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On the dynamic localization conditions for dc–ac electric fields proceeding beyond the nearest-neighbour description

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Abstract

Dynamic localization conditions proceeding beyond the nearest-neighbour description have been established by applying the quasi-energy description. The general energy dispersion laws one deals with concern a periodic but commensurable dc–ac field like $E_0 + E_1 f(t)$, for which $f(t) = f(t+T)$ and $\omega_B = P\omega/Q$. Here $\omega_B = eE_0a/\hbar$ and $\omega = 2\pi/T$ stand for the Bloch and ac field frequencies, respectively, while P and Q are mutually prime integers. A reasonable centre of band generalization of such conditions has been proposed.

1. Introduction

The quantum-mechanical description of a charged particles, say electrons, moving on one-dimensional (1D) lattices under the influence of periodic time-dependent electric fields has attracted much attention over the past two decades [1, 2]. Specifically, there is a periodic return of the electron to the initially occupied site when the ratio of the field magnitude to its frequency is a root of the ordinary Bessel function of order zero [3]. These behaviours serve as a signature to the onset of the dynamic localization effects. Such results are able to be reproduced by resorting to the quasi-energy description, too. In this latter case, the dynamic localization conditions rely on the so-called collapse points of the quasi-energy bands, as discussed before [4]. On the other hand, the dynamic localization properties of electrons on the 1D lattice under the influence of dc–ac electric field like [5]

$$E(t) = E_0 + E_1 f_1(t) \tag{1}$$

where $f_1(t) = f_1(t+T)$ are of a special interest for several applications in quantum electronics, with a special emphasis on semiconductor supperlattices. We shall then use this opportunity to discuss further details concerning localization attributes characterizing such fields, by proceeding beyond the nearest-neighbour description. For this purpose a general energy dispersion law like

$$E_d(k) = \sum_{n=0}^{\infty} R_n \cos(nka) \tag{2}$$

will be used. Here k stands for the wavenumber, a denotes the lattice spacing characterizing the 1D lattice, and R_n are pertinent expansion coefficients. Concrete manifestations of dynamic localization conditions will then be established by resorting to the collapse points characterizing general quasi-energy formulae established before [5, 6]. To this aim a commensurability condition such as given by

$$\omega_{\rm B} = \frac{P}{Q}\omega \qquad (3)$$

where P and Q are mutually prime integers will be accounted for. Note that $\omega_{\rm B} = eE_0a/\hbar$ stands for the Bloch frequency [7], while $\omega = 2\pi/T$. To the best of our knowledge, such conditions have not been written down before in an explicit manner, except for the limiting case in which the quotient P/Q becomes an integer [8]. The influence of a dc-bichromatic electric field has also been discussed, but the results concern only quasi-energy expressions proceeding within the nearest-neighbour description [9]. So there are reasons to say that dynamic localization conditions established before have to be updated by accounting for (2) and (3).

2. Preliminaries and notation

Under the influence of a time-dependent electric field

$$E(t) = \frac{\hbar}{ea}\mathcal{E}_{\rm F} f(t) \qquad (4)$$

the energy dispersion law (2) leads to the discrete time-dependent Schrödinger equation:

$$\mathcal{H}_d(n \geqslant 0)\psi_m = \sum_{n=0}^{\infty} V_n(\psi_{m+n} + \psi_{m-n}) - m\mathcal{E}_{\rm F} f(t)\psi_m = {\rm i}\frac{\rm d}{{\rm d}t}\psi_m(t) \qquad (5)$$

which incorporates a sequence of successive next-nearest-neighbour (NNN) hopping effects. The electric charge of the electron is denoted by $-e < 0$, and $\mathcal{E}_{\rm F}$ denotes the field amplitude which has the dimension of a frequency, while $f(t)$ is a dimensionless function characterizing the field modulation. This proceeds via $R_n = 2\hbar V_m$ as well as by virtue of the rule

$$k \rightarrow \frac{P_{\rm op}}{\hbar} = -{\rm i}\frac{\partial}{\partial x} \qquad (6)$$

which also means that the momentum operator $P_{\rm op}$ is responsible for the related sequence of translations. Accordingly, the free-field Hamiltonian implemented by (2) proceeds as

$$\mathcal{H}_d^{(0)}\psi(x) = E_d\left(-{\rm i}\frac{\rm d}{{\rm d}x}\right)\psi(x) \qquad (7)$$

which produces the hopping terms characterizing (5) in terms of the discretization $\psi_m = \psi(ma)$. It is clear that the usual nearest-neighbour (NN) equation gets reproduced as soon as $V_n = 0$ for $n \geqslant 2$. In addition, the $n = 0$-term in (5) can be incorporated in a pure phase factor:

$$\psi_m(t) = {\rm e}^{-{\rm i}2V_0t}c_m(t) \qquad (8)$$

so that

$$\mathcal{H}_d(n \geqslant 1)c_m(t) = {\rm i}\frac{\rm d}{{\rm d}t}c_m(t) \qquad (9)$$

where

$$\mathcal{H}_d(n \geqslant 1) = \mathcal{H}_d^{(0)}(n \geqslant 1) - m\mathcal{E}_{\rm F} f(t). \qquad (10)$$

Resorting to a orthonormalized Wannier basis, say $\langle m|m'\rangle = \delta_{m,m'}$, we have to realize that the Fourier transform (2) relies on the matrix element of the underlying free-field Hamiltonian as follows [5, 9]:

$$\langle 0|H_0|m\rangle = \frac{1}{2\pi}\int_{-\pi}^{\pi} E_d(\widetilde{k})\exp(-\mathrm{i}\widetilde{k}m)\,\mathrm{d}\widetilde{k} = 0 \tag{11}$$

where by now $\widetilde{k}$ stands for ka. We have restricted ourselves to the first Brillouin zone $\widetilde{k} \in [-\pi, \pi]$ as usual.

3. Applying general quasi-energy formulae

The Hamiltonian characterizing (5) and/or (9) is periodic in time with period T. This opens the way to apply the Floquet factorization:

$$C_m(t) = \exp(-\mathrm{i}Et)u_m(t) \tag{12}$$

where $u_m(t+T) = u_m(t)$ such as has been discussed in some more detail before [5, 6]. In order to handle the commensurability condition (3), one resorts to an extra wavenumber discretization like

$$\widetilde{k} = s + 2\pi\frac{l}{Q} \tag{13}$$

where $s \in [-\pi/Q, \pi/Q)$ and $l = 0, 1, 2, \ldots, Q-1$. This latter equation also shows that the Q-denominator is responsible for the number of quasi-energy bands. The quasi-energy is then given by [5]

$$E_{n_1} = \frac{1}{T}\sum_j \langle 0|H_0|Qj\rangle \exp(\mathrm{i}Qjs)\int_0^T \mathrm{d}t\,\exp(\mathrm{i}Qj\theta(t)) + \frac{\omega n_1}{Q} \tag{14}$$

where j and n_1 are integers. Now one has $f_1(t) = \cos(\omega t)$, so that

$$f(t) = \frac{\omega_\mathrm{B}}{\mathcal{E}_\mathrm{F}} + \cos(\omega t) \tag{15}$$

in accord with (1) and (4), which also means that

$$\theta(t) = \mathcal{E}_\mathrm{F}\int_0^t f(t')\,\mathrm{d}t' = \omega_\mathrm{B}t + \frac{\mathcal{E}_\mathrm{F}}{\omega}\sin(\omega t). \tag{16}$$

Using (2) and (11) and inserting $n_1 = 0$ then gives the quasi-energy

$$E_0(s) = \frac{\omega}{4\pi}\sum_{n'=1}^{\infty}(-1)^{Pn'}R_{n'Q}\exp(-\mathrm{i}ns)J_{n'P}\left(n'Q\frac{\mathcal{E}_\mathrm{F}}{\omega}\right) \tag{17}$$

in accord with (2), where the sum is over positive integer realizations n' of the quotient n/Q. It should be specified that $J_m(z)$ denotes the Bessel function of the first kind and of order m. Intermediary relationships like

$$\exp(\mathrm{i}z\sin\omega t) = \sum_{m=-\infty}^{\infty} J_m(z)\exp(-\mathrm{i}m\omega t) \tag{18}$$

and

$$\int_{-\pi}^{\pi}\mathrm{d}\widetilde{k}\cos(j\widetilde{k})\cos(n\widetilde{k}) = \pi\delta_{j,n} \tag{19}$$

have been accounted for, too.

After having arrived at this stage, we have to establish, at the beginning, the collapse points of the quasi-energy band in terms of parameter values for which

$$E_0 = E_0(s; \omega_B/\omega, \mathcal{E}_F/\omega) = 0. \tag{20}$$

One realizes, however, that (20) is unlikely to be fulfilled irrespective of $s \in [-\pi/Q, \pi/Q)$ when the quasi-energy such as is given by (17) contains several terms instead of a single one. In this context, a reasonable 'centre of band' generalization of (20) like

$$E_0(s = 0, \omega_B/\omega, \mathcal{E}_F/\omega) = 0 \tag{21}$$

can be written down just by inserting $s = 0$ instead of $s \in [-\pi/Q, \pi/Q)$. This amounts to considering a selected sequence $Q\widetilde{k}/2\pi = 0, 1, \ldots, Q-1$ instead of $\widetilde{k}/2\pi \in [0, 1)$.

4. Concrete realization of the dynamic localization condition

Let us start with a fixed value of the Q-denominator characterizing (3). Assuming that $R_Q \neq 0$, but $R_{2Q} = R_{3Q} = \cdots = 0$, gives the dynamic localization condition

$$F_1 \equiv J_P\left(Q\frac{\mathcal{E}_F}{\omega}\right) = 0 \tag{22}$$

in accord with (17), which proceeds this time both in terms of (20) and (21). The interesting point is that the complementary contributions to the energy dispersion law for which $R_n \neq 0$ are irrelevant to the dynamic localization condition. More exactly, the dynamic localization occurs irrespective of $\mathcal{E}_F/\omega$ when $R_1 = R_2 = \cdots = R_{Q-1} = 0$. Equation (22) shows that the dynamic localization occurs when $Q\mathcal{E}_F/\omega$ is a root of the Bessel function of first kind and of order P. This equation generalizes the result which has been presented before for the special case in which P/Q becomes an integer [8].

Proceeding step by step, let us now consider that $R_Q \neq 0$ and $R_{2Q} \neq 0$ such that $R_{3Q} = R_{4Q} = \cdots = 0$. This time (20) is ruled out, but (21) yields the dynamic localization conditions like

$$F_2 \equiv R_Q J_P\left(Q\frac{\mathcal{E}_F}{\omega}\right) + (-1)^P R_{2Q} J_{2P}\left(2Q\frac{\mathcal{E}_F}{\omega}\right) = 0 \tag{23}$$

which provides a higher-order generalization of (22). Of course, (22) gets reproduced as soon as $R_{2Q} \to 0$.

Choosing for example $Q = 3$, $P = 1$, $R_Q = 1$ and $R_{2Q} = 1/4$, one readily finds that (23) yields the condition $4J_1(3x) - J_2(6x) = 0$, where $x = \mathcal{E}_F/\omega$. This leads in turn to the roots

$$x_1 \cong 1.311; \qquad x_2 \cong 2.831; \qquad x_3 \cong 3.426, \ldots \tag{24}$$

which are responsible for the appearance of dynamical localization effects. This results in small corrections to the $\mathcal{E}_F/\omega$ roots implemented by (22) via $J_1(3x) = 0$, i.e. to

$$x_1 \cong 1.266; \qquad x_2 \cong 2.366; \qquad x_3 \cong 3.366, \ldots \tag{25}$$

respectively. The onset of such roots is displayed in figure 1.

5. Conclusions

In this paper we have succeeded in establishing the dynamic localization conditions characterizing the motion of an electron in a 1D lattice with hoppings going beyond the NN description in the presence of dc–ac electric fields like (15) for which the commensurability condition (3) is fulfilled. This proceeds in terms of the collapse points characterizing the centre

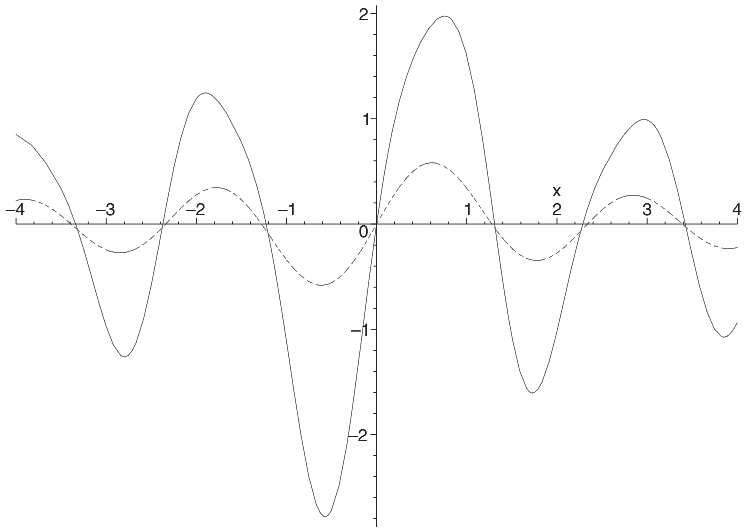

Figure 1. The $\mathcal{E}_F/\omega$-dependence of F_1 (dashed curve) and F_2 (solid curve).

of the quasi-energy band (17), which amounts to considering that $s = 0$. Any such fixing is accord with the very s-independence of (5), which also means that (21) can be viewed as a reasonable generalization of (20). The dynamic localization conditions obtained in this manner are useful in the description of higher harmonic generation [10], but related resonance phenomena characterizing several areas of physics can also be invoked [11]. Moreover, the present results are also able to provide a better understanding of transport and optical properties. The generalization of dynamic localization conditions characterizing dc-bichromatic fields [9] is also of further interest. The same concerns apply to dc-trigonal electric fields discussed recently [12].

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