Finite Translations in Time and Energy

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Commuting time translations and electric translations are used for the specification of time dependent solutions of the Schrödinger equation for a Bloch electron in a periodic in time electric field. Explicit one-band expressions are found for the quasienergies and the corresponding time dependent solutions.

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A well-known and widely used concept in solid state physics is the quasimomentum or the Bloch momentum [1]. The latter is a consequence of finite translational symmetry in space for crystalline solids. It is also possible to define finite translations in momentum space which lead to the concept of a quasicoordinate. The quasimomentum and the quasicoordinate form together a quantum mechanical representation which is called the kq representation [2]. A much less known concept is the quasienergy which is a consequence of finite translational symmetry in time for Hamiltonians containing a periodic function of time [3]. Recently the quasienergy has acquired interest in the framework of laser irradiated superlattices [4]. In analogy with quasimomentum (k) and quasicoordinate (q) it is natural to expect that one can also define, along with quasienergy (ϵ), the concept of quasitime (τ). For this one needs finite translations in energy. Such related translations were defined in connection with the dynamics of a Bloch electron in a constant electric field [5]. A translation in time by T and a translation in energy by $\hbar(2\pi/T)$ commute. They are the fundamental translations in time and energy in the same way the translations by a and $\hbar(2\pi/a)$ are in coordinate and momentum, respectively [2]. It should, however, be pointed out that while a translation in time is a perfectly well-defined quantum mechanical operator [6], this is not the case with a translation in energy [5]. The latter is a multiplication by a time dependent phase, and as such it is a well-defined operation, but it is not a proper operator in quantum mechanics. The concepts of quasienergy and quasitime have recently acquired widespread use in signal processing [7].

In this Letter we define commuting translations in time and energy and show how they are used for the specification of solutions for the time dependent Schrödinger equation for a Bloch electron in a periodic in time electric field. The relevant operator for the symmetry of the problem is $S=i\hbar\,\partial/\partial t-H$ with H being the Hamiltonian. Finding solutions of the time dependent Schrödinger equation is equivalent to finding eigenstates of S corresponding to zero eigenvalue. Finite translations in time $\alpha(T)$ by the period T of the applied electric field commute with S. These translations define the quasienergy [3] with the Brillouin zone $2\pi\hbar/T$. Another operation (we distinguish between an operator and an operation) commuting with S is a combined translation $\beta(a)$ in space and energy [5]: a translation by the lattice constant a in space and by $eE(t)a$ in energy, where $-e$ is the electron charge and $E(t)$ the applied electric field. The translations $\alpha(T)$ and $\beta(a)$ also commute with one another if the zero Fourier component E_0 of the electric field $E(t)$ assumes the values $eE_0a=(2\pi\hbar/T)g$, $g=0,1,2,\ldots$. The meaning of this relation is that the spacing in the Stark ladder [8] of E_0 has to be a multiple of the Brillouin zone for the quasienergy. When this relation on E_0 is satisfied, one uses the commuting operators $\alpha(T)$ and $\beta(a)$ for specifying the solutions of the time dependent Schrödinger equation. In particular, it is shown that the well-known Houston time dependent solutions [9] are eigenfunctions of the commuting translations $\alpha(T)$ and $\beta(a)$. From the eigenvalues of $\alpha(T)$ an explicit analytical expression is found for the quasienergies of a Bloch electron in a time dependent periodic electric field.

We start with the time dependent Schrödinger equation written in the following way:

$$S\psi(x,t)\equiv\left[i\hbar\frac{\partial}{\partial t}-H(t)\right]\psi(x,t)=0\,, \tag{1}$$

where x is the one-dimensional space coordinate. One can consider Eq. (1) as an eigenvalue equation for the operator S with eigenvalue 0. For a Bloch electron in a time dependent periodic electric field $E(t)$, $H(t)$ has the form

$$H(t)=\frac{p^2}{2m}+V(x)+eE(t)x\,. \tag{2}$$

Here $V(x)$ is the periodic potential of the crystal, $V(x+a)=V(x)$, and $E(t+T)=E(t)$. A finite translation in time by T is [6]

$$\alpha(T)\equiv\exp\left[\frac{\partial}{\partial t}T\right]:\exp\left[\frac{i}{\hbar}\epsilon T\right]. \tag{3}$$

It commutes with S [the operator in Eq. (1)]. $\exp[(i/\hbar)\epsilon T]$ in Eq. (3) are the eigenvalues with ϵ being the quasienergy [3]. ϵ is defined modulo $2\pi\hbar/T$, which is the Brillouin zone for the quasienergy. We have

$$\alpha(T)\psi(x,t)=\psi(x,t+T)\,. \tag{4}$$

The wave function $\psi(x,t)$ can be multiplied by a time dependent phase $\exp[if(t)]$. The new function $\exp[if(t)]\psi(x,t)$ satisfies Eq. (1) but with $\hbar[\partial f(t)/\partial t]\psi(x,t)$ on the right-hand side. Such a phase multiplication can therefore be interpreted as a shift in energy by the quantity $\hbar\,\partial f(t)/\partial t$. When $f(t)$ is linear in time, this shift in energy is a constant. The following time dependent phase shifts the energy by the quasienergy Brillouin zone $\hbar(2\pi/T)$:

$$B\left(\frac{2\pi}{T}\right)\equiv\exp\left(i\frac{2\pi}{T}t\right):\exp\left(i\frac{2\pi}{T}\tau\right), \tag{5}$$

where $\exp[i(2\pi/T)\tau]$ is its eigenvalue with τ being the quasitime defined modulo T. $\alpha(T)$ commutes with $B(2\pi/T)$ in Eq. (5) and they form together commuting finite translations in time and energy, respectively. Their eigenvalues are the quasienergy [Eq. (3)] and the quasitime [Eq. (5)]. The translations $\alpha(T)$ and $B(2\pi/T)$ are similar to the translations in coordinate $\exp[(i/\hbar)pa]$ and momentum $\exp[ix(2\pi/a)]$ which define the quasimomentum and quasicoordinate, respectively [2].

Because of the presence of the electric field, the time dependent Hamiltonian in Eq. (2) no longer has translational symmetry of the crystal. However, one can check that a combination of an energy shift and a translation in space exists which commutes with the operator S in Eq. (1). This combination is the known electric translation, and when extended to the case of a time periodic electric field it reads [5]

$$\beta(a)=\exp\left(\frac{i}{\hbar}pa+\frac{iea}{\hbar}\int_0^t E(t')dt'\right), \tag{6}$$

where a is the lattice constant. For simplicity we assume that $E(t)$ contains only one harmonic in its Fourier expansion,

$$E(t)=E_0+E_1\cos\frac{2\pi}{T}t\,. \tag{7}$$

In general $\beta(a)$ does not commute with the time translation $\alpha(T)$ [Eq. (3)], but can be made to commute with it by putting the following condition on the zero Fourier component E_0 of the electric field

$$eE_0a=\hbar\frac{2\pi}{T}g,\quad g=0,1,2,\ldots, \tag{8}$$

where $g=0$ corresponds to the case when $E_0=0$. This condition means that the Stark ladder spacing [8] for E_0 has to be a multiple of the quasienergy Brillouin zone. The part linear in time in the phase of $\beta(a)$ is $\exp[(i/\hbar)eaE_0t]$. By using Eq. (8), this becomes $\exp[i(2\pi/T)tg]$. The latter is nothing else but the power g of the basic energy translation $B(2\pi/T)$ in Eq. (5). It is therefore seen that the basic translation in energy $B(2\pi/T)$ plays an important role in the definition of $\beta(a)$ in Eq. (6).

Having defined $\alpha(T)$ and $\beta(a)$ that commute with one another and both of them commute with S in Eq. (1), one can look for solutions of Eq. (1) that are also eigenfunctions of $\alpha(T)$ and $\beta(a)$. In particular, eigenfunctions of $\alpha(T)$ define the quasienergies [Eq. (3)] of the problem. For finding solutions of Eq. (1) we use the well-known Houston function [9] which for the case of the periodic electric field in Eq. (7) assumes the form

$$\psi_k(x,t)=\exp\left\{-\frac{i}{\hbar}\int_0^t\epsilon[k(t')]dt'\right\}\psi_{k(t)}(x), \tag{9}$$

where

$$k(t)=k-eE_0t/\hbar-(TeE_1/2\pi\hbar)\sin[(2\pi/T)t],$$

$\epsilon[k(t')]$ is a single-band energy spectrum for the unperturbed crystal [for the Hamiltonian in Eq. (2) with $E(t)=0$], $\psi_{k(t)}(x)$ is the corresponding Bloch function for $t'=t$, and the meaning of the subscript k in $\psi_k(x,t)$ will become clear shortly. The Houston function in Eq. (9) is an approximate one-band time dependent solution of Eq. (1). It is interesting to notice that $\psi_k(x,t)$ are eigenfunctions of $\beta(a)$ in Eq. (6) with the eigenvalues $\exp(ika)$,

$$\beta(a)\psi_k(x,t)=\exp(ika)\psi_k(x,t), \tag{10}$$

which explains the subscript k in the Houston function [Eq. (9)]. We now require that $\psi_k(x,t)$ is also an eigenfunction of the finite translation in time $\alpha(T)$ [this can be done, when the condition in Eq. (8) is satisfied, because then $\alpha(T)$ and $\beta(a)$ commute],

$$\psi_k(x,t+T)=\exp\left(-\frac{i}{\hbar}\epsilon T\right)\psi_k(x,t). \tag{11}$$

By using Eqs. (8) and (9) [from the former equation it follows that the Bloch function $\psi_{k(t)}(x)$ does not change when t is replaced by $t+T$], one finds for the quasienergy

$$\begin{aligned}\epsilon(k)&=\frac{1}{T}\int_0^T\epsilon\left(k-\frac{1}{\hbar}eE_0t-\frac{TeE_1}{2\pi\hbar}\sin\frac{2\pi}{T}t\right)dt\\&=\frac{1}{2\pi}\int_0^{2\pi}\epsilon\left(k-\frac{g\theta}{a}-\frac{TeE_1}{2\pi\hbar}\sin\theta\right)d\theta.\end{aligned} \tag{12}$$

In writing Eq. (12), explicit use was made of Eq. (8). Let us assume for $\epsilon(k)$ a tight binding expression $\epsilon(k)=\epsilon_0-(\Delta/2)\cos ka$, where Δ is the bandwidth. It then follows from Eq. (12) for the quasienergy

$$\begin{aligned}\epsilon(k)&=\epsilon_0-\frac{\Delta}{2}\int_0^{2\pi}\cos\left(ka-g\theta-\frac{eE_1a}{\hbar 2\pi/T}\sin\theta\right)d\theta\\&=\epsilon_0-(-1)^g\frac{\Delta}{2}J_g\left(\frac{eE_1a}{\hbar 2\pi/T}\right)\cos ka,\end{aligned} \tag{13}$$

where J_g is the Bessel function. The result in Eq. (13) gives the quasienergy of a Bloch electron in a periodic electric field [Eq. (7)] in the one-band approximation. This result goes over into the result in Ref. [4] when $g=0$

or when $E_0=0$ [see Eq. (8)]. What is striking about the quasienergy in Eq. (13) is that it is a function of k in very much the same way as in the absence of the electric field. Here k varies in the same Brillouin zone as in the pure Bloch case $-\pi/a \le k \le \pi/a$ [see Eq. (10)]. The only difference is in the meaning of k: In Eq. (10), k labels the eigenvalues of the combined electric translation $\beta(a)$ while in the Bloch case, k is the quasimomentum. Another striking feature of Eq. (13) is the appearance of the Bessel function in the bandwidth; the latter is a function of the ratio $eE_1a/(\hbar 2\pi/T)$. In particular, the bandwidth vanishes when this ratio is a zero of the Bessel function J_g (see Ref. [4] for the discussion of an experiment that can detect this band narrowing).

The explicit result in Eq. (13) for the quasienergy is a consequence of the one-band approximation for the Houston function [Eq. (9)]. The wave function corresponding to this quasienergy can be written in the conventional form [3,4]

$$\psi_{\epsilon k}(x,t)=\exp\left(-\frac{i}{\hbar}\epsilon t\right)u_{\epsilon k}(x,t)\,, \tag{14}$$

where $u_{\epsilon k}(x,t+T)=u_{\epsilon k}(x,t)$ and has the form [see Eq. (9)]

$$u_{\epsilon k}(x,t)=\exp\left(\frac{i}{\hbar}\epsilon t\right)\psi_k(x,t)\,. \tag{15}$$

However, the appearance of the labels ϵ and k in the solutions of Eq. (1) has nothing to do with the one-band approximation, and is a completely general feature, connected with the commutation of the commuting translations $\alpha(T)$ and $\beta(a)$ [Eqs. (3) and (6)] with the operator S in Eq. (1). Any general solution of Eq. (1) can be chosen to be an eigenfunction of the translations $\alpha(T)$ and $\beta(a)$, and correspondingly one should expect a band structure for the quasienergies as function of k, when a Bloch electron is subjected to a periodic electric field.

In conclusion, let us remark that solutions of the time dependent Schrödinger equation for a Bloch electron in a periodic electric field can be labeled by a quasienergy ϵ and an additional label k which gives the eigenvalues of a finite electric translation $\beta(a)$ [Eq. (10)]. The latter translation is a combination of a space translation and a translation in energy. The space translation is a well-known operator and forms the basis for Bloch functions. On the other hand, translations in energy deserve some special consideration. The translation in energy in $\beta(a)$ [Eq. (6)] consists of two parts, when the electric field is given by Eq. (7): $\exp[(iea/\hbar)E_0t]$ and $\exp[(iea/\hbar)\times(T/2\pi)E_1\sin(2\pi/T)t]$. The second part commutes with the operator $\alpha(T)$ [Eq. (3)]. For the first part to commute with $\alpha(T)$, E_0 has to satisfy Eq. (8). When the latter is satisfied, $\exp[(iea/\hbar)E_0t]$ assumes the form of $B(2\pi/T)$ in Eq. (5) (or a power of it). The two basic translations for time and energy are therefore $\alpha(T)$ and $B(2\pi/T)$ [Eqs. (3) and (5)]. $\alpha(T)$ is a well-defined operator in quantum mechanics [6]. Being a multiplication by a time dependent phase, $B(2\pi/T)$ is a well-defined operation but is not an operator in quantum mechanics. Similarly, $\beta(a)$ in Eq. (6) is a well-defined operation, but is not an operator in quantum mechanics. $\alpha(T)$ and $B(2\pi/T)$ are finite translations in time and energy and define correspondingly the concepts of quasienergy and quasitime [Eqs. (3) and (5)]. Given a function of t, $\phi(t)$, one can define the quasienergy ϵ, quasitime τ function $C(\epsilon,\tau)$ in complete analogy with the kq function for xp degrees of freedom [10],

$$C(\epsilon,\tau)=\left(\frac{T}{2\pi}\right)^{1/2}\sum_n \exp\left(\frac{i}{\hbar}\epsilon nT\right)\phi(\tau-nT)\,. \tag{16}$$

This transformation has become of wide use in recent years in signal processing [7].

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