Symmetric coordinates in solids: magnetic Bloch oscillations

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Abstract. There has recently been a revival of the Bloch theory of energy bands in solids. This revival was caused, on one hand, by the discovery of topological insulators and the discovery of graphene, and, on the other end, by a very efficient new technique that was developed for creating artificial solids. These are the cold atoms in optical lattices. Last year geometric phases were measured in energy bands of cold atoms in a one-dimensional optical lattice by using Bloch oscillations. These phases are related to the Wyckoff positions, or the symmetry centers in the Bravais lattice. In this lecture a theoretical frame is developed for magnetic Bloch oscillations, meaning oscillations in the presence of a magnetic field. The theory is based on the kq-representation and the symmetric coordinates in solids. It is shown that for a Bloch electron in a magnetic field the orbit quasi-center is a conserved quantity. This is similar to the conservation of the quasi-momentum for an electron in a periodic potential. When an electric field is turned on, the orbit quasi-center oscillates in a similar way to the Bloch oscillations in the absence of a magnetic field. But there is a difference because the magnetic Brillouin zone is different. It depends on the strength of the magnetic field. An analogy is drawn between Bloch oscillations and magnetic Bloch oscillations. By using the magnetic translations it is indicated that a magnetic Wannier-Stark ladder appears in the spectrum of a Bloch electron in crossed magnetic and electric fields. The geometric phases for magnetic Bloch oscillations should be magnetic field dependent.

1. Introduction

The derivation of magnetic Bloch oscillation will be carried out in this talk by using the basic operators in quantum mechanics (x and p being the coordinate and momentum operators)

$$\exp\left(\frac{i}{\hbar}pa\right) \text{ and } \exp\left(ix\frac{2\pi}{a}\right) \tag{1}$$

where a is an arbitrary constant. It can be checked that the operators commute

$$\left[e^{\frac{i}{\hbar}pa}, e^{ix\frac{2\pi}{a}}\right] = 0 \tag{2}$$

These exponentiated operators have a long history. They appear already in the book by Hermann Weyl "The Theory of Groups and Quantum Mechanics" (1928) in connection with the Weyl-Heisenberg group [1]. In the same year, 1928, they appear in Felix Bloch Ph.D. thesis (under Heisenberg) for building the Bloch Theory of Solids [2]. In 1932 von Neumann uses them in his book "Mathematical Foundations of Quantum Mechanics" [3]. In 1960 Julian Schwinger

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uses them in the construction of finite Hilbert spaces [4]. In 1964 they are used in constructing the magnetic translation group [5, 6]. Yakov Zel'dovich uses them in the definition of quasi-energy in 1967 [7]. Finally, in 1967 they are used in the kq-representation [8, 9, 10]. It should be pointed out that there is no classical analog for the commutation relation (2) of these operators: there are no two classical functions, one of x, $f(x)$, and one of p, $g(p)$, that give a vanishing Poisson bracket.

Paul Dirac in "Recollections of an Exciting Era" [11] draws attention to the correspondence between a quantum commutator and a classical Poisson bracket. They differ by a constant. This correspondence does not hold for the exponentiated operators in Eq. (1). According to Noether's theorem [12] in classical physics, continuous symmetries lead to conservation laws. In quantum mechanics Wigner has shown that any transformation, continuous or discrete, that leaves the Hamiltonian unchanged can be expressed by a unitary or anti-unitary operator, which is a conserved quantity [13]. The difference of conserved quantities in classical and quantum mechanics can best be seen by comparing the motion of a free particle with the motion in a periodic potential. For a free particle the Hamiltonian H does not depend on the coordinate x and any continuous translation will not change H. The linear momentum p is conserved both in classical and quantum mechanics. For a particle in a periodic potential the Hamiltonian remains invariant under discrete translations by the period a of the periodic potential. As a consequence of this discrete symmetry there is no conserved quantity in classical mechanics. But in quantum mechanics this invariance of the Hamiltonian under discrete translations leads to the important conservation law of the quasi-momentum (or the Bloch momentum) k.

As was pointed out above the exponentiated operators in Eq. (1) define the kq-representation [8, 9, 10, 14]. The eigenvalues of these operators, k and q, are the symmetric coordinates in solids (in reference [10] these coordinates are called "natural coordinates"). One should compare the k and q in solids with the spherical coordinates r, θ, and φ in atomic physics. In the latter case the potential depends only on the absolute value r of the radius vector $\vec{r}$, while θ and φ appear in the conserved angular momentum $\vec{L}$. By choosing spherical coordinates one simplifies the solution of the problem significantly. In a crystalline solid the potential is a function of the quasi-coordinate q only, $V(q)$, while the quasi-momentum k is a conserved quantity. The operators x and p are connected to k and q in the following way [14]

$$x = i\tfrac{\partial}{\partial k} + q \quad , \quad p = -i\hbar\tfrac{\partial}{\partial q} \tag{3}$$

The wave function $C(k,q)$ in the kq-representation is given by the wave function $\psi(x)$ in the x-representation as follows [14]

$$C(k,q) = \left(\frac{a}{2\pi}\right)^{1/2} \sum_n e^{ikan}\psi(q-na) \tag{4}$$

Here a is like in Eq. (1). The effectiveness of the use of the kq-representation is best demonstrated in the derivation of the acceleration theorem for a Bloch electron in an electric field E. The Hamiltonian for this problem in the kq-representation is [14]

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + V(q) - eE\left(i\frac{\partial}{\partial k} + q\right) = H_0 - eE\left(i\frac{\partial}{\partial k} + q\right) \tag{5}$$

where H_0 is the Bloch Hamiltonian for $E = 0$. From this Hamiltonian the acceleration theorem for the quasi-momentum follows immediately (one needs only to use the simple quantum mechanics rule that the time rate of change of k is given by the commutator of the Hamiltonian with k)

$$\hbar\frac{\mathrm{d}k}{\mathrm{d}t} = i[H,k] = eE \tag{6}$$

Here H is the Hamiltonian in Eq. (5). Eq. (6) is exact [15]! It should be pointed that the existing derivations of the acceleration theorem (6) are not entirely elementary and its validity is restricted to weak electric fields and for k in a small part of the Brillouin zone [16]. For cold atoms in optical lattices the driving force is different from the one in Eq. (6), e.g. gravity [17] or a magnetic field gradient acting on the spin of the atom [18]. A description of the properties of ultracold bosonic and fermionic quantum gases can be found in the review article [19]. The celebrated acceleration theorem in Eq. (6) is of central importance in the Bloch theory of energy bands in solids, in general, and in Bloch oscillations, in particular [20]. In this lecture a similar equation to Eq. (6) is developed for the vector $\vec{k}^{(B)}$ which labels the eigenvalues of the magnetic translations for a Bloch electron in a magnetic field $\vec{B}$. It is shown how $\vec{k}^{(B)}$ is related to the orbit quasi-center $\vec{q}_0$. Using the connection between $\vec{k}^{(B)}$ and $\vec{q}_0$, an elementary equation is developed for the orbit quasi-center $\vec{q}_0$ of a Bloch electron in crossed magnetic and electric fields. It is shown that Bloch-like oscillations may exist also in the presence of a magnetic field $\vec{B}$.

2. Motion in Magnetic and Electric Fields

For a particle of charge e in a periodic potential $V(x, y)$, a magnetic field in the z-direction, and an electric field in the xy-plane, the Hamiltonian is

$$H = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 + V(x, y) - e\vec{E}\cdot\vec{r} \equiv H_0^{(B)} - e\vec{E}\cdot\vec{r} \tag{7}$$

In what follows, we shall use the symmetric gauge for the vector potential $\vec{A} = \frac{1}{2}\vec{B}\times\vec{r}$. For a free particle in a magnetic field $\vec{B}$ the conserved quantity is known to be the orbit center $\vec{r}_0$ [21]:

$$x_0 = x + \tfrac{c}{eB}\left(p_y - \tfrac{eB}{2c}x\right) \quad , \quad y_0 = y - \tfrac{c}{eB}\left(p_x + \tfrac{eB}{2c}y\right) \tag{8}$$

There is a simple picture of this conservation law for a charged particle moving in the plane perpendicular to the magnetic field $\vec{B}$: this particle moves in a circle with a fixed orbit center $\vec{r}_0$. This holds both in classical and quantum mechanics. The difference is that in quantum mechanics $\vec{r}_0$ is an operator with components x_0 and y_0 that do not commute [21]. When in addition to the magnetic field there is also a periodic potential $V(x, y)$ (the Hamiltonian of the problem is $H_0^{(B)}$ in Eq. (7)), the symmetry of the problem is then the magnetic translation group [5, 6]. This group has a subgroup of commuting magnetic translations [22]

$$T\left(\vec{b}_1\right) = \exp\left[\tfrac{1}{\hbar}\left(\vec{p} + \tfrac{e}{2c}\vec{B}\times\vec{r}\right)\cdot\vec{b}_1\right] \quad , \quad T\left(\vec{b}_2\right) = \exp\left[\tfrac{1}{\hbar}\left(\vec{p} + \tfrac{e}{2c}\vec{B}\times\vec{r}\right)\cdot\vec{b}_2\right] \tag{9}$$

where $\vec{b}_1$ and $\vec{b}_2$ are multiples of the periods $\vec{a}_1$ and $\vec{a}_2$ of the periodic potential $V(x, y)$

$$\vec{b}_1 = N_1\vec{a}_1 \quad , \quad \vec{b}_2 = N_2\vec{a}_2 \quad , \quad \vec{b} = m_1\vec{b}_1 + m_2\vec{b}_2 \tag{10}$$

Here m_1, m_2 are integers running from $-\infty$ to ∞, and where N_1, N_2 are positive integers that appear in the rationality condition on the magnetic field B [22]

$$eBb_1b_2 = hc \tag{11}$$

Having in mind the commutation relation of the operators x_0 and y_0 in Eq. (8)

$$[x_0, y_0] = -i\frac{\hbar c}{eB} \tag{12}$$

it is easy to check that the magnetic translations $T\left(\vec{b}_1\right)$ and $T\left(\vec{b}_2\right)$ in Eq. (9) commute; where we have also used the rationality condition in Eq. (11).

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3. Orbit Quasi-center

We are now in a position to define the orbit quasi-center $\vec{q}_0$. Since the magnetic translations in Eq. (9) commute, they have simultaneous eigenfunctions and eigenvalues. We shall denote their eigenvalues in the following way (we use Eq. (8)):

$$T\left(\vec{b}_1\right) = \exp\left(-\frac{ieB}{\hbar c} y_0 b_1\right) \sim \exp\left(i k_x^{(B)} b_1\right) \tag{13}$$

$$T\left(\vec{b}_2\right) = \exp\left(\frac{ieB}{\hbar c} x_0 b_2\right) \sim \exp\left(i k_y^{(B)} b_2\right) \tag{14}$$

In Eqs. (13) and (14) x_0 and y_0 are the operators of the orbit center $\vec{r}_0$, and the magnetic $\vec{k}^{(B)}$-vector labels the eigenvalues of the magnetic translations $T\left(\vec{b}_1\right)$ and $T\left(\vec{b}_2\right)$. The $\vec{k}^{(B)}$-vector has no direct physical meaning. But we can label the eigenvalues of the exponentiated operators in the Eqs. (13), (14) also by the orbit quasi-center $\vec{q}_0$

$$\exp\left(-\frac{ieB}{\hbar c} y_0 b_1\right) \sim \exp\left(-\frac{ieB}{\hbar c} q_{0y} b_1\right) \tag{15}$$

$$\exp\left(\frac{ieB}{\hbar c} x_0 b_2\right) \sim \exp\left(\frac{ieB}{\hbar c} q_{0x} b_2\right) \tag{16}$$

Here q_{0x} and q_{0y} are the x and y-components of the orbit quasi-center $\vec{q}_0$. Eqs. (15), (16) give the definition of the orbit quasi-center $\vec{q}_0$. The reason we call it quasi-center is because it is defined mod $\vec{b}$ in Eq. (10). This is in line with the definition of the quasi-momentum k in the Bloch theory, k is defined modulo the vector of the reciprocal lattice. Since the magnetic translations $T\left(\vec{b}_1\right)$ and $T\left(\vec{b}_2\right)$ commute with the Hamiltonian $H_0^{(B)}$ in Eq. (7), $\vec{q}_0$ is a conserved quantity for a Bloch electron in a magnetic field $\vec{B}$. This is in full analogy with the Bloch theory: for a free particle, the conserved quantity is the momentum p, and when the crystal potential is turned on, the conserved quantity is the quasi-momentum k.

The concept of the orbit quasi-center $\vec{q}_0$ is consistent with the classical Pippard network [23]: a charged particle in a magnetic field moves on a fixed circle with a definite center $\vec{r}_0$; in the presence of a periodic potential, the conserved quantity is $\vec{q}_0$, which is defined mod $\vec{b}$ in Eq. (10) and the particle moves then on a set of circular orbits with centers on the lattice $\vec{b}$, which is the Pippard network [23].

The next step is to consider how $\vec{q}_0$ varies in time when the electric field is turned on. We have

$$\frac{\mathrm{d}}{\mathrm{d}t} T\left(\vec{b}\right) = \frac{i}{\hbar}\left[H, T\left(\vec{b}\right)\right] = -\frac{i}{\hbar}\left[e\vec{E}\cdot\vec{r}_0, T\left(\vec{b}\right)\right] \tag{17}$$

because $T\left(\vec{b}\right)$ commutes with $H_0^{(B)}$ in Eq. (7) and with the components of the operator $\vec{p} + \frac{e}{2c}\vec{B}\times\vec{r}$ that appear in the brackets in Eq. (8) (also, in the Hamiltonian H in Eq. (7)). Having in mind the commutation relation for the operators x_0 and y_0 in Eq. (12), we find by using Eq. (17) that

$$\dot{\vec{q}}_0 = \frac{c\vec{E}\times\vec{B}}{B^2} \tag{18}$$

where $\vec{q}_0$ is the orbit quasi-center in the magnetic field $\vec{B}$, namely, $\vec{q}_0 = \vec{r}_0 \mod \vec{b}$ in Eq. (10). One can check that the same equation as in Eq. (18) holds also for the orbit center $\vec{r}_0$, when $V(x,y) = 0$ in Eq. (7)

$$\dot{\vec{r}}_0 = \frac{c\vec{E}\times\vec{B}}{B^2} \tag{19}$$

The latter equation is well known in classical electrodynamics, where it is called the equation for the drift velocity [24]. Since on the right hand side of Eq. (19) there is a constant vector, the orbit center $\vec{r}_0$ will grow with time indefinitely. The situation is different for the orbit quasi-center $\vec{q}_0$. The latter being defined $\mod \vec{b}$, it will oscillate with time. We call this the magnetic Bloch oscillations of the orbit quasi-center $\vec{q}_0$.

4. Magnetic Bloch Oscillations

There is an analogy between the Eq. (6) for the quasi-momentum k and Eq. (18) for the orbit quasi-center $\vec{q}_0$. In both cases, we have oscillations. This analogy goes much further. For a charged particle in a magnetic field (for the Hamiltonian $H_0^{(B)}$ in Eq. (7) with $V(x, y) = 0$) the energy spectrum consists of sharp Landau levels [21]. In what follows, we shall consider the simplest case of the rationality condition as given by Eq. (11). Under this condition, when a periodic potential is introduced, each Landau level broadens into a magnetic energy band [22] (the more general case of the rationality condition is considered in the calculation of the quantum Hall effect [25]). The energy levels inside the magnetic Bloch band are labeled by the orbit quasi-center $\vec{q}_0$. When the magnetic field $\vec{B} = 0$, the energy levels inside a Bloch band are labeled by the quasi momentum k. As was mentioned in the introduction the acceleration theorem in Eq. (6) forms the basis for the Bloch oscillations for a Bloch electron in an electric field. A similar theorem can be derived for the magnetic $\vec{k}^{(B)}$-vector which labels the eigenvalues of the magnetic translations in Eqs. (13) and (14) when a magnetic field $\vec{B}$ is present. The magnetic translations commute with $H_0^{(B)}$ in Eq. (7). For calculating the time derivative of the magnetic $\vec{k}^{(B)}$-vector we have to find the commutator of the magnetic translation with the electric field energy $-e\vec{E} \cdot \vec{r}$ in Eq. (7). The result is exactly like in Eq. (6) for the quasi-momentum k

$$\hbar \frac{\mathrm{d}\vec{k}^{(B)}}{\mathrm{d}t} = e\vec{E} \tag{20}$$

By comparing Eqs. (13), (14) with Eqs. (15), (16) respectively we find the following relation between the orbit quasi-center $\vec{q}_0$ and the magnetic $\vec{k}^{(B)}$

$$\hbar \vec{k}^{(B)} = \frac{e}{c} \vec{B} \times \vec{q}_0 \tag{21}$$

From Eqs. (20) and (21) we find again Eq. (18) for the orbit quasi-center, which is the main result of the talk [26].

Let us also show that the Hamiltonian in Eq. (7) has a spectrum containing a ladder structure like in the case of the Wannier-Stark ladder [14]. This follows from the following observation. Let ψ_ϵ be an eigenstate of the Hamiltonian in Eq. (7) corresponding to the energy ϵ. We consider the case when the electric field points in the x-direction. The electric field energy in the Hamiltonian (7) is then

$$-eE_x x \tag{22}$$

Consider the magnetic translation (see Eq. (9))

$$T(m\vec{a}_1) = \exp\left(-\frac{ieB}{\hbar c} y_0 a_1 m\right) \tag{23}$$

Its commutation with H in Eq. (7) for the electric field energy in Eq. (22) is

$$T^+(ma_1)\, H T(m\vec{a}_1) = H + m a_1 e E_x \tag{24}$$

Table 1. Conserved quantities and the influence if an electric force on them. $V(x, y)$: periodic potential; $\vec{B}$: magnetic field; $\vec{p}$: momentum; $\vec{r}_0$: orbit center; $\vec{k}$: quasi-momentum; $\vec{q}_0$: orbit quasi-center; $\vec{E}$: electric field. Remark: as explained in the text for neutral atoms $\vec{E}$ and $\vec{B}$ can be created artificially.

	Free space	$V(x, y)$	$\vec{B}$	$\vec{B}$ and $V(x, y)$
Conserved quantities	$\vec{p}$	$\vec{k}$	$\vec{r}_0$	$\vec{q}_0$
Influence of an electric force on them	$\dot{\vec{p}} = e\vec{E}$	$\hbar\dot{\vec{k}} = e\vec{E}$	$\dot{\vec{r}}_0 = \dfrac{c\vec{E} \times \vec{B}}{B^2}$	$\dot{\vec{q}}_0 = \dfrac{c\vec{E} \times \vec{B}}{B^2}$

The result in Eq. (24) was obtained in a way similar to the results in Eqs. (17) and (18). This shows that if ψ_ϵ is an eigenfunction of H in Eq. (7) with the eigenvalue ϵ, then the function $T(ma_1)\psi_\epsilon$ is an eigenfunction of H with the eigenvalue $\epsilon + ma_1eE_x$

$$HT(m\vec{a}_1)\psi_\epsilon = (\epsilon + ma_1eE_x)T(ma_1)\psi_\epsilon \tag{25}$$

for $m = 0, \pm1, \pm2, \ldots$. This shows that the magnetic Wannier-Stark ladder is contained in the spectrum of H. The argument of Eq. (25) was originally used for indicating that a Stark ladder might exist when there is no magnetic field [27].

At the beginning, we pointed out how one mimics an electric force on neutral atoms in optical lattices [17, 18]. There are also ways to mimic artificial vector gauge potentials for neutral particles in an optical lattice [28, 29]. The motion of a charged particle in crossed magnetic and electric fields is more complicated than given by Eq. (19). The particle itself moves on a curve called trochoid [24]. It is the orbit center $\vec{r}_0$ that satisfies the simple equation (19). Eq. (18) is a quantum-mechanical result which is obtained when a periodic potential is turned on. There is no classical analog for Eq. (18).

In Table 1, we summarize the conserved quantities we deal with, and how they are influenced by the "electric" force. The quotation marks are used to indicate that for neutral atoms one uses substitutes for the electric force.

We have started the talk with the exponentiated operators in Eq. (1). The eigenvalues of these operators are the symmetric coordinates, the quasi-momentum k and the quasi-coordinate q, for a Bloch electron in a solid. They are the kq-representaion. The orbit quasi-center $\vec{q}_0$, that was used for the magnetic Bloch oscillations, is defined by the Eqs. (15) and (16). By changing notations

$$x_0 = \tfrac{cP}{eB} \quad , \quad y_0 = X \quad , \quad b_2 = a \quad , \quad b_1 = \tfrac{hc}{eBa} \tag{26}$$

where b_1 is obtained from the rationality condition in Eq. (11), the operators in Eqs. (15) and (16) turn into the exponentiated operators of the kq-representation in Eq. (1)

$$\exp\left(\tfrac{ieB}{\hbar c}x_0b_2\right) \to \exp\left(\tfrac{i}{\hbar}Pa\right) \quad , \quad \exp\left(-\tfrac{ieB}{\hbar c}y_0b_1\right) \to \exp\left(-iX\tfrac{2\pi}{a}\right) \tag{27}$$

The operators X and P form the phase plane of the orbit center $\vec{r}_0$. As was mentioned in the introduction, von Neumann [3] used the exponentiated operators in Eq. (1) or (27) to construct a complete set of functions

$$e^{ix\frac{2\pi}{a}m}e^{\frac{i}{\hbar}pan}\psi_0(x) \tag{28}$$

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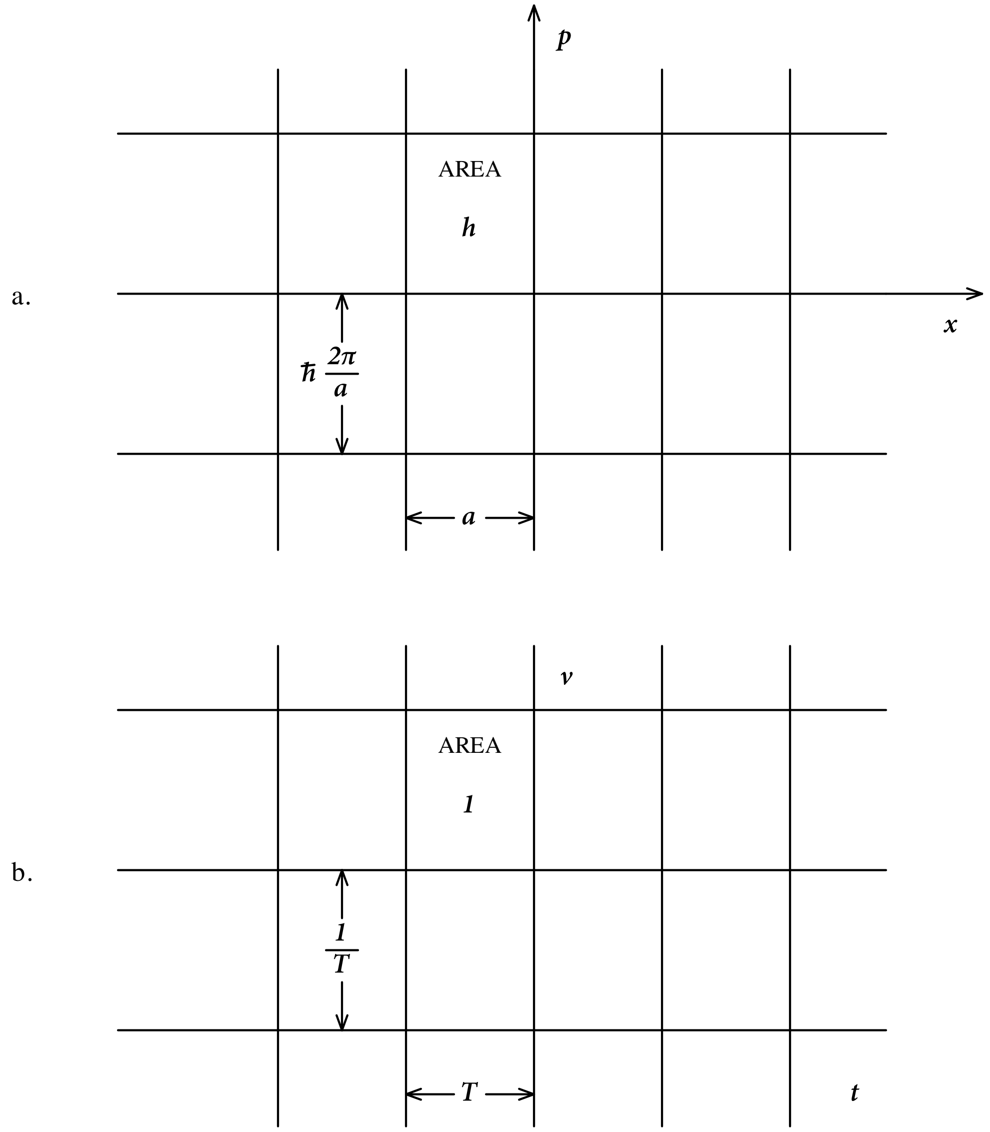

Figure 1. a. von Neumann lattice b. Gabor lattice

where m and n run from $-\infty$ to $+\infty$ and $\psi_0(x)$ is the ground state of the harmonic oscillator. This set is located on a lattice in phase plane as shown in Figure 1 (this figure contains also the lattice in frequency ν and time t plane [30]). In physics this lattice is called the von Neumann lattice, in signal processing it is called the Gabor lattice. What we show here is that this lattice in phase plane xp is closely related to the Pippard network [23] for a Bloch electron in a magnetic field in the coordinate plane x_0y_0 of the orbit center $\vec{r}_0$ in Eq. (8). The points inside the unit cell of area h (the Planck constant) of the von Neumann lattice are related to the orbit quasi-center q_{0x}, q_{0y}, while the lattice points in Figure 1.a are related to b_1 and b_2 in Eq. (26). The complete set of functions in Eq. (28) is very widely used in signal processing [31], where x and p is replaced by time t and frequency ν. It should be pointed out that von Neumann was right when he claimed that the set in Eq. (28) is complete. It turns out however that it is overcomplete by one member [32].

In summary, one deals here with the problem of a Bloch particle in crossed electric and magnetic fields. It is an old problem that has recently attracted wide renewed interest in view of the new techniques of cold atoms in optical lattices subject to synthetic electric and magnetic fields. Our focus is on magnetic Bloch oscillations. For deriving the main result given by Eq. (18), we use the magnetic translations [5, 6]. Their eigenvalues were originally labeled by a magnetic $\vec{k}^{(B)}$-vector, which has no direct physical meaning. As is well known by now, this $\vec{k}^{(B)}$-vector is related to the orbit quasi-center [22]. The main result in Eq. (18) replaces the quasi-momentum acceleration theorem for the case of zero magnetic field. A crucial condition for the use of commuting magnetic translations is the rationality condition given by Eq. (11). They quantize the magnetic flux in the simplest case. Eq. (18) cannot be obtained for an irrational flux because then there are no commuting magnetic translations, Eq. (9). It is pointed out that the Hamiltonian (7) in combination with its symmetry of magnetic translations contains the spectrum of a ladder structure, like in the case of the Wannier-Stark ladder for zero magnetic field. In our case we choose the electric field in the x-direction, Eq. (22), which simplifies to a great extent the derivation of the equations leading to the magnetic Wannier-Stark ladder. In the latter case the experimental observation of the Wannier-Stark levels [20] came much later than their prediction [27]. The theoretical calculation of their lifetime seems to remain a challenging problem [33].

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