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Quasienergy states for a Bloch electron in a constant electric field

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Abstract. A theorem is formulated for constructing quasienergy states for the problem of a Bloch electron in a constant electric field. It is shown that time-dependent solutions of the problem can also be made to be eigenstates of the commuting electric and time translations. The latter define the period of the quasienergy states. The Wannier–Stark ladders and the Bloch oscillations are considered in the framework of the quasienergy states.

Conventionally, quasienergy states can appear when the Hamiltonian is a periodic function of time. One can then construct solutions of the time-dependent Schrödinger equation which are also eigenstates of translations in time by the period T of the problem. By definition these are the quasienergy states [1]. In this context the quasienergy states were recently considered for the problem of a Bloch electron in a periodic-in-time electric field [2–6]. It is instructive to compare quasienergy states with Bloch states in a periodic-in-space potential. While the former are solutions of the time-dependent Schrödinger equation which are also eigenstates of finite translations in time, the latter are eigenstates of both the Bloch Hamiltonian and the finite translations in space. Correspondingly, the eigenvalues of the finite translations in time are the quasienergies [1] and the eigenvalues of the finite translations in space are the quasimomenta [7]. There is also an analogy between these two problems in another aspect. As is well known, one can define Bloch states when the periodic potential is zero. These are the free electron states with a conserved momentum. For them the lattice constant and the quasimomentum Brillouin zone are completely arbitrary. The analogous problem for quasienergy states is the time-independent Hamiltonian with its corresponding stationary states. For the latter the energy is conserved while the time period and the quasienergy Brillouin zone are completely arbitrary.

The problem of a Bloch electron in a constant electric field has a long history [7] and has also been of much recent interest. There are, in general, two aspects to this problem which are not independent. One of them is the stationary approach which has to do with the Wannier–Stark ladders [8]. These ladders were a subject of controversy [9] and theoretically the calculations of their life times seems to remain a challenging problem [10]. On an experimental level, important progress was made when these ladders were observed in superlattices [11, 12]. The other aspect of the constant electric field problem has to do with Bloch oscillations which were already considered in the very early stages of the quantum theory of solids [7]. These oscillations are closely connected to the Wannier–Stark ladders and there are a number of recent publications where they were observed [13–17]. For both aspects of the problem of a Bloch electron in a constant electric field experiment seems to be ahead of the theory. Thus there are no clear theoretical guidelines for the conditions

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under which the Wannier–Stark ladders and the Bloch oscillations should be observable experimentally.

In this paper the problem of a Bloch electron in a constant electric field is considered in the framework of quasienergy states. As mentioned above, the trivial solution would be just to consider the stationary states. However our interest will be in constructing time-dependent solutions which are non-trivial quasienergy states and which are closely related to the Bloch oscillations. For this purpose use is made of the electric translations [18] which are time-dependent operators. In a way similar to the procedure of [5] for a time-dependent electric field, we shall look for quasienergy states for the time-independent Hamiltonian. A general theorem which connects the stationary states of the problem in the kq representation with the time-dependent solutions in the x representation [19] is used. In the one-band approximation the latter states turn out to be the quasienergy solutions for the Bloch oscillations. The quasienergies themselves are calculated including the geometric phase for the corresponding energy band [20].

The time-dependent Schrödinger equation in one dimension for the Bloch electron in a constant electric field E is

$$\mathrm{i}\hbar\frac{\partial\psi(x,\ t)}{\partial t} = \left[\frac{p^2}{2m} + V(x) + eEx\right]\psi(x,\ t) \tag{1}$$

where $V(x)$ is the periodic potential and $V(x+a) = V(x)$ with a being the lattice constant. It is convenient to rewrite equation (1) in the form [5]

$$\left(\mathrm{i}\hbar\frac{\partial}{\partial t} - H\right)\psi(x,\ t) \equiv S\psi(x,\ t) = 0 \tag{2}$$

where H is the Hamiltonian of equation (1) and, by definition, S is the operator

$$S = \mathrm{i}\hbar\frac{\partial}{\partial t} - H. \tag{3}$$

Since the Hamiltonian is time independent there is no special time period for which one can define non-trivial (not stationary) quasienergy states, and any translation in time commutes with S. However, we shall be interested in time-dependent solutions of (1) or (2) which are also eigenstates of the electric translations [18]

$$\beta(a) = \exp\left(\frac{\mathrm{i}}{\hbar}pa + \frac{\mathrm{i}}{\hbar}eEat\right). \tag{4}$$

Such eigenstates will be denoted by $\psi_{k_E}(x,\ t)$, where k_E is the electric quasi-momentum. We have

$$\beta(a)\psi_{k_E}(x,\ t) = \exp\big(\mathrm{i}k_E a\big)\psi_{k_E}(x,\ t). \tag{5}$$

Now $\psi_{k_E}(x,\ t)$ can no longer be chosen as a stationary solution of the Schrödinger equation (equation (1)) despite the fact that the Hamiltonian of this equation is time independent. One can, however, still choose $\psi_{k_E}(x,\ t)$ to be a quasienergy state corresponding to a translation in time $\alpha(T)$ that commutes with the electric translation in equation (4). Such a translation $\alpha(T)$ is

$$\alpha(T) = \exp\left(\frac{\partial}{\partial t}T\right) \tag{6}$$

where the period T is given by [21]

$$T = \frac{2\pi\hbar}{eEa}. \tag{7}$$

It is easy to check that $\alpha(T)$ commutes with $\beta(a)$. Having constructed commuting $\alpha(T)$ and $\beta(a)$ translations one can choose $\psi_{k_E}(x, t)$ in (5) to be an eigenfunction of $\alpha(T)$

$$\alpha(T)\psi_{\zeta k_E}(x, t) = \exp\left(\frac{\mathrm{i}}{\hbar}\zeta T\right)\psi_{\zeta k_E}(x, t). \tag{8}$$

This eigenfunction is a quasienergy state of the Bloch electron in a constant electric field. It is denoted by $\psi_{\zeta k_E}(x, t)$ with ζ being the quasienergy.

We are now going to use a theorem that was formulated in [19] for constructing quasienergy states for a Bloch electron in a constant electric field. For this we write down the eigenvalue Schrödinger equation for the problem in the kq representation [19]

$$\left[-\frac{\hbar^2}{2m}\frac{\partial}{\partial q^2} + V(q) + eE\left(\mathrm{i}\frac{\partial}{\partial k} + q\right)\right]C_\epsilon(k, q) = \epsilon C_\epsilon(k, q) \tag{9}$$

where $C(k, q)$ is the kq wave function which is related to the wave function $\psi(x)$ in the x representation as follows

$$C(k, q) = \sqrt{\frac{a}{2\pi}}\sum_n \exp(\mathrm{i}kna)\psi(q - na). \tag{10}$$

According to the theorem of [19], given an eigenfunction $C_\epsilon(k, q)$ of (9), a time-dependent solution of (1) is

$$\psi(x, t) = \exp\left(-\frac{\mathrm{i}}{\hbar}\epsilon t\right)C_\epsilon\left(k - \frac{1}{\hbar}eEt, x\right). \tag{11}$$

This is an exact result. It is interesting to check whether this is actually a quasienergy state for the Bloch electron in a constant electric field as defined by (1), (5) and (8). For this we just have to denote $\psi(x, t)$ in (11) (we replace ϵ by ζ and k by k_E) by

$$\psi_{\zeta k_E}(x, t) = \exp\left(-\frac{\mathrm{i}}{\hbar}\zeta t\right)C_\zeta\left(k_E - \frac{1}{\hbar}eEt, x\right) \tag{12}$$

and check that the latter function satisfies all three of equations (1), (5) and (8). In checking this we keep in mind that the $C(k, q)$ function satisfies the following boundary conditions [19]

$$C(k, q) = C\left(k + \frac{2\pi}{a}, q\right) = \exp(-\mathrm{i}ka)C(k, q + a). \tag{13}$$

In view of the transformation in (10) from the x to the kq wave function the result in (12) can also be given the following form in the x representation: let $\psi_\zeta(x)$ be the eigenfunction of the time-independent Schrödinger equation in the x representation

$$\left(\frac{p^2}{2m} + V(x) + eEx\right)\psi_\zeta(x) = \zeta\psi_\zeta(x). \tag{14}$$

Then according to (10) and (12), the time-dependent quasienergy state $\psi_{\zeta k_E}(x, t)$ can be written in the following way

$$\psi_{\zeta k_E}(x, t) = \sqrt{\frac{a}{2\pi}}\exp\left(-\frac{\mathrm{i}}{\hbar}\zeta t\right)\sum_n \mathrm{e}^{\mathrm{i}(k_E - \frac{1}{\hbar}eEt)na}\psi_\zeta(x - na). \tag{15}$$

One can check that the time-dependent function $\psi_{\zeta k_E}(x, t)$ satisfies (1) if $\psi_\zeta(x)$ is a solution of (14). This completes the formulation of the theorem for constructing quasienergy states for the problem of a Bloch electron in a constant electric field. Apart from the exponential factor $\exp(-(\mathrm{i}/\hbar)\zeta t)$, (15) is a relation between a Wannier function $\psi_\zeta(x)$ and a Bloch function with a time-dependent quasimomentum $k_E - (\mathrm{i}/\hbar)eEt$. Clearly, for this relation to have a physical meaning the sum in (15) has to converge, or in other words $\psi_\zeta(x)$ has to be sufficiently well localized. As is well known [22] the spectrum of (14) is continuous, and it therefore has no localized eigenstates. This means that the problem of a Bloch electron in a constant electric field has no exact Bloch-like quasienergy states as given by (15).

One can, however, turn to approximate solutions of (14) which have the meaning of resonances. In particular one can consider one-band solutions of (14) [or of the time-dependent equation (1)] which are sufficiently localized, so that the sum in (15) converges. In what follows we are going to consider these one-band solutions, but we refer the reader to [9] and [10] in order to draw attention to the difficulties that are connected with them.

We again turn to (9) in the kq representation. In the one-band approximation one can look for a solution of this equation in the form (we don't write the band index)

$$C_\epsilon(k, q) = B_\epsilon(k)\psi_k(q) \tag{16}$$

where $\psi_k(q)$ is the Bloch function of the band, and $B_\epsilon(k)$ an unknown function. For the function $B_\epsilon(k)$, (9) becomes [19]

$$\left[\mathrm{i}eE\frac{\partial}{\partial k} + \epsilon(k) + eEX(k)\right]B_\epsilon(k) = \epsilon B_\epsilon(k) \tag{17}$$

where

$$X(k) = \frac{2\pi}{a}\mathrm{i}\int u_k^*(q)\frac{\partial}{\partial k}u_k(q)\,\mathrm{d}q \tag{18}$$

with $u_k(q)$ being the periodic part of the Bloch function. The integration in (18) is over a unit cell of the Bravais lattice. The solutions of (17) are well known and they form the Wannier–Stark ladder [8, 19]

$$B_{\epsilon_\nu}(k) = \exp\left(\frac{\mathrm{i}}{eE}\int_0^k\left[\epsilon(k') + eEX(k') - \epsilon_\nu\right]\mathrm{d}k'\right) \tag{19}$$

$$\epsilon_\nu = eEa\nu + \langle\epsilon(k)\rangle + eE\langle X(k)\rangle \tag{20}$$

where the index ν runs over all integers and where the angle brackets define an average over the Brillouin zone of a function $f(k)$

$$\langle f(k)\rangle = \frac{a}{2\pi}\int_0^{2\pi/a} f(k)\,\mathrm{d}k \tag{21}$$

In the kq representation the eigenfunction $C_{\epsilon_\nu}(k, q)$ will be given by (16) with the B function from (19). Since $B_{\epsilon_\nu}(k)$ in (19) is just a periodic in k phase, the eigenfunction $C_{\epsilon_\nu}(k, q)$ in (16) is nothing else but a Wannier function in the kq representation for the energy band under consideration (a Bloch function in the x representation is a Wannier function in the kq representation [19]). The phase of the Bloch function can always be chosen in such a way as to make $X(k)$ in (18) be [20]

$$X(k) = \langle X(k)\rangle. \tag{22}$$

In what follows this choice of phase for the Bloch function will be assumed.

For constructing quasienergy states we shall be interested only in the $\nu = 0$ eigenvalues and eigenfunctions of the Wannier–Stark ladder (the reason for this will become clear below). With this in mind and using (22) we have from (16), (19) and (20)

$$C_{\epsilon_0}(k, q) = \exp\left(\frac{\mathrm{i}}{eE}\int_0^k\left[\epsilon(k') + eE\langle X(k)\rangle - \epsilon_0\right]\mathrm{d}k'\right)\psi_k(q) \tag{23}$$

$$\epsilon_0 = \langle\epsilon(k)\rangle + eE\langle X(k)\rangle. \tag{24}$$

We now use the theorem of [19] (equations (11), (12) and (15)) for constructing a quasienergy state of the Schrödinger equation (1). We have by using (12), (23) and (24)

$$\psi_{\zeta_0} k_E(x,\ t) = \exp\left(-\frac{\mathrm{i}}{\hbar}\zeta_0 t + \frac{\mathrm{i}}{eE}\int_0^{k_E-\frac{1}{\hbar}eEt}\left[\epsilon(k') + eE\langle X(k)\rangle - \epsilon_0\right]\mathrm{d}k'\right)\psi_{k_E-\frac{1}{\hbar}eEt} \qquad (25)$$

$$\zeta_0 = \epsilon_0 = \langle\epsilon(k)\rangle + eE\langle X(k)\rangle. \qquad (26)$$

This is a quasienergy state of (1) in the one-band approximation. It is easy to check that the state in (25) is also an eigenfunction of the commuting operators in (5) and (8). By definition of quasienergy states [1] the quasienergy ζ_0 is defined up to the additive constant $\nu\hbar(2\pi/T)$, where ν is any integer and T is given in (7). We therefore have for the quasienergy ζ_ν (the subscript 0 is replaced by ν)

$$\zeta_\nu = \langle\epsilon(k)\rangle + eE\langle X(k)\rangle + \nu eEa \qquad (27)$$

with ν being an arbitrary integer. The expression for the quasienergy ζ_ν coincides with the Wannier–Stark ladder ϵ_ν in (20). The physical meaning of ζ_ν is, however, different from that of ϵ_ν. While ϵ_ν is an eigenvalue of the one-band approximation eigenvalue equation for a Bloch electron in a constant electric field (equation (17)), ζ_ν is the quasienergy for the same problem in the same approximation. As is well known [1], in a quasienergy state the energy is conserved up to $\hbar(2\pi/T)$ where T is given by (7). In other words, the conservation is for the quasienergy with the Brillouin zone extending from 0 to $\hbar(2\pi/T)$. We come here to the very interesting conclusion that the Wannier–Stark ladder levels are also the quasienergies of the same problem. This is a new interpretation of the Wannier–Stark ladders. As for the quasienergy states (equation (25)), they are closely related to the Houston function [23]

$$\psi(x,\ t) = \exp\left\{-\frac{\mathrm{i}}{\hbar}\int_0^t \epsilon\left(k - \frac{1}{\hbar}eEt'\right)\mathrm{d}t'\right\}\psi_{k-\frac{1}{\hbar}eEt}(x) \qquad (28)$$

The latter, as was shown in [5], is also a quasienergy state. By the substitution $k' = k - (1/\hbar)eEt'$ (and replacing k_E by k) it can be shown that the function in (25) goes over into the one in (28) (up to a constant). The quasienergy ζ_0 [22] (see equation (26)) contains the geometric phase $\langle X(k)\rangle$ [20, 24] which is defined modulo a (the period of the crystal). When the crystal has inversion symmetry $\langle X(k)\rangle$ can be either zero or $a/2$, otherwise it can assume any value between zero and a. The theoretical prediction of Bloch oscillations [7, 13–17] is largely based on the solution in (28). Having shown that the latter function is essentially the quasienergy state in (25) we arrive at a new view of the Bloch oscillations: we can consider them as being related to quasienergy states of the problem. As was pointed out in [1] a system in a quasienergy state has a variable dipole moment and it can radiate. One can therefore consider the Bloch oscillations as coming from the quasienergy states (equation (25)) for a Bloch electron in a constant electric field.

In conclusion we have shown that quasienergy states and quasienergies can be defined for a Bloch electron in a time-independent electric field. Our definition is outside the common framework for the concept of quasienergies where the electric field is a periodic function of time [1–7]. The reason for being able to define quasienergy state (equation (8)) for a constant electric field is that we require them also to be eigenstates of the electric time-dependent translations (equation (4)). It is instructive to consider the same problem in the 'velocity gauge'. To this end, I introduce the vector potential $A(t) = -cEt$. Setting $\tilde{\phi}(x,\ t) = \phi(x,\ t)\exp(\mathrm{i}(e/\hbar c)A(t)x)$, equation (1) becomes

$$\mathrm{i}\hbar\frac{\partial\tilde{\phi}(x,\ t)}{\partial t} = \left(\frac{1}{2m}\left(p + \frac{e}{c}A(t)\right)^2 + V(x)\right)\tilde{\phi}(x,\ t). \qquad (29)$$

Then, substituting $\tilde{\phi}(x,\ t) = u(x,\ t)\mathrm{e}^{\mathrm{i}kx}$, one has

$$\mathrm{i}\hbar\frac{\partial u(x,\ t)}{\partial t} = \left(\frac{1}{2m}\left(p + \hbar k + \frac{e}{c}A(t)\right)^2 + V(x)\right)u(x,\ t). \tag{30}$$

Since k has to be taken modulo $2\pi/a$, the Hamiltonian on the r.h.s. is actually periodic in time with the Bloch period $T_{Bloch} = 2\pi\hbar/(eEa)$. It then becomes immediately obvious why quasienergy states with that period have to play a special role. (The one-band approximation readily yields an explicit example.)

It is clear that these considerations are equivalent to the use of commuting electric and time translations. We have concluded that the quasienergy states for the one-band approximation are identical to the well known Houston states. In order to reach this conclusion we could have used the results in [5] directly without entering into the calculations of this paper. However, the insight gained by our theorem and calculations in equations (9)–(15) leads one to a more general framework for quasienergy states. Thus, according to this theorem, any solution of (14) (not just one-band solutions) leads to a quasienergy state as given by (15). For example we could have considered a two-band solution of (14) or any other localized solution of this equation, and from our theorem one obtains the quasienergy states as given by (15).

Finally, we would like to make the following remark about the result in (15) when considered for the quasienergy ζ_0 (see equation (25)). For simplicity we set the electric quasimomentum $k_E = 0$. We then have

$$\phi_{\zeta_0 0}(x,\ t) = \sqrt{\frac{a}{2\pi}}\exp\left(-\frac{\mathrm{i}}{\hbar}\zeta_0 t\right)\sum_n \exp\left(\frac{\mathrm{i}}{\hbar}eEnat\right)\phi_{\zeta_0}(x - na) \tag{31}$$

Here $\phi_{\zeta_0}(x)$ is a Wannier–Stark ladder function with the spread $(\Delta\epsilon/eE)$ where $\Delta\epsilon$ is the bandwidth under consideration [19]. As a rule this spread is bigger than the lattice constant, and the quasienergy state in the last equation is a superposition of not too sharply localized states corresponding to equidistant Wannier–Stark levels. It is, therefore, to be emphasized that whereas a Wannier–Stark eigenfunction is localized, and gives a single energy eigenvalue, a quasienergy state is an extended state, and gives the whole ladder.

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