Acceleration theorem for Bloch oscillators

Vincenzo Grecchi*
Dipartimento di Matematica, Università di Bologna, Piazza di Porta S. Donato 5, I–40127 Bologna, Italy

Andrea Sacchetti†
Dipartimento di Matematica, Università di Modena e Reggio Emilia, Via Campi 213/B, I–41100 Modena, Italy

(Received 14 July 2000; published 15 May 2001)

In this paper, we give the Heisenberg position operator in the crystal momentum representation and we prove the acceleration theorem for Bloch oscillators. As an application, we discuss the motion of well localized states.

DOI: 10.1103/PhysRevB.63.212303 PACS number(s): 73.21.−b, 03.65.−w, 73.40.Gk

In a previous research,[1] we have given the rigorous behavior of a generic Bloch oscillator (BO) in the crystal momentum representation (CMR). In particular, we have shown the existence of a phase factor, see Eq. (5) below, in the expression of an oscillator that does not undergo a simple uniform translational motion in the crystal-momentum space. It was clear that this phase factor is essential in order to obtain the correct behavior of the state in the position-coordinate space. In particular, it was shown the generic breathing mode motion as a consequence of the same phase factor.

Now, we return to the same problem in order to give the Heisenberg position operator and to prove the acceleration theorem. Moreover, we show the existence of a class of oscillators uniformly localized in the crystal-momentum space and relatively (with respect to the full region of oscillation) localized in the position coordinate space.

In order to understand the new results, let us recall the full problem and the existing results. One of the basic tools in the solid state physics is the so-called acceleration theorem, which concerns the motion of a single electron in a regular crystal subjected to a steady and uniform electric field.[2] Let $\psi(x,t)$ be the electron wave function and let

$$\mathbf{a}(k,t)=(a_n(k,t))_{n\in N}\in\mathcal{H}=\bigoplus_{n=1}^{\infty} L^2(\mathcal{B},dk)$$

be the wave function in the CMR; $\mathcal{B}$ is the Brillouin zone, i.e., it is the torus $\Re/b$ represented by the interval $(-b/2,b/2]$, k, the crystal momentum variable, is an element of $\mathcal{B}$, $b=2\pi/d$ is the period of the reciprocal lattice and d is the period of the crystal.

Let us point out the existence of different definitions for the acceleration theorem. In the Kittel textbook[2] the hypothesis of the uniform translational motion in the crystal momentum space of the states is defined as the acceleration theorem. Thus, the validity of this kind of acceleration theorem should be equivalent to the existence of Bloch oscillators restricted to one band and moving following the equation: $a_n(k,t)=a_n(k-ft/\hbar,0)$. Actually, there is a rigorous version of this theorem given by Calloway,[3] hereafter called the theorem ''of the crystal momentum velocity'' (CMV), which is expressed by the following equation:

$$\langle k\rangle^t=\langle k+ft/\hbar\rangle^0=\langle k\rangle^0+ft/\hbar, \tag{1}$$

where $f=eF$, e is the electron charge and F is the strength of the electric field and

$$\langle k\rangle^t=\sum_{n=1}^{\infty}\int_{-b/2}^{b/2}k|a_n(k,t)|^2\,dk$$

denotes the mean value of the crystal momentum k on the state $\mathbf{a}(k,t)$. This CMV theorem implies that $\langle k\rangle^t$ is a periodic function with period $T_B=2\pi\hbar/fd$, but not the existence of the BO's.[4] Recent studies, both numerical[5] and experimental,[6] have provided a more detailed description of Bloch oscillators. In particular, it has been shown that Bloch oscillators ''breathe,'' that is, the electron wave function $\psi(x,t)$ is localized within an interval that periodically expands and shrinks. Let us recall that the breathing behavior has been previously computed in the case of tight-binding models.[7] As pointed out in Ref. 8 we note that Eq. (1), while predicting the existence of Bloch oscillators, does not afford a full description of these facts. As we will show, this is due to the fact that the CMV theorem (1) is clearly independent of the phase factor (5).

In this paper we consider the asymptotic expression of BO's in the limit of weak electric field from which the theoretical explanation of the breathing behavior in the general case follows.[1] As a result, we give the asymptotic expression of the position's time-dependent operator with its expectation value [see Eq. (9) below] and its variance for weak external field. Moreover, we prove the acceleration theorem giving the expression of the acceleration (called also ''the effective inverse mass'') operator in terms of the second derivatives of the band functions [see formula (12) below].

To this end, we consider the time-dependent Schrödinger equation in the crystal momentum representation

$$i\hbar\frac{\partial\mathbf{a}}{\partial t}=H_f\mathbf{a},\quad H_f=-if\frac{\partial}{\partial k}+E-fX, \tag{2}$$

where $E=\mathrm{diag}(E_n(k))$, $E_n(k)$ are the periodic band functions and $X=[X_{n,m}(k)]_{n,m\in N}$ is the coupling term between the bands. Let us ignore the coupling term fX for the present; in such a case, the operator H_f defined on the Hilbert space $\mathcal{H}$ admits a sequence of ladders of real eigenvalues

$$E_{n,j}=E_{n,0}+j\ df, \quad j\in Z, \tag{3}$$

where $E_{n,0}=(1/b)\int_{-b/2}^{b/2}E_n(k)dk$ with associated eigenvectors $\mathbf{w}^{n,j}(k)=e^{ijdk}w^n(k)\mathbf{e}^n$, where $\mathbf{e}^n=(\delta_m^n)_{m\in N}$, $\delta_m^n=1$ if $n=m$ and 0 otherwise, and

$$w^n(k)=\exp\left[\frac{i}{f}\int_0^k [E_{n,0}-E_n(q)]dq\right].$$

Therefore, if the coupling term is absent, we can write that the solution of Eq. (2) is formally given by

$$\mathbf{a}(k,t)=\sum_{j,n} c_{n,j}e^{-iE_{n,j}t/\hbar}\mathbf{w}^{n,j}(k)$$
$$=\sum_{n\in N} w^n(k)e^{-iE_{n,0}t/\hbar}\left[\sum_{j\in Z} c_{n,j}e^{idj(k-ft/\hbar)}\right]\mathbf{e}^n.$$

The coefficients $c_{n,j}$ are given by

$$c_{n,j}=\frac{1}{b}\langle \mathbf{a}^0,\mathbf{w}^{n,j}\rangle_{\mathcal{H}}=\frac{1}{b}\int_{-b/2}^{b/2}a_n^0(k)e^{-idjk}\overline{w^n}(k)dk,$$

where $\mathbf{a}^0(k)=\mathbf{a}(k,0)$ is the initial state in the crystal momentum representation and $\overline{w^n}$ denotes the complex conjugation of w^n; that is, they are the Fourier coefficients of the function $a_n^0(k)\overline{w^n}(k)$. Hence, the above sum, with respect to the index j, is the Fourier series of $a_n^0\overline{w^n}$ at $k-ft/\hbar$. Combining the terms $e^{-iE_{n,0}t/\hbar}$, $\overline{w^n}(k-ft/\hbar)$, and $w^n(k)$ in a single term $\Phi_n(k,t)$, we obtain the final equation

$$a_n(k,t)=\Phi_n(k,t)a_n^0(k-ft/\hbar), \tag{4}$$

where $\Phi_n(k,t)$ is a phase factor given by

$$\Phi_n(k,t)=e^{i\theta_n(k,t)}, \quad \theta_n(k,t)=-\frac{1}{f}\int_{k-ft/\hbar}^{k}E_n(q)dq, \tag{5}$$

and it is such that

$$\theta_n(k,t)=\theta_n(k+b,t)=\theta_n(k,t+T_B)+bE_{n,0}/f.$$

When we restore the coupling term fX, the ladders of real eigenvalues (3) become ladders of resonances, the so-called Wannier-Stark resonances.[9] Thus it follows that formula (4) must be corrected by means of a slow damping term due to the tunneling effect between the bands and of a remainder term that goes to zero as f goes to zero.[10] Since these corrections can be ignored for any time $t\in[0,T_t]$, where typically $T_t\gg T_B$ for a small electric field,[11] we can conclude that Eq. (4) is (asymptotically) correct for times that are not too great and for a small electric field even if a coupling term is present.

Formula (4) represents the actual behavior of BO's. Let us notice the presence of the phase factor (5) whose motion is not simply a translation on the torus. We emphasize that the phase factor does not contribute to $\langle k\rangle^t$, hence Eq. (4) can be seen as a new version of the CMV theorem that implies Eq. (1). In order to study the time behavior of the Bloch oscillators we go back to the electron wave function in the position coordinate space[12]

$$\psi(x,t)=\sum_{n=1}^{\infty}\int_{-b/2}^{b/2}a_n(k,t)\varphi_n(k,x)dk, \tag{6}$$

where $\varphi_n(k,x)$ are the Bloch functions $\varphi_n(k,x)=e^{ikx}u_n(k,x)$, where $u_n(k,x)=u_n(k,x+d)$ are periodic functions.

If we assume, for the present, that the state is initially prepared in one band, for instance the first one, then the acceleration theorem in the form (4) demonstrates that for any time $t\leqslant T_t$ the electron stays in the same band and that by introducing the new variables $\tau=ft/\hbar$ and $\xi=fx$, the leading term of the right-hand side of Eq. (6) takes the form

$$\int_{-b/2}^{b/2}a_1^0(k-\tau)u_1(k,x)\exp\left[\frac{i}{f}\left(k\xi-\int_{k-\tau}^{k}E_1(q)dq\right)\right]dk$$

which can be evaluated, within the limit of a small f, by means of the stationary-phase theorem. Stationary phase points are the real solutions, belonging to the Brillouin zone $\mathcal{B}$, of the equation

$$E_1(k-\tau)-E_1(k)+\xi=0. \tag{7}$$

Let

$$\eta(\tau)=\max_{k\in\mathcal{B}}[E_1(k-\tau)-E_1(k)] \tag{8}$$

be a periodic function with period $\tau_B=|f|T_B/\hbar=b$ with maximum value at $\tau=b/2$ equal to the width B_1 of the first band and minimum value at $\tau=0$ equal to zero. By definition, Eq. (7) has real solutions belonging to $\mathcal{B}$ when $\xi\in[-\eta(\tau),\eta(\tau)]$, otherwise it has complex solutions with an imaginary part different from zero. Therefore, in the limit of a small electric field and for times that are not too great, the amplitude of the electron wave function (6) is, generically, of the order $\sqrt{f}$ for any $\xi\in[-\eta(\tau),\eta(\tau)]$ and it is exponentially small outside this interval. Hence, we conclude that the Bloch oscillator wave function $\psi(x,t)$, initially prepared in one band, is localized within the interval $[-\eta(\tau)/f,\eta(\tau)/f]$ with amplitude of the order $1/f$, which periodically expands and shrinks, i.e., we replicate the breathing behavior of the Bloch oscillator. The maximum amplitude of this interval is given by $2B_1/f$ according to the Zener tilted band picture.[13]

In order to give a more detailed description of the dynamics of Bloch oscillators we now consider the time behavior of the position's expectation value (called also *center of mass*) defined as

$$\langle x\rangle^t=\int_{-\infty}^{+\infty}x|\psi(x,t)|^2\ dx.$$

It is a matter of simple computation to find, within the limit of a small electric field, that from the time-dependent Schrödinger equation in the form $fx\psi=-i\hbar\dot{\psi}+(p^2/2m)\psi+V\psi$, from Eq. (6), from the fact that $\int_{-\infty}^{+\infty}\overline{\varphi_n}(x,k)\varphi_m(x,k')dx=\delta(k-k')\delta_n^m$, and from the CMV theorem in the form (4) it follows that the leading term is given by

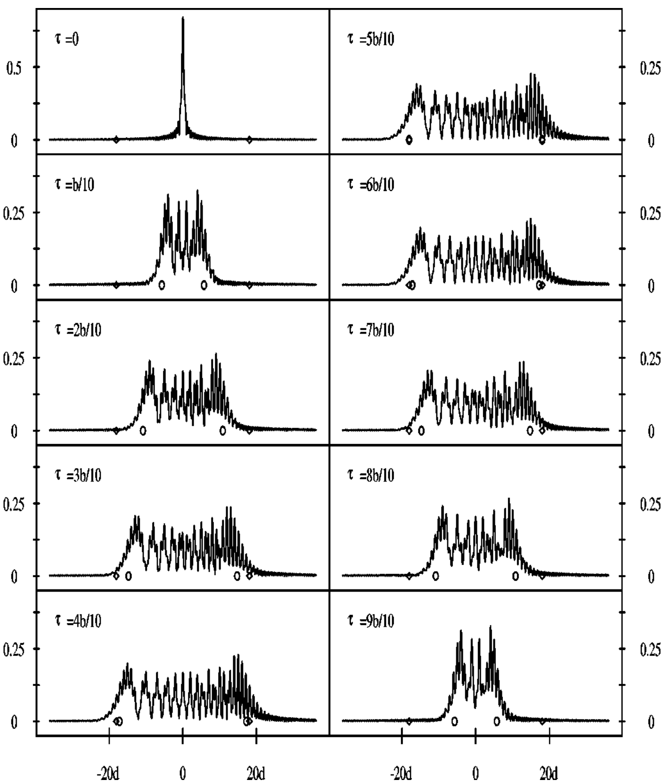

FIG. 1. This picture shows the time evolution of the absolute value $|\psi(x,t)|$ of the electron wave function for different values of τ where $\tau = ft/\hbar$ (Ref. 15). The wave function, initially prepared in an exact Wannier state localized on the zeroth site of the superlattice, symmetrically spreads in space and returns to its initial shape after a Bloch period T_B. As appears from the picture, the wave function is localized inside the interval $[-\eta(\tau)/f, +\eta(\tau)/f]$ and the position's expectation value remains fixed. Circle points denote the values $\pm\eta(\tau)/f$ and diamond points denote the values $\pm B_1/f$.

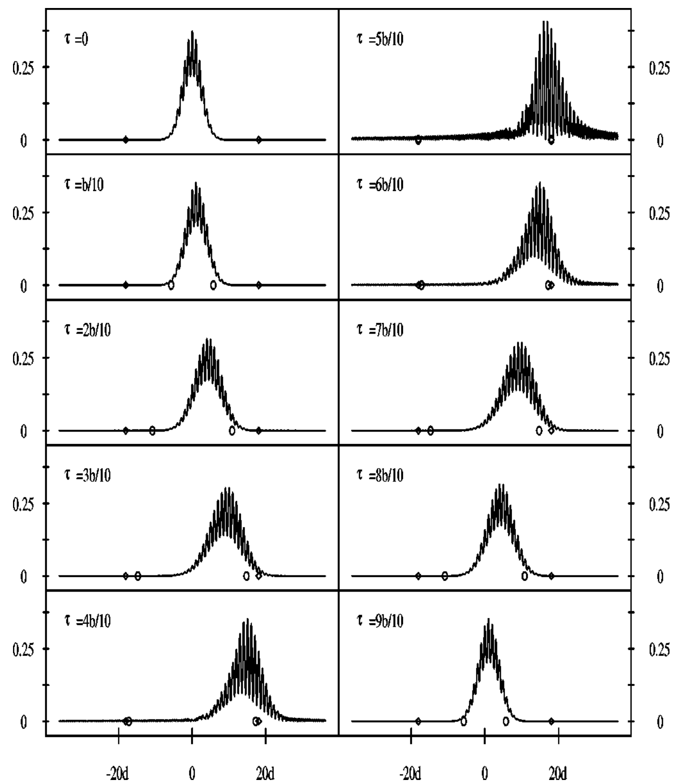

FIG. 2. This picture shows the time evolution of the absolute value of an *optimal* electron wave function that initially is not sharply localized on one site; in such a case we observe an asymmetrical breathing behavior and, in particular, the center of the wave function oscillates in space too, in agreement with Eq. (14). The variance appears almost constant and the wave packet moves with no marked changes in shape.

$$\langle x\rangle^t \sim \sum_n \int_{-b/2}^{b/2} |a_n^0(k)|^2 \Xi_n^t(k)\,dk + x^0, \tag{9}$$

where

$$\Xi_n^t(k) = \frac{1}{f}[E_n(k+ft/\hbar) - E_n(k)] \tag{10}$$

is the multiplicative term of the Heisenberg position operator acting on the nth band space. We point out that $\Xi_n^t(k)$ periodically depends on t. The term x^0 is independent of time and it represents the mean value of the differential part $i\partial/\partial k$ of the Heisenberg's position operator. In particular, $x^0 = 0$ if a_n^0 are real-value functions, i.e., $a_n^0 = \overline{a_n^0}$ for any n. Moreover, it follows that $\langle x\rangle^t = \langle x\rangle^{-t}$ if a_n^0 are even functions, i.e., $a_n^0(-k) = a_n^0(k)$ for any n. As a result of Eq. (9), there immediately follows the acceleration theorem in the coordinate space within the limit of a small electric field

$$\frac{d^2\langle x\rangle^t}{dt^2} \sim \frac{f}{\hbar^2} \sum_n \int_{-b/2}^{b/2} |a_n^0(k)|^2 [E_n''(k+ft/\hbar)]\,dk; \tag{11}$$

the second derivative of the band functions, computed at $k + ft/\hbar$, defines the effective inverse mass operator in the Heisenberg picture.

Regarding the computation of the variance $S^t = \langle [x - \langle x\rangle^t]^2\rangle^t$, the same arguments give that

$$S^t \sim \sum_n \int_{-b/2}^{b/2} |a_n^0(k)|^2 [\Xi_n^t(k)]^2\, dk - (\langle x\rangle^t)^2 + S^0 \tag{12}$$

within the limit of a small electric field, where $S^0 = \sum_n \int_{-b/2}^{b/2} |a_n^0(k)'|^2\, dk$ and where we assume, for the sake of definiteness, that any a_n^0 is a real-value function.

We conclude by considering the time evolution for two different wave packets. In the first case, let us suppose that the electron has been initially prepared in an exact Wannier state, for instance $a_1^0(k) \equiv 1/\sqrt{b}$ and $a_n^0(k) \equiv 0$ for any $n > 1$, that is, the electron wave function is initially localized on one site of the superlattice (see Fig. 1 at $\tau = 0$). The electron wave function given by Eq. (4), (5), and (6) exhibits a symmetrical motion (see Fig. 1); in particular, the center of the wave function remains fixed, i.e., $\langle x\rangle^t \equiv 0$ and the variance is a time-dependent function of the order $1/f^2$.

In the second case, let us suppose that the initial wave function is not sharply localized on one site, for instance,

$$a_1^0(k) = e^{-(k-k_0)^2/2\sigma^2}/[\pi\sigma^2]^{1/4} \tag{13}$$

for some k_0 and $\sigma > 0$ small enough (see Fig. 2 at $\tau = 0$ with $\sigma = 0.1$ and $k_0 = 0$), periodically arranged on the torus $\mathcal{B}$. The electron wave function now exhibits an asymmetrical breathing behavior and, in particular, the center of mass oscillates in space too (see Fig. 2). In particular, for σ small enough, it follows that

$$\langle x \rangle^t \sim \Xi_1^t(k_0)[1 + O(\sigma)], \tag{14}$$

that is, the center of the wave packet oscillates in an interval with amplitude B_1/f. It is also clear that the state is very well localized in the crystal momentum space. Moreover, the square root of the variance giving the spread of the wave packet in the position coordinate space is of order σ/f, that is, it is uniformly small with respect to the range of oscillation. Therefore, the center of mass represents the position of the particle with a reasonable error; in such a case, as explained in Ref. 14, it is expected that by means of an inelastic scattering process, the center of mass of this Bloch oscillator shifts in the field direction contributing to the current.

In conclusion, in this paper we have put on solid bases the usual definition of the effective mass in the case of periodic potential. We have shown the origin of the acceleration theorem from the correct expression of the BO's and the position operator. As a consequence, we have given the behavior of the center of mass and of the spread of a BO. The analytical and numerical applications regard, in particular, well localized states that can be of some experimental interest.

This work was partially supported by the Italian MURST, INDAM-GNFM, and INFN.

*Email address: Grecchi@dm.unibo.it

† Email address: Sacchetti@unimo.it

[1] V. Grecchi and A. Sacchetti, Commun. Math. Phys. **197**, 553 (1998).

[2] See the paper by F. Rossi, in *Theory of Transport Properties of Semiconductor Nanonstructures*, edited by E. Schöll (Chapman and Hall, London, 1998), for a review on this subject. See also the book by C. Kittel, *Quantum Theory of Solids*, 2nd ed. (Wiley, New York, 1987).

[3] See the book by J. Calloway, *Quantum Theory of the Solid State* (Academic Press, New York, 1974); especially formulas (6.1.13a) and (6.1.13b) and the related remarks.

[4] The first theoretical analysis of Bloch oscillators goes back to the paper by Bloch himself, F. Bloch, Z. Phys. **52**, 555 (1928); see F. Bentosela, Commun. Math. Phys. **68**, 173 (1979) for a rigorous proof of the existence of metastable states with a lifetime larger than the Bloch period; C. Waschke, H. Roskos, R. Schwendler, K. Leo, H. Kurz, and K. Köhler, Phys Rev. Lett. **70**, 3319 (1993) gave the experimental evidence of Bloch oscillators in superlattices. Recently, Bloch oscillators have been observed in waveguide arrays too [see T. Pertsch, P. Dannberg, W. Elflein, A. Bräuer, and F. Lederer, *ibid.* **83**, 4752 (1999); R. Morandotti, U. Peschel, J. S. Aitchison, H. S. Eisenberg, and Y. Silberberg, *ibid.* **83**, 4756 (1999)].

[5] A. M. Bouchard and M. Luban, Phys. Rev. B **52**, 5105 (1995).

[6] V. Lyssenko, G. Valusis, F. Löser, T. Hasche, K. Leo, M. Dignam, and K. Köhler, Phys. Rev. Lett. **79**, 301 (1997).

[7] M. Grifoni and P. Hänggi, Phys. Rep. **304**, 299 (1998), Chap. 4.

[8] R. B. Liu and B. F. Zhu, Phys. Rev. B **59**, 5759 (1999).

[9] The existence of Wannier-Stark resonances has attracted great interest; see G. Nenciu, Rev. Mod. Phys. **63**, 91 (1991) for a review. The proof of existence for a class of periodic potentials has been given by V. Grecchi, M. Maioli, and A. Sacchetti, Commun. Math. Phys. **159**, 605 (1994).

[10] In fact, the proof of this result has been given by V. Grecchi and A. Sacchetti, Commun. Math. Phys. **197**, 553 (1998) where it was assumed that the first N gaps are open, for some $N \geqslant 1$ and the others are closed, and that the state is initially prepared in the first N bands.

[11] For an estimate of the tunneling time T_t related to the lifetime of the Wannier-Stark states, see M. Glück, A. R. Kolovsky, and H. J. Korsch, Phys. Rev. Lett. **83**, 891 (1999).

[12] See formula (6.1.4) in Ref. 3.

[13] C. Zener, Proc. R. Soc. London, Ser. A **145**, 523 (1934).

[14] S. Rott, P. Binder, N. Linder, and G. H. Döhler, Phys. Rev. B **59**, 7334 (1999).

[15] For argument's sake, we consider the explicit model with periodic potential given by $V(x) = 2\rho^2 \,\mathrm{sn}^2(x;\rho)$ where $\mathrm{sn}(x;\rho)$ is the Jacobian elliptic function with modulus $\rho \in (0,1)$. In such a case, the first band has amplitude $B_1 = 1 - \rho^2$; it is also possible to obtain an (implicit) expression for the band functions and the Bloch functions, see A. Sacchetti, Maple Tech. Newsl. **4**, 28 (1997). We fix $\rho = 0.8$, $\hbar = 2m = 1$ and the electric field strength such that $f = 0.005$, hence $d \approx 4$ and $2B_1/f = 144 \approx 36d$. Here, we make use of dimensionless units.