible. Defining $\gamma_i(t_i) = 2\pi m_i$, then by construction $m_0 = m_N = 0$ and $m_i = m_{i-1} \pm 1$. We define $g_i(x)$ to be the inverse of $\gamma_i(t)$ and rewrite (9) to make the right-hand side an explicit function of x. We then obtain

$$f(x) = \frac{2\pi}{\tau} \sum_{m,i} |g_i'(x - 2\pi m)|. \tag{10}$$

We first consider two-segment functions ($N = 2$) with $t_0 = 0$, $t_1 = \tau/2$, $t_2 = \tau$, and $\gamma(t_1) = 2\pi$. We write the inverses as $g_1(x) = \tau x/4\pi + h(x)$ and $g_2(x) = \tau(1 - x/4\pi) + h(x)$, where $h(x)$ satisfies $h(0) = h(2\pi) = 0$ and $|h'(x)| < \tau/(4\pi)$, but is otherwise arbitrary. The last condition ensures that $\dot{\gamma}_i(t)$ is single valued, so the electric field is finite. When $h(x) = 0$, we recover the square-wave field described earlier. For $h(x) \neq 0$, we obtain from Eq. (10)

$$f(x) = \frac{2\pi}{\tau}\left[\left|\frac{\tau}{4\pi} + h'(x)\right| + \left|-\frac{\tau}{4\pi} + h'(x)\right|\right]. \tag{11}$$

Since $|h'(x)| < \tau/(4\pi)$, we see that $f(x) = 1$ for any $h(x)$, as required for EDL. To present a simple, concrete example, we take $h(x) = a(x^2 - 2\pi x)$, with $|a| < \tau/(8\pi^2)$ so that $|h'(x)| < \tau/(4\pi)$. After inversion and differentiating with respect to t, we then find the following for the electric field:

$$E(t) = \frac{\hbar}{ed}(Z^2 + 4at)^{-1/2}, \qquad 0 < t < \tau/2, \tag{12}$$

where $Z \equiv \tau/(4\pi) - 2\pi a$, and $E(t + \tau/2) = -E(t)$. This field is shown in Fig. 2(a). Note that this procedure leads to an infinite number of solutions even for $N = 2$, but that very few of these can be inverted in closed form.

By using more than 2 segments, the procedure can be extended to construct many more general fields that yield EDL. Without any loss of generality, we let $g_i(x) = b_i x + a_i + h_i(x)$, where $b_i x + a_i$ is the straight line between $(t_{i-1}, 2\pi m_{i-1})$ and $(t_i, 2\pi m_i)$, and the $h_i(x)$ are arbitrary functions such that $h_i(2\pi m_{i-1}) = h_i(2\pi m_i) = 0$ and $|h_i'(x) + b_i| > 0$. Inserting $g_i(x)$ into (10) we obtain

$$f(x) = \frac{2\pi}{\tau}\sum_{i=1}^{N} |b_i + h_i'(x - 2\pi M_i)|, \tag{13}$$

where $M_i \equiv \min[m_{i-1}, m_i]$. Using the inequality on the derivatives, one can show that $f(x) = 1$ iff

$$\sum_{i=1}^{N} \frac{b_i}{|b_i|} |h_i'(x - 2\pi M_i)| = 0. \tag{14}$$

Thus $N - 1$ functions $h_i(x)$ can be chosen freely, while the remaining function must be chosen to satisfy Eq. (14), the only requirement being that the field does not diverge. *Equation (14) is one of the central results of this work* in that it gives the conditions required of any field that is to yield EDL. Though all such fields lead to EDL, they generally are discontinuous at all t_i. However, the h_i can be chosen such that all nonessential discontinuities disappear, and, in fact, the field can be made arbitrarily smooth at all other t_i. By construction, then, all fields thus obtained have an area between discontinuities that is an integer multiple of $2\pi\hbar/ed$. Thus, we obtain an *area condition*: Electric fields that have only essential discontinuities must have an area between adjacent discontinuities that is an integer multiple of $2\pi\hbar/ed$ if they are to yield EDL; this condition on its own is necessary but not sufficient, as Eq. (14) must also be satisfied.

We now provide numerical examples to illustrate the theory and to examine the validity of the one-band approximation for a realistic structure. We consider a GaAs/$\mathrm{Ga}_x\mathrm{Al}_{1-x}\mathrm{As}$ superlattice with $d = 10$ nm, well and barrier widths of 8.5 and 1.5 nm, respectively, a well depth of $V = 400$ meV, and an electron effective mass of 0.067 that of the free electron mass. These parameters correspond to those of typical systems that have been experimentally investigated [3,4]. We take the ac period to be $\tau = 825$ fs, which is well within the range of experimentally achievable periods for THz fields [9,19]. We solve the time-dependent Schrödinger equation via the split-step Fourier method, including all bands but no dephasing. We take the electron to be initially in the maximally localized Wannier function of the lowest miniband localized about $z = 0$.

In Fig. 1 we show the electron probability density versus position as a function of time for a sinusoidal ac electric field with the amplitude that yields DL in the NNTB limit. The localization is now essentially gone after two periods, even though the ratio $|\varepsilon_2/\varepsilon_1|$ is only 0.0938. Thus, even close to the NNTB regime, it is clearly not sufficient to treat DL in the NNTB limit. Figure 2(b) is similar to Fig. 1, but is for the field in Eq. (12), with $a/\tau = -0.01$ [see Fig. 2(a)]. The electron density is essentially periodic for times much longer than for the sinusoidal field; the irregularity appearing by the fifth period is due, in fact, to transitions to higher minibands. We deliberately chose the large magnitude of a to emphasize the difference with the square wave (the instantaneous field reaches values almost

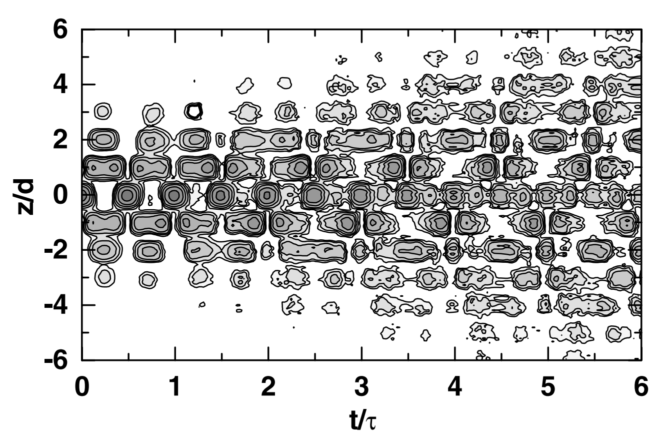

FIG. 1. Electron probability density (log scale) versus time for a sinusoidal electric field with the minimum amplitude that leads to DL in the NNTB approximation.

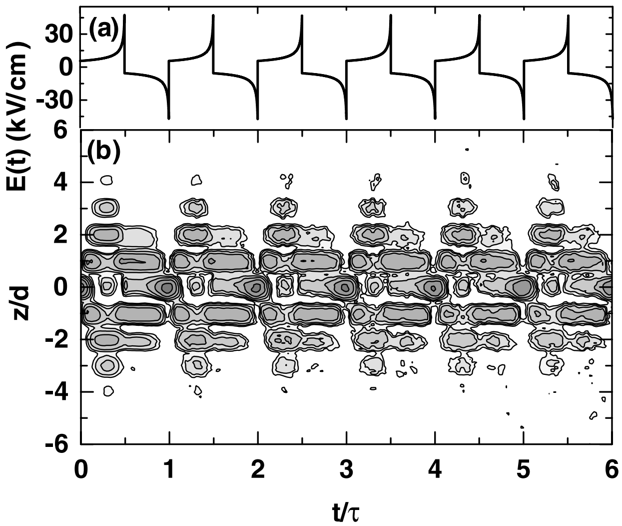

FIG. 2. (a) The electric field of Eq. (12) as a function of time for $a/\tau = -0.01$. (b) The electron probability density (log scale) versus time for the electric field in (a).

5 times that of the square wave with the same period), and to test the theory when coupling to higher bands might not be negligible. Thus, the coupling, while noticeable, does not destroy the effect over times that are much larger than the coherence times (~1 ps) of typical semiconductor superlattice structures [4]. Note that for smoother, lower-intensity fields, or for structures with more widely separated minibands, the tunneling to higher bands is significantly reduced.

The finding that only discontinuous fields lead to EDL, an important conclusion of this work, would seem to be a considerable challenge for the design of experiments. However, numerical experiments, not shown here, indicate negligible changes in the electron density when using finite up- and down-switching speeds that are up to 6% of the total ac period; thus genuinely discontinuous fields are not required for localization for $t \lesssim 6\tau$. Such quasidiscontinuous fields generally yield much better DL than a sine wave. Moreover, in optical systems consisting of arrays of coupled waveguides [7,17] the time variable in electronic systems maps onto a spatial variable in the propagation direction, and the dynamics then takes the form of a dc light beam snaking back and forth in space upon propagation. Because the "ac field" in these arrays can be generated via a spatially varying waveguide curvature [17], "ac fields" that are essentially discontinuous can be constructed in these systems.

In conclusion, we have shown that exact dynamic localization occurs only in ac fields that are discontinuous when changing sign; we have derived an area condition for such fields; and we have demonstrated how to construct such fields. This puts earlier results, obtained in somewhat of an *ad hoc* fashion, into a systematic framework. Our results are well born out by simulations.

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