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Newtonian equations of motion for a Bloch electron

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ABSTRACT. Newtonian equations of motion for a Bloch electron essentially equivalent to Zak's equation are derived in an elementary manner, assuming arbitrary electromagnetic fields, starting with Bloch's theorem and using the Hamiltonian formulation. For very high magnetic fields the velocity must be defined differently form the standard low-field formula.

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1. INTRODUCTION

In the late twenties, Sommerfield, Bloch, Peierls, and other pioneer-physicists applied quantum theory to metals with outstanding successes [1]. A huge amount of literature now exists for the so-called semiclassical dynamics of electrons in metals [2]. The basic equations for a Bloch electron wave packet (Bloch electron) in this theory are [2, Eq. (12.6)]

$$\mathbf{v} = \hbar^{-1} \frac{d}{d\mathbf{k}} E_n(\hbar\mathbf{k}), \tag{1}$$

$$\hbar \frac{d\mathbf{k}}{dt} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}), \tag{2}$$

where $E_n(\hbar\mathbf{k})$ are the energy eigenvalues characterized by the *wave vector* $\mathbf{k}$ and the *zone number* n corresponding to the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \psi_{n,\mathbf{k}}(\mathbf{r}) = E_n(\hbar\mathbf{k}) \psi_{n,\mathbf{k}}(\mathbf{r}). \tag{3}$$

Note the remarkable absence of the force on the right-hand-side (rhs) of Eq. (2) derivable from the *periodic* lattice potential $V(\mathbf{r})$. Equations (1) and (2) have been used to obtain the Fermi energy surfaces for a great many metals and semiconductors. Despite their usefulness, the derivation of Eqs. (1) and (2) from first principles has been a subject of much work and controversy [3]. Zak used the k–q representation to formulate a quantum mechanical derivation but arrived at a gauge-invariant equation, a little different from Eq. (2).

The energy $E_n(\hbar\mathbf{k})$ is defined through the Schrödinger equation with zero electric and magnetic fields ($\mathbf{E} = \mathbf{B} = 0$). Equation (1) should therefore be useful for low fields only. The limitation of Eq. (2) is also obvious. The electromagnetic fields $(\mathbf{E}, \mathbf{B})$ can, of course, vary in space. But since the vector $\mathbf{k}$ is Fourier-conjugate to the position vector $\mathbf{r}$, it cannot depend on this variable. Thus, Eq. (2) may be valid for homogeneous fields only. The main purpose of the present work is to derive Newtonian equations of motion essentially equivalent to Zak's in the presence of arbitrary electromagnetic fields.

In Sect. 2, we derive new equations of motion. In Sect. 3, we discuss their validity, significance and simple applications.

2. Derivation of semiclassical equations of motion

We consider a monovalent metal like Cu. Neglecting the ionic motion, we have a system of interacting electrons moving in the ion-lattice potential. The motion of these electrons is correlated because of the electronic interaction and the Fermi-Dirac statistics. Still, a typical electron may be thought to move in an effective lattice potential V which has the same periodicity as the bare lattice potential. This independent-electron picture (approximation) will be assumed throughout in the present work.

The Schrödinger equation for a single electron is given by Eq. (3). The quantum mechanical calculations, known as the Bloch theorem (function), [4,5] show that the wave function ψ, which satisfies Eq. (3), is of the form

$$\psi_{n,\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r}), \tag{4}$$

where $u_{n,\mathbf{k}}(\mathbf{r})$ has the same lattice periodicity as the potential $V(\mathbf{r})$. the wave vector $\mathbf{k}$ is real for an infinitely extended lattice. The energy eigenvalues E have forbidden regions (energy gaps), and the energy eigenstates are characterized by the wave vector $\mathbf{k}$ and the zone number n, which enumerates the allowed energy bands

$$E = E_n(\hbar\mathbf{k}). \tag{5}$$

By taking the absolute square of Eq. (4), we observe that the stationary electron distribution is lattice-periodic.

Bloch's theorem can also be cast in an alternative form

$$\psi_{n,\mathbf{k}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{n,\mathbf{k}}(\mathbf{r}), \tag{6}$$

where $\mathbf{R}$ is any translation vector under which the lattice potential is invariant. In this form, the limitation imposed on the wave vector $\mathbf{k}$ is clear; the magnitude of $\mathbf{k}$ has an upper bound. For example, the maximum value for each component k_α, $\alpha = x, y, z$, for a sc lattice is limited to π/a_0, where a_0 is the lattice constant. This means that the wavelengths λ of the Bloch waves have lower bounds

$$\lambda > 2a_0. \tag{7}$$

The energy–k relation characterized by (5) can be probed by transport measurements. A metal is perturbed from the equilibrium condition by the applied electric field; the deviations of the electron distribution from the equilibrium move in the crystal so as to reach and maintain a stationary state. Typical deviations, that is, localized Bloch wave packets should extend over several or more lattice sites. This is so because no wave packets constructed from waves of the wave vectors (k_x, k_y, k_z) whose magnitudes have the upper bounds (π/a_0) can be localized within distances less than a_0. the motion of a quantum wave packet in general is known to obey Hamilton's equations of motion [6]. Thus, the Bloch electron should move classical-mechanically under the action of the forces averaged over the lattice constants. The periodic lattice forces generated from the potential V are averaged out to zero since

$$-\int\int dy\,dz\int_0^{a_0} dx\frac{\partial}{\partial x}V(x,y,z) = -\int\int dy\,dz\,[V(a_0,y,z)-V(0,y,z)] = 0. \tag{8}$$

Therefore, practically important forces acting on the Bloch's electron are electromagnetic forces.

We may now formulate dynamics for the Bloch electron as follows: First, we introduce a model Hamiltonian,

$$H_0(p_x,p_y,p_z) = E_n(\hbar k_x,\hbar k_y,\hbar k_z), \tag{9}$$

which generates the energy eigenvalue (5). we shall hereafter consider the motion of the electron within a fixed zone and drop the zone number n. Second, we generate classical equations of motion with the aid of this Hamiltonian. Before actually executing this program let us generalize our Hamiltonian to include the electromagnetic interaction energy

$$\begin{aligned} H &= H_0(p_x - qA_x, p_y - qA_y, p_z - qA_z) + q\phi(x,y,z,t) \\ &\equiv H_0(p_1 - qA_1, p_2 - qA_2, p_3 - qA_3) + q\phi(x_1,x_2,x_3,t), \end{aligned} \tag{10}$$

where $(A_1, A_2, A_3) \equiv \mathbf{A}$ and ϕ are vector and scalar potentials generating the electric and magnetic fields $(\mathbf{E}, \mathbf{B})$ such that

$$\mathbf{E} = -\nabla\phi(\mathbf{r}, t) - \frac{\partial}{\partial t}\mathbf{A}(\mathbf{r}, t),$$

and

$$\mathbf{B} = \nabla \times \mathbf{A}(\mathbf{r}, t). \tag{11}$$

By using the standard procedures, we then get Hamilton's equations of motion

$$\dot{x}_j \equiv v_j = \frac{\partial H}{\partial p_j} = \frac{\partial}{\partial p_j} H_0(p_1 - qA_1, p_2 - qA_2, p_3 - qA_3) \tag{12}$$

and

$$\dot{p}_j = -\frac{\partial H}{\partial x} = \frac{\partial H_0}{\partial x_j} - q\frac{\partial \phi}{\partial x_j} \qquad (j = 1, 2, 3). \tag{13}$$

The first set of equations define the velocity $\mathbf{v} \equiv (v_1, v_2, v_3)$. Notice that in the zero-field limit these definition equations are in agreement with Eq. (1). In the presence of electromagnetic fields Eqs. (12) give a relationship between $\{p_j - qA_j\}$ and $\{v_j\}$. Inverting this relation, we have

$$p_j - qA_j = f_j(v_1, v_2, v_3). \tag{14}$$

Using these and Eqs. (13), we then obtain

$$\frac{df_j}{dt} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})_j. \tag{15}$$

These are the desired equations of motion. Since f_j are functions of (v_1, v_2, v_3), these equations describe how the velocity $\mathbf{v}$ changes by the Lorentz force. That is, they are Newtonian equations.

3. Discussions

A. Validity

The velocity $\mathbf{v}$ [see Eqs. (9) and (12)] was defined in terms of the derivatives of $E_n(\hbar\mathbf{k})$, which is the energy eigenvalue of the zero-field Schrödinger equation (3). The energy E must therefore be a continuous analytic function of $\mathbf{k}$, which is true for an infinitely extended lattice. For low fields, this definition should be useful. If a high constant magnetic field is applied, the quantum states are characterized by the Landau-like quantum numbers quite distinct from the Bloch quantum numbers $(n, \mathbf{k})$ [7]. We must then abandon the standard definition (1) for $\mathbf{v}$. We shall discuss this case separately in subsection C.

The Hamiltonian H_0 constructed from the energy $E_n(\hbar\mathbf{k})$ represents a kinetic energy although this energy is not a simple quadratic function of $p's$. Dirac demonstrated in his famous book [6] that for *any* functional dependence of H_0 on $p's$. the center of a quantum wave packet moves in accordance with Hamilton's equations of motion. As we stated earlier in (8) *any* lattice-periodic force averaged over the periods vanishes.

The electromagnetic fields $(\mathbf{E}, \mathbf{B})$ may vary in space and time. Since the velocity $\mathbf{v}$ are not conjugate to the position $\mathbf{r}$, Eqs. (15) are correct for inhomogeneous fields while Eq. (2) cannot as pointed out in Sect. 1.

Electromagnetic radiations such as microwaves and visible lights which are used to probe the states of conduction electrons, have wavelengths much greater than the lattice constants a_0. The Bloch electron should then respond to the electromagnetic fields carried by the radiation as represented by Eqs. (15). If radiations such as X-rays and γ-rays, whose wavelengths are comparable to, or smaller than, the lattice constant are applied to a solid, the picture of the interaction between the Bloch electron (spread over several lattice sites) and the radiation should break down. Rather, the picture of the interaction between a (nearly) free electron and the radiation should prevail as this picture has routinely been used for the theory of the photo-electric effect and the Compton scattering. In other words, Eqs. (15) are valid for the fields varying slowly over the lattice constant.

B. Significance

The physical meaning of Eqs. (15) is transparent when the effective mass approximation is applicable. The dispersion relation for an orthorhombic lattice may be represented by $E = (2m_1)^{-1}\hbar^2k_1^2 + (2m_2)^{-1}\hbar^2k_2^2 + (2m_3)^{-1}\hbar^2k_3^2$. Then, Eqs. (15) are then simplified to

$$m_j\frac{dv_j}{dt} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})_j, \tag{16}$$

which have a familiar form: (mass) × (acceleration) = force.

Clearly, Eqs. (15) are gauge-invariant in contrast with the commonly adopted Eq. (2). In the homogeneous limit, Eqs. (15) approach Zak's equation [3]. Only Eqs. (15) are consistent with the fact of principle that no static magnetic fields can alter the energy of the Bloch electron. This energy conservation law can simply be proved by multiplying Eqs. (15) with $\mathbf{E} = 0$ and $\mathbf{B} = \mathbf{B}(x, y, z)$ by v_j, summing the results over j, and obtaining

$$\sum_j v_j\frac{df_j}{dt} = \frac{d}{dt}H_0(p_1 - qA_1, p_2 - qA_2, p_3 - qA_3) = q(\mathbf{v} \times \mathbf{B}) \cdot \mathbf{v} = 0. \tag{17}$$

In the zero magnetic field limit, $B = 0$, and in the homogeneous limit, in which $\mathbf{v} = \mathbf{v}(\mathbf{r}, t)$ and $\mathbf{E} = \mathbf{E}(\mathbf{r}, t)$, Eqs. (15) are reduced to Eq. (2). In the great majority of

the cases in which experiments such as the de Haas-van Alphen effect on conductors were analyzed with the aid of Eq. (2), Onsager's formula [2] and others valid for intermediate magnetic fields (high Landau oscillator numbers) are used to map the Fermi energy surfaces [8]. Corrections to the Fermi surfaces after the analyses of the experimental data at low fields by using Eqs. (15) in place of Eq. (2) appear to be negligible.

Equations (15) are Newtonian equations in the direct lattice space. This allows a sensible interpretation of the cyclotronic motion of a Bloch electron as expounded in the following subsection.

C. Strong magnetic fields

In the absence of the lattice potential V, the stationary quantum states of a free electron subjected to a constant magnetic field $\mathbf{B}$ are characterized by the Landau quantum numbers, which are very different from the k-vector. By analogy, the energy of a crystal electron under a high magnetic field cannot be characterized by (k_x, k_y, k_z). This means that the velocity $\mathbf{v}$ for a Bloch-Landau electron cannot be defined in the standard form (1). It is, however, still possible to generate semiclassical dynamics with a new definition of the velocity as follows.

Let us take wurtzite ZnS, which has highly anisotropic transport properties [9], and which may be thought to have a set of parallel "conducting planes" perpendicular to the c-axis, each plane containing a hexagonal array of ions. If a constant magnetic field $\mathbf{B}$ is applied along the c-axis, the conduction electrons may orbit around the field $\mathbf{B}$ and passing through a series of + ions forming hexagons of various sizes. The quantum energies for closed hexagonal orbitals should be of the form

$$(\nu + \tfrac{1}{2})\hbar\omega_0^*, \quad \nu = 0, 1, 2, \ldots,$$

where $\omega_0^* \equiv eB/m_t$ is the cyclotron frequency. The molecular orbitals are highly degenerate since the centres of the hexagons can be anywhere in each plane. Since the crystal-atom arrays and therefore the crystal potential V is periodic in the z-direction (c-axis), the electron is unlocalized in this direction, and the energy E should depend on the wave number k_z by Bloch's theorem. In summary, we may then represent the energy E near the band edge E_0 by

$$E = E_0 + \frac{\hbar^2 k_z^2}{2m_\ell} + (\nu + \tfrac{1}{2})\hbar\omega_0^*. \tag{18}$$

The effective masses (m_t, m_ℓ) should be different from each other. The transverse mass m_t is the effective mass associated with the motion in the conducting plane. In contrast, the longitudinal mass m_ℓ is connected with the quantum tunneling along the c-axis and should be much greater than the transverse mass m_t.

The energy levels represented by (18) may be regarded as those for a quasi-particle with with charge q and anisotropic masses (m_t, m_ℓ), characterized by the Hamiltonian

$$H = \frac{1}{2m_t}\left[(p_x - qA_x)^2 + (p_y - qA_y)^2\right] + \frac{1}{2m_\ell}(p_z - qA_z)^2, \tag{19}$$

with $\mathbf{A}$ being chosen such that $\mathbf{B} = \nabla \times \mathbf{A}$ may point in the positive z-axis.

Let us now consider a general case in which the field $\mathbf{B}$ is applied in an arbitrary orientation (θ, ϕ) relative to the c-axis. The motion of the quasi-electron may be characterized by the Hamiltonian H in (19) with a choice of $\mathbf{A}$ such that $\mathbf{B} = \nabla \times \mathbf{A}$. Using the Hamiltonian formulation, we can then generate Newtonian equations of motion. The results are identical with those given in (16) with $m_1 = m_2 = m_t, m_3 = m_\ell$ and $\mathbf{E} = 0$. By solving the equations of motion, we can then obtain the following expression for the cyclotron frequency ω [7]

$$\omega = (\omega_t^2 \cos^2\theta + \omega_\ell \omega_t \sin^2\theta)^{1/2}, \quad \omega_t \equiv \frac{eB}{m_t}, \quad \omega_\ell \equiv \frac{eB}{m_\ell}. \tag{20}$$

No cyclotron resonance experiments for this crystal are available at the present time.

In the early fifties, Dresselhaus, Kip and Kittel observed first ever cyclotron resonance in Ge and Si and reported [10] that there are a number of resonance peaks for electrons and holes, and that the peak positions (frequencies) depend on the orientation of the magnetic field relative to the crystal axes. They successfully discussed the orientation dependence of the resonance peaks for electrons by using formula (20), [which was obtained a little differently, starting with the k-space dynamics]. Recently, we rederived the same formula (20), as outlined here, and interpreted their data from the direct-lattice dynamics [7]. Briefly, every resonance peak for the electron $(q = -e)$ or the hole $(q = e)$ can be identified with the cyclotron frequency ω associated with the hexagonal orbitals on one of the four $\{111\}$ planes or that associated the square-base orbitals on one of the three $\{100\}$ planes. As the orientation of the magnetic field $\mathbf{B}$ is varied, each peak moves, following formula (20). We stress that the present direct-lattice interpretation is more appealing to our common sense than the alternative (and original) interpretation in terms of the energy surfaces in the k-space.

The cyclotron radius r_0 corresponding to the lowest Landau states $\nu = 0$ is given by $r_0 \equiv (\hbar/eB)^{1/2}$, which is independent of the particle mass. This radius r_0 must be greater than the lattice constant a_0 for the validity of the continuous dynamical description. The values of r_0 are approximately 1800 (8) Å at $B = 0.02(1000)$ T. Therefore, semiclassical dynamics represented by Eqs. (15) and (19) should hold for all practical ranges of experimental fields.

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RESUMEN. Se derivan, en forma elemental, ecuaciones newtonianas de movimiento para un electrón de Bloch que son totalmente equivalentes a las ecuaciones de Zak. La derivación se hace utilizando el teorema de Bloch y la formulación hamiltoniana suponiendo campos electromagnéticos arbitrarios. Para campos magnéticos muy grandes, la velocidad se debe definir de manera diferente a la fórmula de campo débil.