Zitterbewegung (trembling motion) of electrons in narrow-gap semiconductors

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Abstract

The theory of trembling motion (Zitterbewegung (ZB)) of charge carriers in various narrow-gap materials is reviewed. Nearly free electrons in a periodic potential, InSb-type semiconductors, bilayer graphene, monolayer graphene and carbon nanotubes are considered. General features of ZB are emphasized. It is shown that, when the charge carriers are prepared in the form of Gaussian wavepackets, ZB has a transient character with a decay time of femtoseconds in graphene and picoseconds in nanotubes. Zitterbewegung of electrons in graphene in the presence of an external magnetic field is mentioned. A similarity of ZB in semiconductors to that of relativistic electrons in a vacuum is stressed. Possible ways of observing trembling motion in solids are mentioned.

1. Introduction

Zitterbewegung (trembling motion) was theoretically devised by Schroedinger [1] after Dirac had proposed his equation describing free relativistic electrons in a vacuum. Schroedinger showed that, due to a non-commutativity of the quantum velocity with the Dirac Hamiltonian, relativistic electrons experience Zitterbewegung (ZB) even in the absence of external fields. The frequency of ZB is about \( \omega = 2m_0c^2/h \) and its amplitude is about the Compton wavelength \( \lambda_c = h/m_0c \approx 3.86 \times 10^{-3} \text{ Å} \). It was later understood that the phenomenon of ZB is due to an interference of electron states with positive electron energies (\( E > m_0c^2 \)) and those with negative energies (\( E < m_0c^2 \)). In other words, ZB results from the structure of the Dirac Hamiltonian, which contains both positive and negative electron energies. It is a purely quantum effect as it goes beyond Newton’s first law (see the discussion in [2]). To our knowledge, ZB for free electrons has never been directly observed. However, in the presence of the Coulomb potential ZB is manifested in the appearance of the so-called Darwin term. It was pointed out that Zitterbewegung may also occur in non-relativistic two-band systems in solids [3]. Since the appearance of papers by Zawadzki [4] and Schliemann et al [5] the subject of ZB became popular and it was demonstrated that this phenomenon should occur in various situations in solids [6–14]. It is the purpose of the present review to outline main features of ZB in narrow-gap semiconductors.

We begin by elementary considerations based on the Schroedinger equation. In the absence of external fields the Hamiltonian is \( \hat{H} = \hat{p}^2/2m \) and the velocity is \( \hat{v}_j = \partial \hat{H}/\partial \hat{p}_j = \hat{p}_j/m \). The time derivative of velocity is easily calculated to give \( \dot{\hat{v}}_j = 1/i\hbar [\hat{v}_j, \hat{H}] = 0 \). This means that \( \dot{\hat{v}}_j(t) = \text{const} \), which is equivalent to first Newton’s law stating that in absence of external forces the velocity is constant.

The situation is different when a Hamiltonian \( \hat{H} \) has a matrix form, as in the Dirac equation for relativistic electrons in a vacuum or in case of two or more interacting energy bands in solids. Then the quantum velocity \( \hat{v}_j = \partial \hat{H}/\partial \hat{p}_j \), which is also a matrix, does not commute with the Hamiltonian and the quantum acceleration \( \ddot{\hat{v}}_j/\text{dr} \) does not vanish even in the absence of external fields. Below we consider such situations and investigate their consequences for the electron motion.

2. Theory and results

We consider first the case of InSb-type narrow-gap semiconductors (NGS), see [4]. Their band structure is well described by the model of \( \Gamma_9 \) (conduction), \( \Gamma_8 \) (light and heavy hole) and \( \Gamma_7 \) (split-off) bands and it is represented by an 8 \( \times \) 8 operator matrix. Assuming the spin–orbit energy \( \Delta \gg \varepsilon_g \), neglecting the free-electron terms and taking the momentum components \( \hat{p}_z \neq 0 \) and \( \hat{p}_x = \hat{p}_y = 0 \), one obtains for the conduction and light-hole bands the Hamiltonian

\[
\hat{H} = u\hat{a}_3\hat{p}_z + \frac{4}{3}\varepsilon_g\hat{p}, \tag{1}
\]
where $\hat{a}_3$ and $\hat{p}$ are the well known $4 \times 4$ Dirac matrices and $\mu = (E_g/n_0^2)^{1/2} \approx 1 \times 10^8$ cm s$^{-1}$ is the maximum velocity. Hamiltonian (1) has the form appearing in the Dirac equation. The electron velocity is $\hat{z} = (1/\hbar)[\hat{z}, \hat{H}] = i\hbar \hat{a}_3$. To determine $\hat{a}_3(t)$ one calculates the commutator of $\hat{a}_3$ with $\hat{H}$ and integrates the result with respect to time. This gives $\hat{z}(t)$, and $\hat{z}(t)$ is calculated integrating again. The result is

$$\hat{z}(t) = \hat{z}(0) + \frac{u^2}{\hbar} \hat{p} + \frac{i\hbar}{2\hbar} \Lambda_0 \left[ \exp \left( \frac{-2i\hat{H}t}{\hbar} \right) - 1 \right],$$  \hspace{1cm} (2)$$

where $\Lambda_0 = \hat{a}(0) - u\hat{p}/\hbar$. The first two terms represent the classical motion. The third term describes time-dependent oscillations with the frequency $\omega_Z \approx E_g/\hbar$. Since $\Lambda_0 \approx 1$, the amplitude of oscillations is $\hbar u/\hat{H} \approx \hbar/(m_0^* u) = \lambda_Z$. Here

$$\lambda_Z = \frac{\hbar}{m_0^* u}$$  \hspace{1cm} (3)$$
is an important quantity analogous to the Compton wavelength $\lambda_c = \hbar/(m_0 c)$ for relativistic electrons in a vacuum. The oscillations analogous to those described in (2) are called Zitterbewegung. The quantity $\lambda_Z$ can be measured. The energy for electrons in NGS can be written in a 'semi-relativistic' form (see [15])

$$E = \pm \hbar u (\lambda_Z^{-2} + k^2)^{1/2}.$$  \hspace{1cm} (4)$$

For $k^2 > 0$ this formula describes the conduction and light-hole bands. For imaginary values of $k$ we have $k^2 < 0$ and the above formula describes the dispersion in the energy gap. This region is classically forbidden but can become accessible through quantum tunneling. Figure 1 shows the data for the dispersion in the gap of InAs obtained from tunneling experiments. The fit gives $\lambda_Z \approx 41.5$ Å and $u \approx 1.33 \times 10^8$ cm s$^{-1}$, in good agreement with the estimation for InAs ($m_0^* \approx 0.024 m_0$). Similar data for GaAs give $\lambda_Z$ between 10 and 13 Å [16], again in good agreement with the theoretical predictions ($m_0^* \approx 0.066 m_0$).

To demonstrate the universality of the two-band situation we consider the well known case of nearly free electrons in a solid in which the periodic lattice potential $V(r)$ is treated as a perturbation (see [10]). Near the Brillouin zone boundary the Hamiltonian has, to a good approximation, a $2 \times 2$ form

$$\hat{H} = \begin{pmatrix} \epsilon_{k+q} & V_q^* \epsilon_k \\ V_q & \epsilon_k \end{pmatrix},$$  \hspace{1cm} (4)$$

where $V_q^* = V_{-q}$ are the Fourier coefficients in the expansion of $V(r)$, and $\epsilon_k = \hbar^2 k^2/2m_0$ is the free-electron energy. The $2 \times 2$ quantum velocity $\hat{v}_z$ can now be calculated and the acceleration $\hat{a}_z$ is computed in the standard way. Finally, one calculates the displacement matrix $\hat{z}_{ij}$.

Until now we treated the electrons as plane waves. However, Lock [18] in his important paper observed that such a wave is not localized and it seems to be of a limited practicality to speak of rapid oscillations in the average position of a wave of infinite extent. Since ZB is by its nature not a stationary state, but a dynamical phenomenon, it is natural to study it with the use of wavepackets. These became a practical instrument when femtosecond pulse technology emerged (see [19]). Thus, in a more realistic picture the electrons are described by a wavepacket

$$\psi(z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp \left( -\frac{i}{2}d^2(k_z - k_{z,0})^2 \right) \times \exp(ik_z z) \, dk_z \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$  \hspace{1cm} (5)$$

In figure 2 we show ZB oscillations of $\hat{z}_{11}(t)$ averaged over wavepacket (5). The essential result is that, in agreement with Lock’s general predictions, the ZB oscillations of a wavepacket have a "transient" character, i.e. they disappear with time on a femtosecond scale. The frequency of oscillations is $\omega_Z = E_g/\hbar$, where $E_g = 2|V_q|$. Now we turn to interesting and intensively studied materials: bilayer and monolayer graphene and carbon

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**Figure 1.** Energy-wavevector dependence in the forbidden gap of InAs. Various symbols show the experimental data of Parker and Mead [17]. The solid line is a theoretical fit. The determined parameters are $\lambda_Z = 41.5$ Å and $u \approx 1.33 \times 10^8$ cm s$^{-1}$ (after [4]).

**Figure 2.** Transient Zitterbewegung oscillations of nearly free electrons versus time, calculated for a very narrow wavepacket centered at various $k_{z,0}$ values. The band parameters correspond to GaAs.
and the decay time is about \( \Gamma_Z^{-1} = 40 \) fs (after [11]).

The energy spectrum is \( \mathcal{E} = \pm \hbar^2 k^2/2m^* \), i.e. there is no energy gap between the conduction and valence bands. The position operator in the Heisenberg picture is \( \hat{x}(t) = \exp(i\hat{H}_Mt/\hbar)\hat{x}\exp(-i\hat{H}_Mt/\hbar) \). We calculate

\[
x_{11}(t) = x(0) + \frac{k_y}{k} \left[ 1 - \cos \left( \frac{\hbar k^2 t}{m^*} \right) \right],
\]

where \( k^2 = k_x^2 + k_y^2 \). The third term represents Zitterbewegung with the frequency \( \hbar \omega_z = 2\hbar^2 k^2/2m^* \), corresponding to the energy difference between the upper and lower energy branches for a given value of \( k \). In order to have ZB in the \( x \) direction one needs a non-vanishing momentum \( k_y \) in the \( y \) direction. If the electron is represented by a two-dimensional Gaussian wavepacket similar to that given in equation (5), the integrals of interest can be calculated analytically. In figure 3 we show observable physical quantities related to ZB. It can be seen that they have a transient character.

To look for the reason for the transient character of ZB the electron wavepacket is decomposed into sub-packets corresponding to positive and negative electron energies. It turns out that the ‘positive’ and ‘negative’ sub-packets move in opposite directions with the same velocity \( v = \hbar k_{0x}/2m^* \), where \( h k_{0x} \) is the initial value of momentum. The relative velocity is \( v^{rel} = \hbar k_{0y}/m^* \). Each of these packets has an initial width \( d \) and it spreads (slowly) in time. After a time \( \Gamma_Z^{-1} = d/v^{rel} \) the distance between the two packets equals \( d \), so the sub-packets cannot interfere and the ZB amplitude diminishes. This reasoning gives the decay constant \( \Gamma_Z = \hbar k_{0y}/m^*d \), in agreement with the analytical results [11]. Thus, the transient character of the ZB oscillations in a collisionless sample is due to an increasing spatial separation of the sub-packets corresponding to the positive and negative energy states.

Now, we turn to monolayer graphene. The two-dimensional band Hamiltonian describing its band structure is [22]

\[
\hat{H}_M = u \left( \hat{\mathbf{p}}_x + i \hat{j}_y, \hat{\mathbf{p}}_y - i \hat{j}_x \right),
\]

where \( u \approx 1 \times 10^8 \) cm s\(^{-1}\). The resulting energy dispersion is linear in momentum: \( \mathcal{E} = \pm u\hbar k \), where \( k = \sqrt{k_x^2 + k_y^2} \). The quantum velocity in the Schroedinger picture is \( \hat{v}_j = \partial\hat{H}_M/\partial j_j \), it does not commute with the Hamiltonian. In the Heisenberg picture we have \( \hat{v}(t) = \exp(i\hat{H}_M t/\hbar)\hat{v}\exp(-i\hat{H}_M t/\hbar) \). Using equation (8) we calculate

\[
v^{(11)}_y = u \frac{k_y}{k} \sin(2u kt).
\]

The above equation describes trembling motion with the frequency \( \omega_z = 2uk \), determined by the energy difference between the upper and lower energy branches for a given value of \( k \). As before, ZB in the direction \( x \) occurs only if there is a non-vanishing momentum \( \hbar k_x \). The results for the current \( j_x = e\bar{v}_x \) are plotted in figure 4 for \( k_{0y} = 1.2 \times 10^9 \) m\(^{-1}\) and different packet widths \( d \). It is seen that the ZB frequency does not depend on \( d \) and is nearly equal to \( \omega_z \), as given above for the plane wave. On the other hand, the amplitude of the ZB does depend on \( d \) and we deal with decay times of the order of femtoseconds.

Finally, we consider monolayer graphene sheets rolled into single semiconducting carbon nanotubes (CNT). The band Hamiltonian in this case is similar to equation (8) except that, because of the periodic boundary conditions, the momentum \( \hat{\mathbf{p}}_x \) is quantized and takes discrete values \( \hbar k_x = \hbar k_{nv} \), where \( k_{nv} = (2\pi/L)(n - v/3) \), \( n = 0, \pm 1, \ldots, v = \pm 1 \), and \( L \) is the length of circumference of CNT [23]. As a result, the free-electron motion can occur only in the direction \( y \), parallel to the tube axis. The geometry of CNT has two important consequences. First, for \( v = \pm 1 \) there always exists a non-vanishing value of the quantized momentum \( \hbar k_{nv} \). Second, for
quantization of the electron spectrum

features of ZB, which results from an interference of positive
to cause no interband electron transitions, so the essential
two carriers are described by different quantum numbers

The last subject we consider is the trembling motion of
each value of \(k_{\alpha}\), there exists \(k_{-\alpha,-\nu} = -k_{\alpha,\nu}\), resulting in the
same subband energy \(E = \pm E\), where \(E = \hbar u \sqrt{k_{\alpha,\nu}^2 + k_{\gamma}^2}\).

The time-dependent velocity \(v(t)\) and the displacement \(\hat{y}(t)\) can be calculated for the plane electron wave in the usual
way and they exhibit ZB oscillations (see [8]). For small
momenta \(k_{\gamma}\) the ZB frequency is \(\hbar \omega = E_{g}\), where \(E_{g} = 2\hbar\omega_{k_{\alpha}}\). The ZB amplitude is \(\lambda_{Z} \approx 1/k_{\alpha}\). However, we are
again interested in the displacement \(\hat{y}(t)\) of a charge carrier
represented by a one-dimensional wavepacket analogous to
that described in equation (5), see [11]. Figure 5 shows the
ZB oscillations calculated for a Gaussian wavepacket of two
widths. The decay times are of the order of picoseconds,
i.e. much larger than in bilayer and monolayer graphene.
The reason is that ZB oscillations occur due to the ‘built in’
momentum \(k_{\gamma}\), arising from the tube’s topology. In other words,
the long decay time is due to the one-dimensionality of the
system.

The last subject we consider is the trembling motion of
electrons in monolayer graphene in the presence of an external
magnetic field \(B \parallel z\), see [12]. The magnetic field is known
to cause no interband electron transitions, so the essential
features of ZB, which results from an interference of positive
and negative energy states of the system, are expected not to be
destroyed. On the other hand, introduction of an external field
provides an important parameter affecting the ZB behavior.
The essential feature introduced by the magnetic field is a
quantization of the electron spectrum \(E_{n} = s\hbar \omega \sqrt{n}\), where
\(n = 0, 1, \ldots\) and \(s = \pm 1\) for the conduction and valence
bands, respectively. The basic energy is \(\hbar \omega = \sqrt{2\hbar u/L}\),
with \(1/L = (eB/h)^{1/2}\). The velocity operators can again be
calculated in the time-dependent Heisenberg picture. These
are subsequently averaged over a Gaussian wavepacket and
they exhibit trembling motion. The presence of a quantizing
magnetic field has very important effects on ZB.

(1) For \(B \neq 0\) the ZB oscillations are permanent, for \(B = 0\) they are transient.
(2) For \(B \neq 0\) many ZB frequencies appear, for \(B = 0\) only
one frequency is at work.
(3) For \(B \neq 0\) both interband and intraband (cyclotron)
 frequencies contribute to ZB, for \(B = 0\) there are no
intraband frequencies.
(4) Magnetic field intensity changes not only the ZB
frequencies but the entire character of the ZB spectrum.

3. Discussion

It follows from the recent theoretical papers that the
phenomenon of ZB should appear quite often in solids.
Whenever one deals with interacting energy bands, charge
carriers having a non-vanishing momentum should experience
a trembling motion. Its frequency \(\omega_{Z}\) is about \(\hbar \omega_{Z} \approx \Delta E\),
where \(\Delta E\) is the energy separation between the interacting
‘positive’ and ‘negative’ states. If the real energy gap \(\Delta E\) exists,
there is \(\Delta E = E_{g}\) if \(E_{g} = 0\) the energy separation \(\Delta E\) is caused
by the non-vanishing value of momentum. The amplitude
\(\lambda_{Z}\) goes as \(\lambda_{Z} \propto 1/\Delta E\). The latter can reach the values of
tens of nanometers in narrow-gap semiconductors. As
mentioned in section 1, a similar phenomenon should occur
for free relativistic electrons in a vacuum, but both its frequency
and amplitude are much less favorable than for electrons in
semiconductors, see [24, 25]. This correspondence of the
trembling motions illustrates a general analogy between the
behavior of electrons in narrow-gap semiconductors and that
of relativistic electrons in a vacuum [25]. Zitterbewegung
was also proposed for other systems [26, 27], and it has
some interesting analogies in quantum optics [28]. As
to the ways of observing ZB, one can try to detect directly the
moving charge at corresponding frequencies using scanning
probe microscopy [29, 30]. One can also try to measure the
ac current related to the oscillating charge, see figures 3, 4
and reference [12]. Finally, and this is probably the most
 promising way, the oscillating charges should produce an
observable dipole radiation. An external magnetic field can
continuously change the frequency of such radiation. It
appears that graphene in the presence of a magnetic field
provides the most favorable conditions for an observation of
the fascinating phenomenon of Zitterbewegung. Very recently,
an acoustic analogue of Zitterbewegung was observed in a two-
dimensional sonic crystal [31].

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