Semiconductor Physics, Quantum Electronics & Optoelectronics, 2026. V. 29, No 2. P.130-135.

Editorial

Anatomy of electrons in the periodic potential of the crystal lattice in semiconductors

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Abstract. This review article describes in a concise form some of the latest achievements in semiconductor physics related to the topological and quantum properties of electron dynamics, in particular, in strong electric fields; new concepts in electronics based on the quantum degrees of freedom of electrons, which have led to the emergence of new branches distinct from traditional charge-based electronics. The recent emergence of picosecond-to-attosecond time-resolved and scanning spectroscopy has prompted the development of quantum theory describing the detailed high-frequency behavior of electrons on very short temporal and spatial scales, of the order of a few interatomic distances. In fact, such a precise spatiotemporal dynamical picture represents, in a sense, the anatomy of electrons in the periodic potential of a crystal lattice. Specifically, our attention is focused on the following issues that have been actively discussed in leading scientific journals over the past decade: the Berry phase, orbitronics, Zitterbewegung (trembling motion), and effective mass dynamics. Although several specialized reviews already have devoted to the addressed topics, we believe that such review digest including most recent references can help the readers, including authors of SPQEO, to get more information about current trends in the modern semiconductor theory and applications.

Keywords: slectron dynamics, strong electric fields, Berry's phase, orbitronics, Zitterbewegung, effective mass dynamics.

https://doi.org/10.15407/spqeo29.02.130
PACS 03.65.Vf, 72.20.-i, 72.25.-b, 87.15.hj

Manuscript received 06.04.26; revised version received 11.05.26; accepted for publication 10.06.26; published online 23.06.26.

1. Introduction

The fundamental aspects of semiconductor physics and, in general, solid-state physics form the basis of contemporary electronics and optoelectronics, where various electronic, optical, acoustical, and other effects and processes provide an advanced performance of modern devices. A large number of researchers from various scientific groups are working on the discovery and implementation of new physical phenomena and effects for potential innovative functional devices. The existing trend towards aggressive miniaturization of electronic devices makes the dynamics of electrons especially significant, since the frequency of electric currents associated with the movement of charge carriers in conduction bands determines the limits of device speed and operating frequency, and, consequently, the speed of information processing.

Today, the emergence of experimental methods with time resolution from picoseconds to attoseconds and a number of various scanning technologies allows the study of the motion of charges, currents, spins, *etc.* on the scales of elementary crystal cells and relevant times. Theoretical and experimental investigations of physical properties of early-time electron dynamics in strong electric fields have emerged as an area of central interest. The features of the electron behavior in nanoscale and particularly their wave functions (the Bloch functions) are important and open new ways for unexpected applications. This stimulates a more detailed study of electron behavior on very short temporal and spatial scales, corresponding to several interatomic distances thereby unfolding inherent electron anatomy in semiconductor crystals.

What happens to an electron in the periodic potential of semiconductor crystal lattice under the influence of an external electric field? Scientists have been trying to answer this question for many decades, permanently discovering new properties and details of electron behavior in new low-dimensional materials and structures, thereby reflecting the well-known dialectical viewpoint that "the electron is just as inexhaustible as the atom".

In this work, we collect and review in a digest-type form some of latest achievements in theoretical and experimental studies associated with quantum and topological properties of electron dynamics and transport in semiconductors focused on potential electronic applications.

It should be noted that the discovery of graphene, as well as many other related two-dimensional (2D) materials with unusual physical properties, has led to the emergence and rapid development of new branches of electronics – spintronics (*i.e.*, spin plus electronics or spin transport electronics) followed by others, such as valleytronics, orbittronics, straintronics, *etc.* We choose topics to address below mainly based on our own scientific interests and the area of research, where we work directly.

The organization of this review is as follows. Section 1 is an introduction describing the general background, the aim, and the article structure. In Sections from 2 to 5, we address sequentially quantum phenomena of the Berry phase, the Zitterbewegung (trembling motion), the orbitronics, and the effective mass dynamics. Section 6 provides the concluding remarks.

2. Berry's phase, connection, and curvature [1–10]

Currently, the concept of Berry phase of the electronic wave function of quantum states is closely associated with a wide range of new quantum phenomena, such as quantum Hall effect (QHE), anomalous Hall effect (AHE), spin Hall effect (SHE), and valley Hall effect (VHE), as well as various solid-state applications. Importantly, the notion of Berry phase makes the significant contribution to the understanding of various fundamental aspects of solid-state physics.

In a time-dependent problem, when considering a physical system described by a Hamiltonian that depends on time by means of a set of parameters, which are defined in the parameter space $\boldsymbol{R}(t)$, the Hamiltonian solutions are time dependent through $\boldsymbol{R}(t)$; they represent the *instantaneous eigenstates and eigenvalues.* The wave function of a state $n(\boldsymbol{R})$ contains an arbitrary phase factor γ_n in addition to the usual dynamical phase determined by the time integral along a path C in the parameter space $\boldsymbol{R}(t)$; the integral is taken in the limits from the initial point $\boldsymbol{R}(t = 0)$ to the final point $\boldsymbol{R}(t = T)$. Being gauge dependent, γ_n can be compensated under gauge transformation by a factor acquired during the system evolution along the path C between the initial and final points $[\boldsymbol{R}(0) \neq \boldsymbol{R}(T)]$. Then, only the dynamical phase factor may be taken into account. For this reason, the mentioned phase γ_n has commonly been regarded as unimportant and neglected in the theory and interpretation of experimental results. However, the situation is radically changed, as it has been shown by Berry (1984) for the cyclic evolution of the system along a *closed path*, when the initial and final points coincide $[\boldsymbol{R}(0) = \boldsymbol{R}(T)]$. In this case, the phase is changed by an integer multiple of 2π only, which makes it being gauge-invariant physical quantity that cannot be dropped. In general, the Berry phase is a *geometrical phase*, *i.e.*, it depends only on topological properties of the path C, and is independent on the explicit time dependence of $\boldsymbol{R}(t)$. Compared to the Berry phase, which is always associated with a closed path, several fundamental quantities can be introduced to provide a local description of the geometric properties of the parameter space. These are the *Berry connection* and the *Berry curvature* defined through $\gamma_n(\boldsymbol{R}) = \int_C \mathrm{d}\boldsymbol{R}\cdot\boldsymbol{A}_n(\boldsymbol{R}) = \int_S \mathrm{d}\boldsymbol{S}\cdot\boldsymbol{\Omega}_n(\boldsymbol{R})$. Here, $\boldsymbol{A}_n(\boldsymbol{R}) = i\langle n(\boldsymbol{R})|\partial/\partial\boldsymbol{R}|n(\boldsymbol{R})\rangle$ is called the Berry vector or the Berry connection for $n(\mathbf{R})$ state, S is an arbitrary surface enclosed by the path C, and $\boldsymbol{\Omega}_n(\boldsymbol{R}) = \nabla_{\boldsymbol{R}}\times\boldsymbol{A}_n(\boldsymbol{R})$ is the Berry curvature (gauge invariant). The latter can be interpreted as an effective magnetic field in the parameter space. As distinct from the Berry phase defined through a closed loop, the Berry curvature is a local quantity. It characterizes geometrical properties of the parameter space. Since the parameters can be dynamical variables, the Berry curvature participates in the dynamics itself. In the Bloch band theory, it represents an intrinsic property of the band structure. For example, being nonzero in crystals with broken inversion symmetry, it gives rise to the transverse velocity of the electrons, leads to a Hall current in the *absence of magnetic field*, and the valley Hall effect in multivalley semiconductors, where electrically control of the valley electron density and valley magnetic domains has been predicted and analyzed. The Berry curvature of energy bands $\varepsilon_n(\boldsymbol{k})$ in semiconductor crystals is defined by the vector product of a bra-state $\langle\boldsymbol{\nabla}_{\boldsymbol{k}}\mathrm{u}_n(\boldsymbol{k})|$ and a ket-state $|\boldsymbol{\nabla}_{\boldsymbol{k}}\mathrm{u}_n(\boldsymbol{k})\rangle$ vectors:

$$\boldsymbol{\Omega}_{n\boldsymbol{k}} = i\langle\boldsymbol{\nabla}_{\boldsymbol{k}}\mathrm{u}_n(\boldsymbol{k})|\times|\boldsymbol{\nabla}_{\boldsymbol{k}}\mathrm{u}_n(\boldsymbol{k})\rangle;$$

here, $u_{n\boldsymbol{k}}$ is the cellular Bloch function and $\boldsymbol{k}$ is the electron wave vector. The average electron velocity $\boldsymbol{v}_n(\boldsymbol{k})$ in a state $(n, \boldsymbol{k})$ in an electric field $\boldsymbol{E}$ acquires quantum correction proportional to the Berry curvature in addition to the well-known quasi-classical term

$$\boldsymbol{v}_n(\boldsymbol{k}) = \frac{1}{\hbar}\boldsymbol{\nabla}_{\boldsymbol{k}}\varepsilon_n(\boldsymbol{k}) - \frac{e}{\hbar}\boldsymbol{E}\times\boldsymbol{\Omega}_{n\boldsymbol{k}}.$$

The second term on the right-hand side is called the *anomalous velocity*, which is transverse to the electric field direction and gives rise to the Hall current in the absence of magnetic field.

In summing up, the Berry phase plays the important role in electronic structure and electron dynamics of solid-state crystals. It has generated much interest throughout various fields of solid-state physics and practical applications.

3. Orbitronics [11–16]

Orbitronics is a recently emerging research area, which exploits the electron orbital angular momentum (OAM) degree of freedom in solid-state systems similar to spintronics, which is based on the use of a spin angular momentum as an information carrier. By analogy with spintronics (spin transport electronics), orbitronics utilizes orbital currents, which can be generated, transmitted, and detected.

The existence of orbital currents originates from the orbital character of Bloch states in crystals. It can be described resulting from various atomic orbital states, for example, *s*- and 3*p*-atomic orbitals (s, p_x, p_y, p_z) using the tight-binding approximation. In centrosymmetric crystals, the OAM $\boldsymbol{L}$ is zero due to the requirements of time reversal and spatial inversion symmetry properties; so that it can be induced only under an external electric field $\boldsymbol{E}$, which breaks the inversion symmetry. In this case, OAM appears due to the orbital hybridization along the direction of vector product $\boldsymbol{k}\times\boldsymbol{E}$, so that electrons with opposite direction of $\boldsymbol{L}$ propagate in the opposite directions perpendicular to both $\boldsymbol{L}$ and $\boldsymbol{E}$. This transport phenomenon is called the orbital Hall effect (OHE), similar to the SHE in spintronics. In noncentrosymmetric crystals, like monolayer gapped graphene or transition metal dichalcogenide (TMD) semiconductors, the OAM $\boldsymbol{L}$ is nonzero and of opposite direction corresponding to opposite sign of the Berry curvature (and the anomalous velocity) of Bloch states associated with the two inequivalent valleys in the mentioned above multivalley crystals. At that, the total OAM is zero due to the time reversal symmetry. Thus, there exist two opposite flows of the electrons, carrying the opposite orbital angular momentum due to the anomalous velocity governed by the Berry curvature, which gives the electron OAM Hall current. This effect is accompanied by accumulation of the OAM (and corresponding orbital magnetic moment) at the sample edges, which can be observed in experiments using Kerr rotation microscopy and magneto-optical Kerr rotation.

In addition, the orbital transport can mediate other transport phenomena, such as SHE and VHE. We recall that the classical Hall effect arises in a magnetic field perpendicular to the electric current (flow of charges) producing a voltage in the direction transverse to the current (in an open circuit configuration) or a transverse current (in a short-circuited circuit configuration). Similarly, the SHE transforms electric current into a transverse flow of polarized spins due to strong spin-orbit coupling (SOC) without magnetic field. In VHE, the electrons from different valleys move in the opposite transverse directions relative to a longitudinal (*i.e.*, along the conducting channel) electric current in the absence of magnetic field. It arises from the opposite-sign Berry curvatures in different valleys of multivalley semiconductor crystals with broken inversion symmetry.

Unlike spintronics, orbitronics is not based on spin-orbit interaction, which allows for the use of a wide range of different nonmagnetic materials. As well, orbitronics addresses 2D materials such as graphene and other similar 2D semiconductors, where orbital effects can exhibit themselves even in a more pronounced way. Orbitronics also involves the use of lasers and microwave waves to generate and study orbital currents. Orbitronics creates new possibilities for information processing, new more energy-efficient and compact devices.

Thus, orbitronics constitutes a promising branch of electronics due to expected creation of new types of memory devices, logic elements, and possible applications in terahertz technologies, for example, generating terahertz radiation through orbital currents.

4. Zitterbewegung (Trembling motion) [17–22]

The term and the phenomenon *Zitterbewegung* (ZB, trembling motion) was introduced into the theory of electron dynamics in a vacuum by E. Schrödinger (1930). He showed how the interference of quantum states in the two energy bands led to the electron velocity not being a constant of motion in the absence of external fields, but exhibiting, in addition to classical motion, very rapid periodic oscillations over time. However, the estimated amplitude (about 4×10^{-3} Å) and frequency (about 1 MeV, in energy units), corresponding to the positive and negative electron energies resulting from the Dirac equation, demonstrated that they were far beyond capability of the existing experimental techniques. Many years later, a large deal of interest in ZB phenomenon has been generated by the work of Zawadzki (2005), who showed that the electron ZB-phenomenon would have much more favorable amplitude and frequency characteristics in narrow-gap semiconductors than those in a vacuum. The reason was in more favorable values of the critical parameters determining the basic ZB characteristics: namely, the narrow energy gap, the electron effective mass (instead of the bare mass), and the maximum electron velocity (instead of the light velocity in vacuum). For narrow-gap semiconductors, the_latter has much less numerical values compared with those in a vacuum. Since then, this area of research has begun to develop rapidly. Many detailed features have been clarified, such as its transient character (*i.e.*, it disappears with time), the effect of multiband structure, *etc.* Numerous different models predicting ZB-like behavior have been proposed and analyzed. Among them, we can mention the models based on the Bychkov–Rashba and/or Dresselhaus spin splitting caused by structure/crystal inversion asymmetry in 2D semiconductors and many other related systems, which demonstrates universality of ZB phenomenon in the two-band situation.

It has been proposed to observe the trembling motion of electrons by detecting the oscillating current related to the ZB velocity, as well as the increase of electric high-frequency noise at the ZB characteristic frequency. Another possible way is to detect electromagnetic waves radiated from the trembling electrons.

5. Effective mass dynamics [23–35]

The effective mass m_{eff} and, more generally, the energy dispersion $\varepsilon_n(\boldsymbol{k})$ of the band electrons are the main characteristics, that determine the equilibrium and non-equilibrium electronic properties of semiconductors. They are of primary importance both for semiclassical and quantum phenomena, and are thoroughly studied theoretically and measured experimentally, especially for new low-dimensional semiconductor materials and structures. Two qualitatively different situations can be noted, in which the effective mass plays a decisive role. One of the cases is when the most important electronic states are located only in the immediate vicinity of the minimum of the electron energy $\varepsilon_n(\boldsymbol{k})$; then, m_{eff} determines the value of the electron mobility and contributes to the kinetic effects. The electron effective mass is an important factor for electron-phonon interaction, which is beyond the scope of this article. In another case, the effective mass (defined as a second derivative of $\varepsilon_n(\boldsymbol{k})$ on the wave vector) plays a key role in a certain part of the energy band dispersion or throughout the entire band. For example, the presence of energy dispersion regions with a negative effective mass leads to qualitatively new effects – electrical instabilities, the possibility of generating terahertz oscillations, *etc*. In addition, in the case of a more complex dispersion relation, such as a "Mexican hat" type dispersion, it becomes possible to form a new class of electronic states – bi-electron quasiparticles.

One of the fundamental statements of semiconductor theory is that an electron (or hole) in a Bloch state of the crystal accelerates under the action of an external force field F as a free particle with an effective mass m_{eff}; the rate of change of the mean velocity is equal to F/m_{eff}. In the multiband Bloch theory, the effective mass can be interpreted through the interaction between the states of different Bloch bands, which is determined by matrix elements of the momentum operator and the corresponding band-energy gaps summed over all bands.

The parameter m_{eff} is involved in describing electron dynamics in the Brillouin zone. It should be noted here that the use of m_{eff} over very short time intervals (of the order of or less than the energy gap divided by the Planck constant) may raise questions. The reason is that just after initial injection of a free-mass electron into a crystal band, it responses like a bare mass electron, rather than the effective mass one. The original discussion of this point was initiated by Adams and Argyres (1956). Contemporary theoretical and experimental studies confirm this idea. Today, owing to available high-speed femtosecond-attosecond time-resolved spectroscopy methods, the basic unfolding of detailed dynamical picture of the Bloch electron in strong electric field over a wide temporal range allows to follow how the effective mass arises. The recent theoretical analysis has showed that the changing inertia from early injection of a free-mass electron is the result of the bare mass electron dressing-up into the multiband states of the crystal to become an effective mass electron. The estimation of the transition time from real mass to effective mass demonstrates that this is the time for electron to traverse several lattice spaces. As we have noted above, the classical ZB-like phenomena are most pronounced in the two-band Dirac-like systems. However, for real multiband semiconductor systems, the non-negligible coupling between the bands gives rise to necessary sum over all band states. This multiband coupling leads to the two-band model ZB effects being over time, probabilistically, smeared out thus resulting in the dynamic effective mass picture. Note that a similar problem arises for electron transfer at the heterostructure interface (for example, an AlGaAs/GaAs heterostructure), where the electron must change its effective mass.

Thus, the concept of effective mass is of interest not only from the scientific point of view, but also allows generating new ideas in applied aspects of semiconductor physics, for example, possible generation of terahertz oscillations based on the negative effective mass picture.

6. Concluding remarks

Summing up, we conclude that recently an advanced technology has emerged called spintronics, where the electron spin (but not the electron charge) is used to carry information. This offers opportunities for creating new devices, which combine standard electronics with spin-dependent effects. This technology is quickly developing and spreading to involve other electron *quantum numbers*, thereby producing new similar branches such as valleytronics, orbitronics, *etc*. Topological features and quantum properties of electron dynamics have the important influence on the effects used in the base of new developing branches. It is important to note that the expected advantages of such new devices will be increased data processing speed, decreased electric power consumption, and higher integration element density on the chip. Despite the fact that the research areas discussed above are new, some authors claim the existence of potential and functional demonstration devices.

Acknowledgments

This work was supported in part (V.A.K.) by the Long-Term Program for the Ukrainian research teams at the Polish Academy of Sciences with financing by the U.S. National Academy of Sciences (Project LTP-NAS-A7-11-0008).

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Анатомія електронів у періодичному потенціалі кристалічної решітки напівпровідників

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Анотація. У цій оглядовій статті в стислій формі описано деякі останні досягнення у фізиці напівпровідників, пов’язані з топологічними та квантовими властивостями динаміки електронів, зокрема у сильних електричних полях; нові концепції в електрониці, основані на квантових ступенях свободи електронів, які привели до виникнення нових галузей, відмінних від традиційної електроніки, що базується на заряді. Недавня поява часово-розділеної та скануючої спектроскопії у піко- та атосекундному діапазонах стимулювала розвиток квантової теорії, що описує детальну високочастотну поведінку електронів на дуже коротких часових та просторових масштабах порядку кількох міжатомних відстаней. Насправді така точна просторово-часова динамічна картина представляє, у певному сенсі, анатомію електронів у періодичному потенціалі кристалічної решітки. Зокрема, наша увага зосереджена на наступних питаннях, які активно обговорювались у провідних наукових журналах протягом останнього десятиліття: фаза Беррі, орбітроніка, ціттербевегунг (тремтливий рух) та динаміка ефективної маси. Хоча кілька спеціалізованих оглядів уже присвячено зазначеним темам, ми вважаємо, що такий оглядовий дайджест, що включає найновіші посилання, може допомогти читачам, включаючи авторів SPQEO, отримати більше інформації про сучасні тенденції в теорії та застосуваннях напівпровідників.

Ключові слова: електронна динаміка, сильні електричні поля, фаза Беррі, орбітроніка, циттербевегунг, динаміка ефективної маси.