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2007 J. Phys.: Condens. Matter 19 136219

(http://iopscience.iop.org/0953-8984/19/13/136219)

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **19** (2007) 136219 (18pp) doi:10.1088/0953-8984/19/13/136219

Zitterbewegung of nearly-free and tightly-bound electrons in semiconductors

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Received 10 September 2006, in final form 21 January 2007
Published 15 March 2007
Online at stacks.iop.org/JPhysCM/19/136219

Abstract

We show theoretically that non-relativistic nearly-free electrons in solids should experience a trembling motion (Zitterbewegung, ZB) in the absence of external fields, similarly to relativistic electrons in a vacuum. The ZB is directly related to the influence of the periodic potential on the free electron motion. The frequency of the ZB is $\omega \approx E_g/\hbar$, where E_g is the energy gap. The amplitude of the ZB is determined by the strength of periodic potential and the lattice period, and it can be of the order of nanometres. We show that the amplitude of the ZB does not depend much on the width of the wavepacket representing an electron in real space. An analogue of the Foldy–Wouthuysen transformation, known from relativistic quantum mechanics, is introduced in order to decouple electron states in various bands. We demonstrate that after the bands are decoupled electrons should be treated as particles of a finite size. In contrast to nearly-free electrons we consider a two-band model of tightly-bound electrons. We show that in this case also the electrons should experience the trembling motion. It is concluded that the phenomenon of ZB of electrons in crystalline solids is the rule rather than the exception.

1. Introduction

Zitterbewegung (a trembling motion) was theoretically devised by Schrödinger [1] after Dirac had proposed his equation describing free relativistic electrons in a vacuum. Schrödinger showed that, due to a non-commutativity of the quantum velocity $\hat{v} = \partial \hat{H}_D/\partial \boldsymbol{p}$ with the Dirac Hamiltonian $\hat{H}_D$, relativistic electrons experience Zitterbewegung (ZB) even in the absence of external fields. The frequency of the ZB is about $\omega = 2m_0c^2/\hbar$ and its amplitude is about the Compton wavelength $\lambda_c = \hbar/m_0c \approx 3.86 \times 10^{-3}$ Å. It was later understood that the phenomenon of the ZB is due to the interference of electron states with positive electron energies ($E > m_0c^2$) and negative energies ($E < m_0c^2$) (see [2–4]). In other words, ZB results

from the structure of the Dirac Hamiltonian, which contains both positive and negative electron energies, and it is a purely quantum effect as it goes beyond Newton's first law.

An important step in the understanding of ZB was made by Foldy and Wouthuysen [5], (see also [6, 7]), who showed that in the absence of external fields there exists a unitary transformation that transforms the Dirac Hamiltonian into a Hamiltonian in which positive and negative electron energies are decoupled. While solutions of the Dirac equation are four-component functions, the transformed states for the positive energies have only two upper non-vanishing components and those for the negative energies have only two lower non-vanishing components. Now the above-mentioned interference between the positive and negative energy states cannot occur and there is no ZB. Instead, in the new representation the electron is not a point-like particle but acquires a 'quantum radius' of the size λ_c. The interpretation of the two pictures is not quite clear at present (see [8–14]). To our knowledge, ZB has never been directly observed for free electrons. However, in the presence of the Coulomb potential the ZB is manifested in the appearance of the so-called Darwin term [2–4].

It was pointed out some time ago that Zitterbewegung may also occur in non-relativistic two-band systems in solids [15]. It was shown that, similarly to the relativistic case in a vacuum discussed above, the consequence of the ZB is that it is impossible to localize the electron better than to a certain finite volume. Recently, an analogy between the Dirac description of electrons in a vacuum and the coupled-band $\boldsymbol{k}\cdot\boldsymbol{p}$ formalism for electrons in narrow-gap semiconductors (NGS) and carbon nanotubes (CNT) was used to demonstrate that ZB should occur in these systems [16, 17]. It was shown that, in agreement with the 'semi-relativistic' analogy [18, 19], the ZB frequency is always $\omega \approx E_g/\hbar$, where E_g is the energy gap between the conduction and valence bands. The amplitude of Zitterbewegung in NGS and CNT was estimated to be $\lambda_Z = \hbar/m_0^* u$, where m_0^* is the effective electron mass and $u \approx 10^8$ cm s^{-1} is the maximum electron velocity in the system. The ZB length in NGS and CNT turns out be 10–100 Å, i.e. 10^4–10^5 times larger than in a vacuum. A much lower ZB frequency and its much higher amplitude, as compared to a vacuum, should make ZB much more readily observable in semiconductors. Zitterbewegung was also recently proposed in two-dimensional systems exhibiting spin splitting due to structure and bulk inversion asymmetry [20], and in 2D graphite [21]. A phenomenon similar to the ZB was proposed for electrons in degenerate valence bands in the presence of an external electric field [22]. Very recently, a unified description of the ZB of electrons in different solid state systems was attempted [23].

In view of this recently published work we want to investigate the question of whether the phenomenon of ZB in solids is the rule rather than the exception or vice versa. To this end we consider two limiting models for electrons in solids: nearly-free electrons, for which the periodic potential of the lattice may be treated as a weak perturbation, and tightly-bound electrons, for which the periodic potential may not be treated as a perturbation. Since we are interested in the general properties of ZB, we do not insist on details of the band models in question but rather concentrate on essential features that result in this phenomenon. Although we deal with non-relativistic electrons in solids, we use methods of relativistic quantum mechanics to investigate an alternative picture in which the trembling motion is replaced by a kind of electron 'smearing' in real space. The reason that the somewhat mysterious phenomenon of the ZB of electrons in a vacuum has never been observed seems to be related to its very high frequency and very small amplitude. The corresponding phenomenon in solids would have a much lower frequency and a much larger amplitude. The underlying hope motivating our work is that a more thorough theoretical understanding of the trembling motion will lead to an experimental detection of the phenomenon. This would not only deepen our knowledge of electrons in solids but also represent a great success for the relativistic quantum theory.

Our paper is organized in the following way. In section 2 we give the basis of the nearly-free electron formalism. Section 3 treats the resulting ZB using Schrödinger's method of the equation of motion. In section 4 a more realistic description of the ZB is presented in which electrons are treated as wavepackets. In section 5 we use the Foldy–Wouthuysen transformation known from the relativistic quantum mechanics to obtain an alternative electron picture. Section 6 treats the ZB in case of tightly-bound electrons. In section 7 we discuss the obtained results and compare them with previous work. The paper is concluded by a summary.

2. Nearly-free electrons

The beginning of this section is standard, but it is needed for further developments. We consider an electron in the presence of an external periodic potential $V(\boldsymbol{r}) = V(\boldsymbol{r} + \boldsymbol{r}_\mathrm{a})$, where $\boldsymbol{r}_\mathrm{a}$ is a translation vector of the lattice. The periodic potential $V(\boldsymbol{r})$ may be expressed by the Fourier series $V(\boldsymbol{r}) = \sum_{\boldsymbol{l}} V_{\boldsymbol{l}} \exp(\mathrm{i}\boldsymbol{l}\boldsymbol{r})$, where $\boldsymbol{l}$ are reciprocal lattice vectors and $V_{\boldsymbol{l}}$ are Fourier components of the periodic potential. For a real potential there is $V_{\boldsymbol{l}}^* = V_{-\boldsymbol{l}}$. The wavefunction of an electron has the Bloch form

$$\Psi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{\mathcal{V}}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{r}} \sum_{\boldsymbol{l}} a_{\boldsymbol{l}} \mathrm{e}^{\mathrm{i}\boldsymbol{l}\boldsymbol{r}}, \tag{1}$$

where $\mathcal{V}$ is the crystal volume and $\boldsymbol{k}$ is the wavevector. Inserting the wavefunction $\Psi_{\boldsymbol{k}}(\boldsymbol{r})$ into the Schrödinger equation one obtains the well-known equation for the energy E and the coefficients $a_{\boldsymbol{l}}$

$$\left(E - \frac{\hbar^2}{2m_0} (\boldsymbol{k} + \boldsymbol{l})^2 \right) a_{\boldsymbol{l}} = \sum_{\boldsymbol{g}} V_{\boldsymbol{g}} a_{\boldsymbol{l}-\boldsymbol{g}}, \tag{2}$$

where m_0 is the free electron mass and $\boldsymbol{g}$ are reciprocal lattice vectors.

In the absence of a periodic potential there is $a_{\boldsymbol{l}} = 0$, $a_0 = 1$, and $E = \hbar^2\boldsymbol{k}^2/2m_0 \equiv \epsilon_{\boldsymbol{k}}$ is the free electron energy. For a weak periodic potential we may treat $V(\boldsymbol{r})$ as a perturbation and approximate $a_{\boldsymbol{l}}$ for $\boldsymbol{l} \neq 0$ by retaining only linear terms in $V_{\boldsymbol{l}}$. We then obtain

$$a_{\boldsymbol{l}} = \frac{V_{\boldsymbol{l}}}{\epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k}+\boldsymbol{l}}} \tag{3}$$

and $a_0 = 1$. The perturbed energy is

$$E = \epsilon_{\boldsymbol{k}} + \sum_{\boldsymbol{l}\neq 0} \frac{|V_{\boldsymbol{l}}|^2}{\epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k}+\boldsymbol{l}}}. \tag{4}$$

For weak potentials the correction to the free electron energy is small. This, however, is true only if $\epsilon_{\boldsymbol{k}} \neq \epsilon_{\boldsymbol{k}+\boldsymbol{l}}$. For $\boldsymbol{k}$ and $\boldsymbol{l} = \boldsymbol{q}$ such that $\epsilon_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}+\boldsymbol{q}}$ we expect $a_{\boldsymbol{q}}$ to be comparable to a_0 and the potential may not be treated as a weak perturbation. The well-known way to treat this problem is to use the approximation for nearly degenerate levels in which we neglect in (2) all $a_{\boldsymbol{l}}$ except a_0 and $a_{\boldsymbol{q}}$. We then find

$$\begin{aligned} (E - \epsilon_{\boldsymbol{k}}) a_0 &= V_{-\boldsymbol{q}} a_{\boldsymbol{q}} \\ (E - \epsilon_{\boldsymbol{k}+\boldsymbol{q}}) a_{\boldsymbol{q}} &= V_{\boldsymbol{q}} a_0. \end{aligned} \tag{5}$$

Equations (5) are equivalent to dealing with the Hamiltonian

$$\hat{H} = \begin{pmatrix} \epsilon_{\boldsymbol{k}+\boldsymbol{q}} & V_{\boldsymbol{q}} \\ V_{\boldsymbol{q}}^* & \epsilon_{\boldsymbol{k}} \end{pmatrix}, \tag{6}$$

which is valid for $\boldsymbol{k}$ such that $\epsilon_{\boldsymbol{k}+\boldsymbol{q}} \approx \epsilon_{\boldsymbol{k}}$. Hamiltonian (6) has two eigen-energies

$$E_{1(2)} = \frac{\epsilon_{\boldsymbol{k}+\boldsymbol{q}} + \epsilon_{\boldsymbol{k}}}{2} \pm \sqrt{|V_{\boldsymbol{q}}|^2 + \left(\frac{\epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}}}{2} \right)^2}, \tag{7}$$

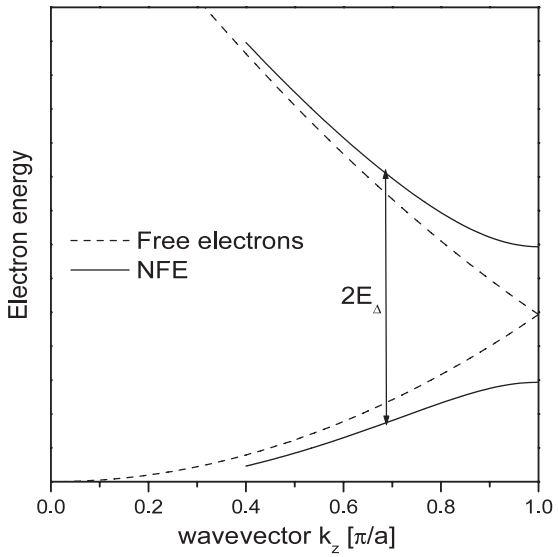

Figure 1. Energy versus k_z for free and nearly-free electrons (schematically). The dashed line shows $E = \hbar^2 k_z^2/2m_0$ dispersion for free electrons plotted in the first Brillouin zone. The solid line indicates $E(k_z)$ dispersion for the free motion weakly perturbed by a periodic potential.

and two eigen-states

$$|1\rangle = \frac{1}{N}\begin{pmatrix} E_\Delta + \Delta \\ V_q^* \end{pmatrix} \tag{8a}$$

$$|2\rangle = \frac{1}{N}\begin{pmatrix} -V_q \\ E_\Delta + \Delta \end{pmatrix}, \tag{8b}$$

where

$$\Delta = \frac{1}{2}(\epsilon_{k+q} - \epsilon_k) = \frac{\hbar^2}{2m_0}\left(\boldsymbol{kq} + \frac{q^2}{2}\right), \tag{9}$$

$$E_\Delta = \sqrt{|V_q|^2 + \Delta^2} \tag{10}$$

and $N = \sqrt{2E_\Delta(E_\Delta + \Delta)}$.

Taking only one vector $\boldsymbol{q}$ in the reciprocal lattice we are in reality considering a one-dimensional problem. To concentrate our attention we consider the symmetry of a simple cubic lattice. For the two points in the reciprocal lattice (see (5)) it is convenient to take $\boldsymbol{l} = 0$ and $\boldsymbol{l} = \boldsymbol{q} = [0, 0, -2\pi/a]$, where a is the lattice period. Then the two parabolas ϵ_k and ϵ_{k+q} in (4) cross at $\boldsymbol{k} = [0, 0, \pi/a]$, which determines the Brillouin zone boundary on the positive k_z axis (see figure 1). The energy gap at the zone boundary is $E_g = 2|V_q|$. The energies Δ and E_Δ depend in reality only on k_z. When using the nearly-degenerate perturbation theory based on (6) we should keep in mind that this procedure is only valid near the degeneracy point $k_z = \pi/a$, but it progressively ceases to work as k_z is lowered toward zero.

We note that E_Δ of (10) is analogous to the relativistic dispersion relation $E(p) = [(m_0c^2)^2 + c^2p^2]^{1/2}$. Thus $|V_q|^2 = (E_g/2)^2$ corresponds to $(m_0c^2)^2$, while Δ^2, which is quadratic in momentum, corresponds to c^2p^2.

It is convenient to split the Hamiltonian (6) into two parts:

$$\hat{H} = \hat{H}_\Delta + \hat{H}_k, \tag{11}$$

where

$$\hat{H}_\Delta = \begin{pmatrix} \Delta & V_q \\ V_q^* & -\Delta \end{pmatrix} \tag{12}$$

and

$$\hat{H}_k = \tfrac{1}{2}(\epsilon_{k+q} + \epsilon_k) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{13}$$

In terms of the Pauli matrices the Hamiltonian (12) reads

$$\hat{H}_\Delta = \Delta\hat{\sigma}_z + \mathrm{Re}(V_q)\hat{\sigma}_x - \mathrm{Im}(V_q)\hat{\sigma}_y. \tag{14}$$

Hamiltonian $\hat{H}_\Delta$ has a form reminiscent of the Dirac Hamiltonian for relativistic electrons in a vacuum, while the part $\hat{H}_k$ is proportional to the unity matrix and can be treated as a c-number. The decomposition (11) is directly related to the two terms in the energy (7).

The quantum velocity is $\hat{\boldsymbol{v}} = \partial\hat{H}/\partial(\hbar\boldsymbol{k})$. We calculate

$$\hat{\boldsymbol{v}} = \hat{\boldsymbol{v}}_\Delta + \hat{\boldsymbol{v}}_k = \boldsymbol{u}_\Delta\hat{\sigma}_z + \boldsymbol{u}_k\mathbf{1}, \tag{15}$$

where $\boldsymbol{u}_\Delta = \partial\Delta/\partial(\hbar\boldsymbol{k}) = (\hbar/m_0)\boldsymbol{q}/2$ and $\boldsymbol{u}_k = (\hbar/m_0)(\boldsymbol{k} + \boldsymbol{q}/2)$. It follows from (15) that the quantum velocity $\hat{\boldsymbol{v}}$ is an operator, not a number. Since Δ depends only on k_z, the only non-vanishing component of $\hat{\boldsymbol{v}}_\Delta$ is $\hat{v}_{\Delta z}$. In the following we drop the index z.

Eigen-values of the quantum velocity $\hat{v}_\Delta$ are $\mp(\hbar/m_0)(\pi/a)$. This seems paradoxical, as it means that the quantum velocity takes only two constant (and extreme) values. A similar result is obtained for the Dirac equation describing relativistic electrons in a vacuum, for which the eigen-values of the quantum velocity are $\pm c$. It is known that this feature is related to the ZB phenomenon.

3. Zitterbewegung

It can easily be verified that the quantum velocity (15) does not commute with the Hamiltonian (6). This means that $\mathrm{d}\hat{\boldsymbol{v}}/\mathrm{d}t$ does not vanish. Schrödinger's original derivation is based on the quantum equation of motion (see also [12]). Let us calculate the time dependence of $\hat{\boldsymbol{v}}$. We have

$$\mathrm{i}\hbar\frac{\mathrm{d}\hat{\boldsymbol{v}}}{\mathrm{d}t} = [\hat{v}_\Delta, \hat{H}] + [\hat{\boldsymbol{v}}_k, \hat{H}]. \tag{16}$$

Since $\hat{H}_k$ and $\hat{\boldsymbol{v}}_k$ are unity matrices, they commute with any number matrices. Therefore $\mathrm{d}\hat{\boldsymbol{v}}_k/\mathrm{d}t = 1/(\mathrm{i}\hbar)[\hat{\boldsymbol{v}}_k, \hat{H}] = 0$, so that $\hat{\boldsymbol{v}}_k(t) = \boldsymbol{v}_{k0}$. Thus

$$\mathrm{i}\hbar\frac{\mathrm{d}\hat{v}_\Delta}{\mathrm{d}t} = [\hat{v}_\Delta, \hat{H}_\Delta] = 2\hat{v}_\Delta\hat{H}_\Delta - \{\hat{v}_\Delta, \hat{H}_\Delta\}, \tag{17}$$

where the anti-commutator of $\{\hat{v}_\Delta, \hat{H}_\Delta\} = 2u_\Delta\Delta$. Hence

$$\mathrm{i}\hbar\frac{\mathrm{d}\hat{v}_\Delta}{\mathrm{d}t} = 2\hat{v}_\Delta\hat{H}_\Delta - 2u_\Delta\Delta. \tag{18}$$

Let us calculate the second time derivative of $\hat{v}_\Delta$

$$\begin{aligned}\mathrm{i}\hbar\frac{\mathrm{d}^2\hat{v}_\Delta}{\mathrm{d}t^2} &= \left[\frac{\mathrm{d}\hat{v}_\Delta}{\mathrm{d}t}, \hat{H}_\Delta\right] = \frac{1}{\mathrm{i}\hbar}[2\hat{v}_\Delta\hat{H}_\Delta - 2u_\Delta\Delta, \hat{H}_\Delta] \\ &= \frac{2}{\mathrm{i}\hbar}[\hat{v}_\Delta, \hat{H}_\Delta]\hat{H}_\Delta = 2\frac{\mathrm{d}\hat{v}_\Delta}{\mathrm{d}t}\hat{H}_\Delta.\end{aligned} \tag{19}$$

This represents a differential equation for $\mathrm{d}\hat{v}_\Delta/\mathrm{d}t$. Its solution is

$$\frac{\mathrm{d}\hat{v}_\Delta}{\mathrm{d}t} = \hat{A}_0 \exp(-2\mathrm{i}\hat{H}_\Delta t/\hbar), \tag{20}$$

where $\hat{A}_0$ is a constant operator. Inserting (20) into (18)

$$\mathrm{i}\hbar\hat{A}_0 \exp(-2\mathrm{i}\hat{H}_\Delta t/\hbar) = 2\hat{v}_\Delta\hat{H}_\Delta - 2u_\Delta\Delta. \tag{21}$$

Solving (21) for $\hat{v}_\Delta$ we obtain

$$\hat{v}_\Delta(t) = \tfrac{1}{2}\mathrm{i}\hbar\hat{A}_0 \exp(-2\mathrm{i}\hat{H}_\Delta t/\hbar)\hat{H}_\Delta^{-1} + u_\Delta\Delta\hat{H}_\Delta^{-1}. \tag{22}$$

Integrating (22) with respect to time and adding the term due to the z component of $\hat{\boldsymbol{v}}_{\boldsymbol{k}}$ we finally find

$$\hat{z}(t) = z_0 + v_{k_z0}t + u_\Delta\Delta\hat{H}_\Delta^{-1}t - \tfrac{1}{4}\hbar^2\hat{A}_0(\exp(-2\mathrm{i}\hat{H}_\Delta t/\hbar) - 1)\hat{H}_\Delta^{-2}. \tag{23}$$

In order to find $\hat{A}_0$ we use (21) for $t = 0$

$$\hat{A}_0 = \frac{1}{\mathrm{i}\hbar}\left(2\hat{v}_\Delta\hat{H}_\Delta - 2u_\Delta\Delta\right) = \frac{2u_\Delta}{\mathrm{i}\hbar}\begin{pmatrix} 0 & V_q \\ -V_q^* & 0 \end{pmatrix}. \tag{24}$$

At $t = 0$ there is $\hat{z}(0) = z_0$. Similarly, it follows from (22) and (24) that $\hat{v}_\Delta(0)$ is equal to the z component of the initial velocity $\hat{v}_\Delta$ from (15).

In order to interpret the result (23) we observe that the eigen-energy of $\hat{H}_\Delta$ is $\pm E_\Delta$, where E_Δ is given by (10). There is $\hat{H}_\Delta^{-1} = \hat{H}_\Delta/{E_\Delta}^2$ and $\hat{H}_\Delta^{-2} = 1/{E_\Delta}^2$. The exponential term in (23) is (see the appendix)

$$\exp\left(\frac{-2\mathrm{i}\hat{H}_\Delta t}{\hbar}\right) = \cos\left(\frac{2E_\Delta t}{\hbar}\right) - \mathrm{i}\frac{\hat{H}_\Delta}{E_\Delta}\sin\left(\frac{2E_\Delta t}{\hbar}\right). \tag{25}$$

The first three terms in (23) describe the classical motion. The last term, according to (25), describes oscillations with the frequency $\omega = 2E_\Delta/\hbar$. This frequency corresponds directly to the interband energy $2E_\Delta$, as seen in figure 1.

Since the Hamiltonian $\hat{H}_\Delta$ is a matrix, the position $\hat{z}(t)$ is also a matrix. We have explicitly

$$\hat{z}(t) = \begin{pmatrix} z_{11}(t) & z_{12}(t) \\ z_{21}(t) & z_{22}(t) \end{pmatrix}, \tag{26}$$

where

$$\hat{z}_{11}(t) = \frac{\hbar u_\Delta|V_q|^2}{2{E_\Delta}^3}\sin\left(\frac{2E_\Delta t}{\hbar}\right) + \frac{u_\Delta\Delta^2 t}{{E_\Delta}^2} + v_{k_z0}t + z_0. \tag{27}$$

The component $\hat{z}_{22}(t)$ has negative signs of the first two terms. Further

$$\hat{z}_{21}(t) = -\frac{\hbar u_\Delta V_q^*}{2{E_\Delta}^2}\left\{\mathrm{i}\left[\cos\left(\frac{2E_\Delta t}{\hbar}\right) - 1\right] + \frac{\Delta}{E_\Delta}\sin\left(\frac{2E_\Delta t}{\hbar}\right)\right\} + \frac{u_\Delta\Delta V_q^* t}{{E_\Delta}^2}, \tag{28}$$

where $z_0 = z(0)$ and $\hat{z}_{12}(t) = \hat{z}_{21}(t)^*$.

The amplitude of the oscillating term in (27) is $\hbar u_\Delta|V_q|^2/2{E_\Delta}^3 \approx \pi\hbar^2/(2m_0a|V_q|) = \lambda_Z/2$, where the ZB length is defined as

$$\lambda_Z = \frac{\pi\hbar^2}{m_0a|V_q|}. \tag{29}$$

This corresponds to the Compton wavelength in relativistic quantum mechanics. Its numerical estimation is given below.

In agreement with the history of the subject, as described in section 1, we can legitimately call the above oscillations the ZB. We shall discuss the subject of the ZB more thoroughly below. Here we emphasize how *little* we have assumed to obtain the trembling motion—we have only perturbed the free electron motion by a periodic potential.

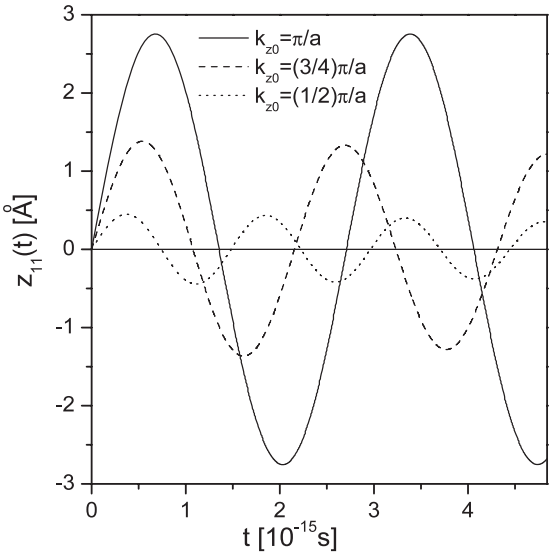

Figure 2. Zitterbewegung oscillations of nearly-free electrons versus time, calculated for a very narrow wavepacket centred at various k_{z0} values. The band parameters correspond to GaAs (see text).

4. Wavepacket

Now we consider a more realistic picture describing an electron in terms of a wavepacket. Taking, as before, $\boldsymbol{q} = [0, 0, -2\pi/a]$ and using the fact that Δ and E_Δ depend only on k_z, we take a Gaussian packet in the form

$$\psi(z) = \frac{1}{\sqrt{2\pi}} \frac{d^{1/2}}{\pi^{1/4}} \int_{\infty}^{\infty} \exp\left(-\frac{1}{2} d^2 (k_z - k_{z0})^2\right) \exp(\mathrm{i} k_z z)\, \mathrm{d}k_z \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{30}$$

where d determines the packet's width and k_{z0} fixes its centre in k_z space. Averaging the oscillating part of the motion over the wavepacket we obtain from (26)

$$\langle \psi(z) | \hat{z}^{\mathrm{osc}}(t) | \psi(z) \rangle = \frac{d}{\sqrt{\pi}} \int_{-\infty}^{\infty} \hat{z}_{11}^{\mathrm{osc}}(t) \exp(-d^2 (k_z - k_{z0})^2)\, \mathrm{d}k_z, \tag{31}$$

where $\hat{z}_{11}^{\mathrm{osc}}(t)$ is given in (27).

To begin, let us take the packet to be a delta function in k_z space centred at k_{z0}. This corresponds to a completely non-localized packet in real space. We can then take various k_{z0} values beginning with $k_{z0} = \pi/a$ at the zone boundary. In figure 2 we show the calculated ZB oscillations of $z_{11}(t)$ for different values of k_{z0}. It can be seen that as k_{z0} diminishes from π/a toward the zone centre, the amplitude of ZB quickly drops. This should not be surprising since, as is well known (see figure 1), the effect of the periodic potential on the free electron motion is the strongest at the zone boundary $k_z = \pi/a$, where the minimum gap occurs. (We do not consider here the gap at $k_z = 0$ for the upper branch.) Figure 3 shows the amplitude of the ZB for $d = \infty$ and $d = 20 r_{\mathrm{B}}^{-1}$, as calculated from (31). The quantity $r_{\mathrm{B}} = 0.53$ Å is the Bohr radius. For $d = \infty$ we deal in (30) and (31) with a delta function and the solid line in figure 3 follows the dependence $\hbar u_\Delta |V_q|^2/(2E_\Delta{}^3)$ of (27). When the width of the wavepacket increases (d decreases) the amplitude of the ZB for $k_{z0} \approx \pi/a$ diminishes and, as k_{z0} is lowered, it becomes independent of the width. Since our model is not valid for k_{z0} near zero, we are limited in our considerations to not too small d and k_{z0} values.

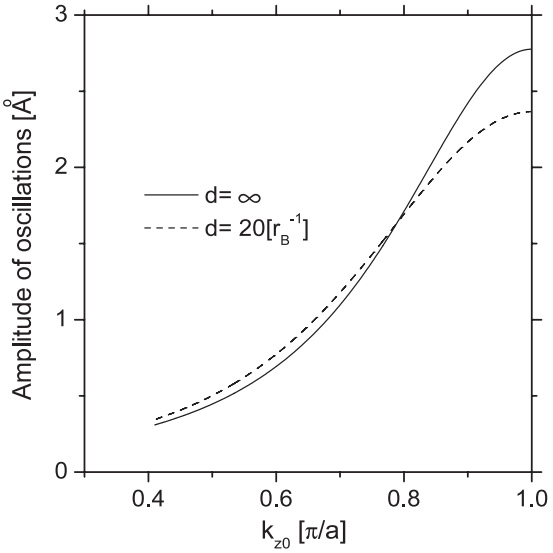

Figure 3. Amplitude of the ZB of nearly-free electrons versus the packet centre k_{z0}, calculated for two widths of the wavepacket. The symbol r_B denotes the Bohr radius. Material parameters correspond to GaAs.

However, since the ZB amplitude diminishes so quickly with diminishing k_{z0}, it is justified to limit the considerations of ZB to the vicinity of the band extremes. It can be seen from figure 2 that, with decreasing k_{z0}, the frequency of ZB increases. This increase follows from the behaviour of the gap $2E_\Delta$, as illustrated in figure 1.

In order to calculate numerical values for the ZB we need to specify material parameters. As an example we take $V_q = E_g/2 = 0.76$ eV and $a = 5.6$ Å, corresponding to GaAs. This gives $\lambda_Z = 5.6$ Å. This value can be compared with $\lambda_Z = 10$–13 Å for GaAs, as obtained with the use of $\boldsymbol{k}\cdot\boldsymbol{p}$ theory for the fundamental gap in GaAs at $\boldsymbol{k} = 0$ [16]. The above estimation of λ_Z based on the simple model is better than one could expect. Clearly, if we take the V_q value corresponding to $E_g = 0.23$ eV for InSb, λ_Z would be seven times larger.

Next we calculate an observable quantity, that is the electric current caused by ZB. It is given by the velocity multiplied by the charge. The oscillatory part of the velocity is given by the first term in (22). We average it using the wavefunction (30) which selects the component $\hat{v}_{11}(t)$

$$\hat{v}_{11}(t) = \frac{u_\Delta |V_q|^2}{E_\Delta^2} \cos\left(\frac{2E_\Delta t}{h}\right) + \frac{u_\Delta \Delta^2}{E_\Delta^2}. \tag{32}$$

The results for the velocity, computed with the Gaussian wavepacket (30), are plotted in figure 4. They are quantitatively similar to those shown in figure 2, the ZB frequency is clearly the same and the amplitude decreases with increasing k_{z0}. The phase, however, is different and the velocity $\hat{v}_{11}(t)$ is not zero at $t = 0$ but is equal to u_Δ from (15). Also, the velocity does not oscillate around zero, it oscillates around the value $v_{11}^{(0)}$ resulting from the second term in (32). For $k_{z0} = \pi/a$ we can find $v_{11}^{(0)}$ analytically:

$$v_{11}^{(0)} = u_\Delta\{1 - \sqrt{\pi}\,\zeta \exp(\zeta^2)[1 - \mathrm{erf}(\zeta)]\}, \tag{33}$$

where $\zeta = d/\lambda_Z$ and $\mathrm{erf}(x)$ is the error function. For narrow packets (large d) the shift $v_{11}^{(0)}$ tends to zero.

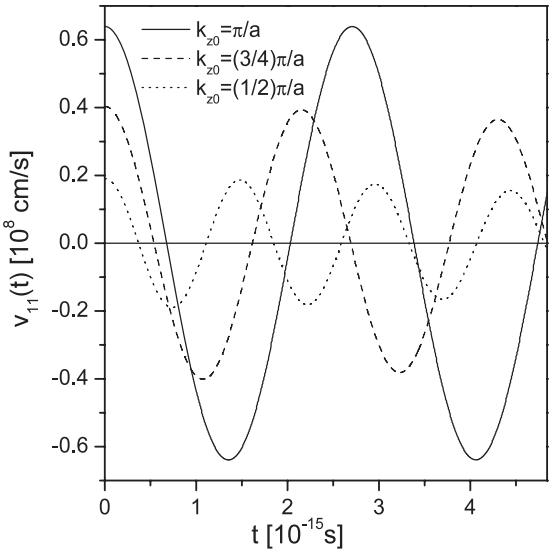

Figure 4. Contribution of ZB to the velocity for nearly-free electrons versus time, calculated for a very narrow wavepacket centred at various k_{z0} values. The band parameters correspond to GaAs (see text).

5. Foldy–Wouthuysen transformation

As mentioned in section 1, Foldy and Wouthuysen [5] proposed a transformation which, in the absence of external fields, transforms the Dirac Hamiltonian for relativistic electrons in a vacuum into a form in which positive and negative electron energies are separated. It was recently shown by Zawadzki [16, 17] that similar transformations exist for the $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonians describing band structures in narrow gap semiconductors and carbon nanotubes. Since the Hamiltonian $\hat{H}_\Delta$ of (12) also bears a similarity to the Dirac Hamiltonian, we can expect that a similar transformation exists for nearly-free electrons as well. This is indeed the case.

We define a unitary transformation

$$\hat{U} = \frac{E_\Delta + \hat{\beta}\hat{H}_\Delta}{\sqrt{2E_\Delta(E_\Delta + \Delta)}}, \tag{34}$$

where $\hat{\beta} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$. It is easy to verify that $\hat{U}\hat{U}^\dagger = 1$. Further

$$\hat{U}\hat{H}_\Delta\hat{U}^\dagger = E_\Delta\hat{\beta} \tag{35}$$

and obviously $\hat{U}\hat{H}_k\hat{U}^\dagger = \hat{H}_k$ since $\hat{H}_k$ is proportional to the unity matrix (see (13)). Thus, for the transformed Hamiltonian the eigen-energy problem factorizes into two independent problems for positive and negative E_Δ energies. This means that the wavefunction corresponding to the positive energy has the lower component equal to zero while the wavefunction for the negative energy has the upper component equal to zero. However, this is also true for other wavefunctions in the transformed representation, as we show below.

We consider an arbitrary wavefunction $\Psi(z)$ in the two-component representation. It can be expressed in general in the form

$$\Psi(z) = \int_{-\infty}^{\infty} u(k_z')\exp(\mathrm{i}k_z' z)\,\mathrm{d}k_z' = \Psi_+(z) + \Psi_-(z), \tag{36}$$

where

$$\Psi_{\pm}(z) = \frac{1}{2}\int_{-\infty}^{\infty}\left(1 \pm \frac{\hat{H}_{\Delta}}{E_{\Delta}}\right) u(k_z')\exp(\mathrm{i}k_z' z)\,\mathrm{d}k_z'. \tag{37}$$

Let us now transform the above functions using the $\hat{U}$ operator: $\Psi'_{\pm}(z) = \hat{U}\Psi_{\pm}(z)$. After some manipulations we obtain

$$\Psi'_{\pm}(z') = \frac{1 \pm \hat{\beta}}{2}\int_{-\infty}^{\infty}\left(\frac{E_{\Delta}}{2(E_{\Delta}+\Delta)}\right)^{1/2}\left(1 \pm \frac{\hat{H}_{\Delta}}{E_{\Delta}}\right) u(k_z')\exp(\mathrm{i}k_z' z')\,\mathrm{d}k_z'. \tag{38}$$

The k_z'-dependent function under the square root may be put under the integral sign, as explained in [5].

The functions $\Psi'_{\pm}(z')$ have the above-mentioned property of having only the upper or the lower non-vanishing components, which is guaranteed by the pre-factors $(1 \pm \hat{\beta})$. Using the inverse Fourier transform

$$u(k_z') = \frac{1}{2\pi}\int_{-\infty}^{\infty}\Psi(z')\exp(-\mathrm{i}k_z' z')\,\mathrm{d}z', \tag{39}$$

we have

$$\Psi'_{\pm}(z) = \int_{-\infty}^{\infty}\mathcal{K}^{\pm}(z, z')\Psi(z')\,\mathrm{d}z', \tag{40}$$

where

$$\mathcal{K}^{\pm}(z, z') = \frac{1 \pm \hat{\beta}}{2}\frac{1}{2\pi}\int_{-\infty}^{\infty}\left(\frac{E_{\Delta}}{2(E_{\Delta}+\Delta)}\right)^{1/2}\left(1 \pm \frac{\hat{H}_{\Delta}}{E_{\Delta}}\right)\exp(\mathrm{i}k_z'(z - z'))\,\mathrm{d}k_z'. \tag{41}$$

The kernels $\mathcal{K}^{\pm}(z, z')$ are not point transformations. To illustrate this we will transform the eigen-function of the position operator $\hat{z}'$ in the old representation, i.e. the Dirac delta function multiplied by a unit vector

$$\Psi(z') = \delta(z' - z_0)\begin{pmatrix}1\\0\end{pmatrix}. \tag{42}$$

The transformed functions are

$$\Psi'_{+}(z) = \mathcal{K}^{+}_{11}(z, z_0)\begin{pmatrix}1\\0\end{pmatrix} \tag{43}$$

and

$$\Psi'_{-}(z) = \mathcal{K}^{-}_{21}(z, z_0)\begin{pmatrix}0\\1\end{pmatrix}, \tag{44}$$

where

$$\mathcal{K}^{+}_{11}(z, z_0) = \frac{1}{2\pi\sqrt{2}}\int_{-\infty}^{\infty}\sqrt{1 + \frac{\Delta}{E_{\Delta}}}\mathrm{e}^{\mathrm{i}k_z'(z-z_0)}\,\mathrm{d}k_z' \tag{45}$$

and

$$\mathcal{K}^{-}_{21}(z, z_0) = \frac{-V_q}{2\pi\sqrt{2}}\int_{-\infty}^{\infty}\frac{\mathrm{e}^{\mathrm{i}k_z'(z-z_0)}}{\sqrt{E_{\Delta}(E_{\Delta}+\Delta)}}\,\mathrm{d}k_z'. \tag{46}$$

It is seen explicitly that the transformed functions $\Psi'_{+}(z)$ and $\Psi'_{-}(z)$ have vanishing lower or upper components, respectively. Both $\mathcal{K}^{+}_{11}(z, z_0)$ and $\mathcal{K}^{-}_{21}(z, z_0)$ are normalized to delta functions. To demonstrate that the transformed functions are characterized by a certain width,

we calculate their second moments $\mathcal{M}_2^{\pm}$. Since $\mathcal{K}_{11}^{+}(z, z_0) = \mathcal{K}_{11}^{+}(\zeta)$, where $\zeta = z - z_0$, we have

$$\mathcal{M}_2^{+} = \int_{-\infty}^{\infty} (\mathcal{K}_{11}^{+}(\zeta))^{\dagger} \zeta^2 \mathcal{K}_{11}^{+}(\zeta)\, \mathrm{d}\zeta$$
$$= \frac{1}{(2\pi)^2} \int\int\int \mathrm{e}^{-\mathrm{i}k_z'\zeta} \sqrt{1 + \frac{\Delta_{k_z'}}{E_{\Delta_{k_z'}}}}\, \mathrm{e}^{\mathrm{i}k_z''\zeta} \sqrt{1 + \frac{\Delta_{k_z''}}{E_{\Delta_{k_z''}}}}\, \zeta^2\, \mathrm{d}\zeta\, \mathrm{d}k_z'\, \mathrm{d}k_z''. \quad (47)$$

In (47) we used subscripts k_z' and k_z'' to indicate the variables of the integration. Using relations $\zeta = \mathrm{i}(\mathrm{d}/\mathrm{d}k_z') \exp(-\mathrm{i}k_z'\zeta)$ and similarly for k_z'' the triple integral is reduced to

$$\mathcal{M}_2^{+} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left(\frac{\mathrm{d}}{\mathrm{d}k_z'} \sqrt{1 + \frac{\Delta_{k_z'}}{E_{\Delta_{k_z'}}}} \right)^2 \mathrm{d}k_z' = \frac{1}{32} \lambda_Z, \quad (48)$$

where λ_Z is defined in (29). The above result has been calculated directly using Δ and E_{Δ} from (9) and (10). Note that since $\mathcal{K}_{11}^{+}(\zeta)$ has the dimension (m^{-1}), the dimension of $\mathcal{M}_2^{+}$ is (m).

Similar calculations for the second moment of $\mathcal{K}_{21}^{-}(\zeta)$ give $\mathcal{M}_2^{-} = \lambda_Z/32$. Thus the transformed functions for the upper and lower energies are characterized by the same widths, as should be expected. We will discuss physical implications of the above calculations in section 7.

When transforming various wavefunctions from the two-component representation to the one-component representation with the use of (40), it is important to know more about the kernels $\mathcal{K}^{\pm}(z - z')$, as given by (41). As an example we will calculate and plot $\mathcal{K}_{11}^{+}(\zeta)$ given by (45).

Because both Δ and E_{Δ} are centred at $k_z' = -q_z/2 = (\pi/a)$, it is convenient to change the variables $k_z' \to k_z - q_z/2$. Then we obtain

$$\mathcal{K}_{11}^{+}(\zeta) = \exp(-\mathrm{i}q_z\zeta/2) \times K_{11}^{+}(\zeta), \quad (49)$$

where

$$K_{11}^{+}(\zeta) = \frac{1}{2\pi\sqrt{2}} \int_{-\infty}^{\infty} \sqrt{1 + \frac{\Delta^0}{E_{\Delta}{}^0}}\, \exp(\mathrm{i}k_z\zeta)\, \mathrm{d}k_z, \quad (50)$$

$$\Delta^0 = \frac{\hbar^2}{2m_0} k_z q_z, \quad (51)$$

and $E_{\Delta}{}^0 = \sqrt{|V_q|^2 + (\Delta^0)^2}$. The quantities Δ^0 and $E_{\Delta}{}^0$ are centred at $k_z = 0$. After the change of variables, we singled out the rapidly oscillating part of $\mathcal{K}_{11}^{+}(\zeta)$, which is related to the position of band extremes in $\boldsymbol{k}$ space. The remaining part $K_{11}^{+}(\zeta)$ is a smoothly varying function of ζ with a singularity at $\zeta = 0$.

We consider the integrand in (50)

$$B(k_z) = \frac{1}{\sqrt{2}} \sqrt{1 + \frac{\Delta^0}{E_{\Delta}{}^0}}. \quad (52)$$

For $k_z \to \infty$ the function $B(k_z)$ tends to unity as $1 - \mathrm{O}(k_z^2)$, while for $k_z \to -\infty$ it tends to zero as $\mathrm{O}(k_z)$. Therefore the integral (52) is poorly convergent. Nevertheless, we can calculate it with the help of the Heaviside function $\Theta(k_z)$, which has a similar behaviour to the integrand (52) for $k_z \to \pm\infty$. We have

$$K_{11}^{+}(\zeta) = \frac{1}{2\pi} \left(\int_{-\infty}^{\infty} \left[B(k_z) - \Theta(k_z) \right] \exp(\mathrm{i}k_z\zeta)\, \mathrm{d}k_z + \int_{-\infty}^{\infty} \Theta(k_z) \exp(\mathrm{i}k_z\zeta)\, \mathrm{d}k_z \right). \quad (53)$$

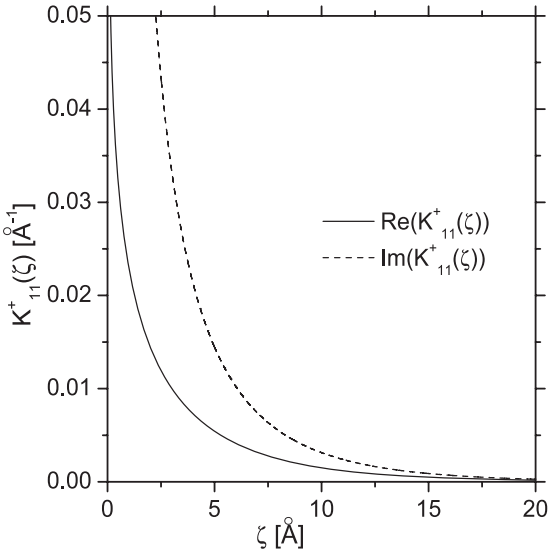

Figure 5. Real and imaginary parts of the kernel of Foldy–Wouthuysen transformation for nearly-free electrons (the smooth component) versus $\zeta = z - z_0$. Material parameters correspond to GaAs.

The second integral is $\int_{-\infty}^{\infty} \Theta(k_z) \exp(\mathrm{i}k_z\zeta)\,\mathrm{d}k_z = \mathrm{i}/\zeta + \pi\delta(\zeta)$. Thus the real and imaginary parts of $K_{11}^{+}(\zeta)$ are

$$\mathrm{Re}[K_{11}^{+}(\zeta)] = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left[B(k_z) - \Theta(k_z)\right]\cos(k_z\zeta)\,\mathrm{d}k_z + \frac{1}{2}\delta(\zeta) \tag{54}$$

and

$$\mathrm{Im}[K_{11}^{+}(\zeta)] = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left[B(k_z) - \Theta(k_z)\right]\sin(k_z\zeta)\,\mathrm{d}k_z + \frac{1}{2\pi\zeta}. \tag{55}$$

The above integrations are carried out numerically. The results are plotted in figure 5. Both $\mathrm{Re}[K_{11}^{+}(\zeta)]$ and $\mathrm{Im}[K_{11}^{+}(\zeta)]$ are singular at $\zeta = 0$ and for large ζ they decay exponentially.

Since we are dealing with weakly convergent integrals it is of interest to verify the accuracy of the above numerical calculations. To this end, we check two sum rules holding for $K_{11}^{+}(\zeta)$ defined in (50) (see [2]). The first rule is

$$\mathcal{S}_0^{+} = \int_{-\infty}^{\infty} K_{11}^{+}(\zeta)\,\mathrm{d}\zeta = \frac{1}{\sqrt{2}}\sqrt{1 + \frac{\Delta^0}{{E_\Delta}^0}}\bigg|_{k_z=0} = \frac{1}{\sqrt{2}}. \tag{56}$$

Now we verify that the same result is obtained from the numerical calculations of integrals in (54) and (55). Since the imaginary part of $K_{11}^{+}(\zeta)$ is an odd function of ζ, it gives no contribution to $\mathcal{S}_0$. The numerical calculation of the real part of $K_{11}^{+}(\zeta)$ gives $1/\sqrt{2}$ with an accuracy of 10^{-3}.

The second sum rule is related to the second moment of $K_{11}^{+}(\zeta)$. Calculations similar to those presented above give

$$\begin{aligned}\mathcal{S}_2^{+} &= \int_{-\infty}^{\infty} K_{11}^{+}(\zeta)\zeta^2\,\mathrm{d}\zeta \\ &= -\frac{1}{\sqrt{2}}\frac{\mathrm{d}^2}{\mathrm{d}k_z^2}\sqrt{1 + \frac{\Delta^0}{{E_\Delta}^0}}\bigg|_{k_z=0} = \frac{1}{\sqrt{2}}\left(\frac{\lambda_Z}{2}\right)^2.\end{aligned} \tag{57}$$

Taking into account the normalization (56) we obtain the extension of the K_{11}^{+} function to be $\lambda_Z/2$, which is in exact analogy to the relativistic Dirac electrons [2] (see also [16]). Similar results are obtained for the $\mathcal{S}_0^-$ and $\mathcal{S}_2^-$ integrals defined using the K_{21}^- function.

The Foldy–Wouthuysen transformation is not the only transformation which can decouple positive and negative energies in the field-free case. In the relativistic quantum mechanics described by the Dirac equation other transformations were devised (see for example Cini–Touschek [24]). In a recent paper Mulligan [25] introduced still another transformation separating the 4×4 Dirac equation into two 2×2 equations for the electron and anti-electron, respectively. It is possible that an analogous transformation would be possible for the nearly-free non-relativistic electrons considered above.

6. Tightly-bound electrons

In the preceding sections we considered the case of a weak periodic potential acting on free electrons and we showed that this potential leads to the ZB. Now we consider the opposite limit of a strong periodic potential.

An effective treatment of a strong periodic potential is the tight-binding method. We use here as an example the so-called empirical tight binding method. In this model one takes one s orbital per cation and three p orbitals per anion including nearest-neighbour and second nearest-neighbour interactions. Spherical approximation is assumed, so all sp and p bands are isotropic and their $\boldsymbol{k}$-dependence is given by the Γ–X dispersion. The model was used for calculating magnetic interactions in dilute magnetic semiconductors, approximating the band structure of $Cd_{1-x}Mn_xTe$ within the whole Brillouin zone [26]. This scheme provides a good semi-quantitative description of both upper valence bands as well as the lowest conduction band. In the basis x_a, y_a, z_a, s_c, (c, cation; a, anion) the Hamiltonian is

$$\hat{H} = \begin{pmatrix} t_k^{(2)} & 0 & 0 & \mathrm{i}V_k \\ 0 & t_k^{(3)} & 0 & 0 \\ 0 & 0 & t_k^{(3)} & 0 \\ -\mathrm{i}V_k & 0 & 0 & t_k^{(1)} \end{pmatrix}, \tag{58}$$

where

$$t_k^{(1)} = \epsilon_c + 4C[1 + 2\cos(\tfrac{1}{2}ak)], \tag{59}$$

$$t_k^{(2)} = \epsilon_a + 4A_2 + 8A_1\cos(\tfrac{1}{2}ak)], \tag{60}$$

$$t_k^{(3)} = \epsilon_a + 4A_1[1 + \cos(\tfrac{1}{2}ak)] + 4A_2\cos(\tfrac{1}{2}ak), \tag{61}$$

$$V_k = 4V_{ca}\sin(\tfrac{1}{4}ak). \tag{62}$$

Six parameters in (59)–(62), namely $\epsilon_c = 3.16$ eV, $\epsilon_a = 0.1$ eV, $V_{ca} = 1.103$ eV, $C = 0.015$ eV, $A_1 = 0.13$ eV and $A_2 = 0.15$ eV, are the Slater–Koster parameters in the notation used in [26], and $a = 6.482$ Å is the CdTe lattice constant. The parameters ϵ_c (ϵ_a) are cation (anion) on-site energies, V_{ca} is a single nearest-neighbour hopping parameter, while C, A_1, A_2 are the second-neighbour parameters.

Hamiltonian (58) can be factorized giving one doubly degenerate energy band $E_{2,3} = t_3(k)$ coming from p_y and p_z orbitals, and two energy bands coming from the s–p_x interaction. The sp_x Hamiltonian can be written in the form

$$\hat{H}_{sp} = \begin{pmatrix} \Delta_k & -\mathrm{i}V_k \\ \mathrm{i}V_k & -\Delta_k \end{pmatrix} + \Gamma_k \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{63}$$

where $\Delta_k = \frac{1}{2}(t_k^{(1)} - t_k^{(2)})$ and $\Gamma_k = \frac{1}{2}(t_k^{(1)} + t_k^{(2)})$. The Hamiltonian (63) is very similar to

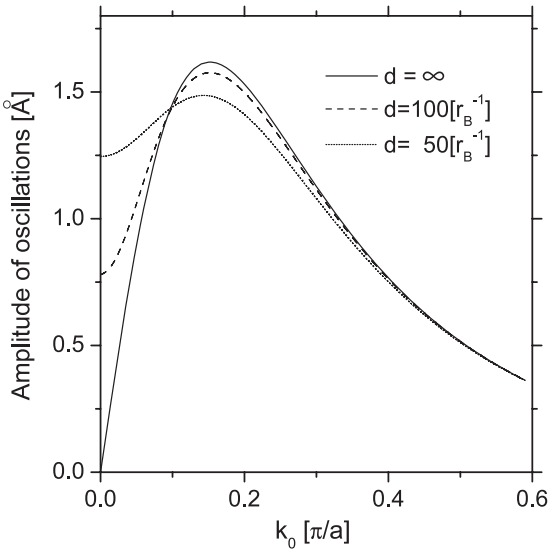

Figure 6. Amplitude of ZB of tightly-bound electrons versus packet centre k_0, calculated for three widths of the wavepacket. Symbol r_B denotes the Bohr radius. Material parameters correspond to CdTe (see text).

that for nearly-free electrons of (11)–(13). The difference is that Δ_k and V_k depend on the absolute value of $|\boldsymbol{k}|$. Also, the minimum band gap now occurs at $k = 0$. All eigen-energies of the Hamiltonian $\hat{H}_{\rm sp}$ have the periodicity of the reciprocal lattice. The quantum velocity $\hat{\boldsymbol{v}} = \partial \hat{H}_{\rm sp}/(\partial \hbar \boldsymbol{k})$ does not commute with $\hat{H}_{\rm sp}$. To calculate $\hat{r}(t)$ we use the Heisenberg picture

$$\hat{r}(t) = \exp(\mathrm{i}\hat{H}_{\rm sp}t/\hbar)\hat{r}(0)\exp(-\mathrm{i}\hat{H}_{\rm sp}t/\hbar), \tag{64}$$

which gives for the $\hat{r}(t)$ matrix

$$\hat{r}_{11}(t) = \left(\frac{V_k\Delta_k' V_k - V_k\Delta_k V_k'}{2{E_\Delta}^3}\right)\sin\left(\frac{2E_\Delta t}{\hbar}\right) + \left(\frac{\Delta_k V_k V_k' + \Delta_k^2\Delta_k'}{{E_\Delta}^2\hbar}\right)t + v_\Gamma t + r_0. \tag{65}$$

The component $\hat{r}_{22}(t)$ is given by (65) with the changed signs of the first two terms. Further

$$\hat{r}_{21}(t) = \frac{\Delta_k V_k' - \Delta_k' V_k}{2{E_\Delta}^2}\left\{\left[\cos\left(\frac{2E_\Delta t}{\hbar}\right) - 1\right] - \mathrm{i}\frac{\Delta}{E_\Delta}\sin\left(\frac{2E_\Delta t}{\hbar}\right)\right\} - \mathrm{i}\left(\frac{V_k^2 V_k' + V_k\Delta_k\Delta_k'}{\hbar{E_\Delta}^2}\right)t, \tag{66}$$

and $r_{12} = r_{21}^*$. In (65) and (66) the prime denotes a differentiation with respect to k, and $v_\Gamma = \partial\Gamma_k/(\partial\hbar k)$. Equations (65) and (66) are formally similar to (27) and (28), the main difference is that now there appear terms related to the dependence of V_k on k.

We calculated the ZB oscillations of $\hat{r}_{11}(t)$, as given by (65), using the Gaussian packet of the form (30). The results are similar to those illustrated in figure 2. In figure 6 we show the calculated amplitudes of the ZB as functions of the packet centre k_0 for three widths of the packet. Here the k_0 dependence does not have a maximum at $k_0 = 0$, because at this point the interaction V_k between the bands vanishes (see (62)).

The presence of a strong periodic potential leads to two effects. First, the quadratic dispersion relation $E_{\boldsymbol{k}} \propto \boldsymbol{k}^2$ for free electrons is replaced by a periodic one. Second, the potential mixes s and p_x states to form two sp_x energy bands. This mixing leads to the ZB.

7. Discussion

The main result of our work is that both in the case of nearly-free electrons and in the opposite case of tightly-bound electrons we predict the ZB phenomenon. Comparing this result with the previous work, in which ZB was predicted with the use of LCAO [15] and $\boldsymbol{k}\cdot\boldsymbol{p}$ theory [16, 17], we conclude that ZB is not due to a particular approach. In fact, the mathematics is quite similar in all the above theories and, although we deal with non-relativistic electrons, it resembles the formulation of relativistic quantum mechanics for free electrons in a vacuum. It is clear that the fundamental underlying reason for the appearance of ZB in solids is the periodic potential of the lattice. Particularly instructive in this respect are figures 2 and 3 of the present paper which show that the amplitude of ZB is directly related to the effect of the periodic potential on the free electron motion.

This result is not surprising. Without specifying any particular band model we deal in solids with the periodic Hamiltonian $\hat{H} = \hat{\boldsymbol{p}}^2/2m_0 + V(\boldsymbol{r})$ and the electron velocity is $\hat{\boldsymbol{v}} = \partial\hat{H}/\partial\hat{\boldsymbol{p}} = \hat{\boldsymbol{p}}/m_0$. It follows that $\mathrm{d}\hat{\boldsymbol{v}}/\mathrm{d}t = 1/(\mathrm{i}\hbar)[\hat{\boldsymbol{v}}, \hat{H}] \neq 0$, i.e. the velocity is not constant in time because of the periodic potential $V(\boldsymbol{r})$. In this perspective the various models mentioned above simply illustrate how this result comes about.

Clearly, the velocity does not commute with the Hamiltonian in the presence of other potentials as well. However, the periodic potential is special because, due to the Bloch theorem, the electrons can propagate in the perfect crystal without scattering and the quasi-momentum $\hbar\boldsymbol{k}$ is a good quantum number. For this reason it is possible to treat the electrons as almost free particles and replace the influence of the periodic potential by an effective electron mass. Still, as demonstrated in [16, 17] and the present paper, within two-band models the basic non-commutativity of $\hat{\boldsymbol{v}}$ and $\hat{H}$ mentioned above remains in the form of non-commuting 2×2 matrices with the resulting ZB. If the bands are completely separated, we have $\hat{H}_{\mathrm{eff}} = \hat{\boldsymbol{p}}^2/2m^*$ and $\hat{\boldsymbol{v}} = \hat{\boldsymbol{p}}/m^*$, so that $\hat{H}_{\mathrm{eff}}$ and $\hat{\boldsymbol{v}}$ commute and the ZB disappears. However, there is a price to pay for this separation. It is shown in [16, 17] and in the present paper that, once the electrons are described by a one-band equation (so that their energy is completely specified), they should be treated as objects of a finite size. The last effect is observable in the presence of an external potential due to appearance of the so-called Darwin term for free relativistic electrons [2–4, 10] as well as semiconductor electrons [16].

As emphasized throughout our paper (see also [16, 17]), in the two-band model the ZB of non-relativistic electrons in solids is in close analogy to the ZB of relativistic electrons in a vacuum, as first proposed by Schrödinger. The Hamiltonians for the two cases are very similar, and in both systems the ZB results from an interference of electron states corresponding to positive and negative electron energies [2–4]. If, with the use of Foldy–Wouthuysen transformation, the states of positive and negative energies are separated in the Hamiltonian and in the wavefunctions, ZB does not occur because the positive energy state (say) has nothing to interfere with. This corresponds to the separation of bands mentioned above and the conclusions of the two lines of reasoning agree.

Thus we are confronted with the following choice: (1) we use a two-band description, the electrons are point-like particles and they experience the ZB; (2) we use a one-band description, the electrons do not experience the ZB but they are characterized by a quantum radius of the size equal to the ZB amplitude.

The last point is illustrated by (57) describing the average 'smearing' of the transformed delta function. It is equal to the amplitude of ZB given by (27). One can say that the separation of energy bands by the Foldy–Wouthuysen transformation is equivalent to a certain averaging of the ZB motion.

It was observed [11] that, since the ZB had been predicted for plane Dirac waves, it is not quite clear what the trembling motion means for an electron uniformly distributed in space. In this connection it is important that the amplitude does not vary much when the electron is represented by a wavepacket localized in real space (see figure 3).

Passing to more specific points of our treatment, we emphasize again how little we had to assume to derive the ZB in the case of nearly-free electrons—it was enough to perturb the free electron motion by a periodic potential. This case has certain particularities. In the 'typical' two-band situations, both in a vacuum [2, 4, 10] and in solids [16, 17], there exists a maximum velocity in the system which plays an important role in the theory. In case of nearly-free electrons there is no maximum velocity since the perturbed energy branches tend asymptotically to the free electron parabola $E = \hbar^2 \boldsymbol{k}^2/2m_0$ (see figure 1). This is reflected in the velocity $\hat{v}_{\boldsymbol{k}}$, while the velocity $\hat{v}_\Delta$ has the typical 'two-band' behaviour and is responsible for the ZB. In fact, the velocity $\hat{v}_\Delta$ has the maximum value. It is equal to $(\hbar/m_0)(\pi/a)$ (see our eigen-value considerations after (15)). For $a = 5.6$ Å the maximum velocity is 6.4×10^7 cm s^{-1}, which should be compared with $u = 1.3 \times 10^8$ cm s^{-1} obtained from the $\boldsymbol{k} \cdot \boldsymbol{p}$ theory for GaAs and other III–V compounds [16]. Again, our simple model gives quite a reasonable estimation. In the nearly-free electron model λ_Z is proportional to $1/V_{\boldsymbol{q}} \sim 1/E_{\mathrm{g}}$ (see (29)), which agrees with the $\boldsymbol{k} \cdot \boldsymbol{p}$ approach [16], where $\lambda_Z \sim 1/m_0^* \sim 1/E_{\mathrm{g}}$. In narrow gap materials λ_Z can be as large as tens of angstroms.

As far as the phenomenon of ZB is concerned, the behaviour of nearly-free and tightly-bound electrons is quite similar. The main difference comes from the fact that in the nearly-free case the Fourier coefficients of the periodic potential do not depend on the wavevector $\boldsymbol{k}$, whereas in the tightly-bound case they go to zero for vanishing k. As a result, in the first case (see figure 3) the ZB amplitude is highest for the k_{z0} corresponding to the minimum energy gap, while in the second case (see figure 6) the maximum amplitude is shifted with respect to the minimum gap. For the tightly-bound case the electrons in $t_k^{(3)}$ bands (see (61)) would not exhibit ZB, but we do not insist on this point since these two bands are not realistically described by the model.

In order to illustrate that, after the Foldy–Wouthuysen transformation has been carried out, the former Dirac delta function is 'smeared' into the kernel $\mathcal{K}_{11}^+$ of (45), we not only calculate it numerically (see figure 5) but also calculate its second moment $\mathcal{M}_2^+$ (see (48)) and the sum rule $\mathcal{S}_2^+$ of (57). The second moment has the advantage of using the standard quantum mechanical probability distribution $(K_{11}^+)^\dagger K_{11}^+$ (see (47)). Its disadvantage is that this probability distribution is normalized to the Dirac delta function and not to a number. As to the sum rules using the single K_{11}^+ function, their advantage is that both the normalization (56) and the sum rule $\mathcal{S}_2^+$ (57) are numbers, and (57) can be simply interpreted as a square of 'smearing' (this procedure was used for free relativistic electrons by Rose [2]). The disadvantage of using the single K_{11}^+ is that we have to separate out its 'smooth' part (see (49)). The oscillatory part $\exp(-\mathrm{i}q_z\zeta)$ would not appear if we considered the nearly-free electron gap at $k_z = 0$.

Methods for observing the ZB should clearly be adjusted to the investigated materials, but it seems that an appropriate tool would be scanning probe microscopy which can produce images of coherent electron flow [27, 28]. This technique uses a sharp mobile tip which can sense the electron charge. If one used dilute magnetic semiconductors of the CdMnTe type [26] one could employ the magnetic effects caused by electron oscillations.

The second category of possible observable effects is related to the problem of what happens when electrons are confined to dimensions smaller than λ_Z. In relativistic quantum mechanics one finds statements that a measurement of the position of a particle, if carried out with greater precision than the Compton wavelength, would lead to pair production [8]. It is clear, however, that the pairs created this way can only be virtual, otherwise their recombination

would lead to the production of energy out of nothing. The virtual carriers could be observed in screening or in magnetism. An alternative point of view states that a stiff confinement is equivalent to an infinite potential well having the width $\Delta r < \lambda_Z$, and the electrons will simply occupy the lowest energy level in such a well. It is, however, certain that if an electron is confined to dimensions $\Delta r < \lambda_Z$, its energy (or its uncertainty) is of the order of the gap E_g between the positive and negative electron energies, which means that a one-band description is not adequate. We are then back to the two-band model, which was our starting point.

There remain many unanswered questions concerning the trembling motion but it appears that in crystalline solids it represents the rule rather than the exception. According to the theory, the ZB in semiconductors has decisive advantages over the corresponding effect in a vacuum. Thus an experimental detection of the trembling motion in solids may be possible in the near future.

8. Summary

We considered theoretically non-relativistic nearly-free electrons in solids for which the periodic potential of the lattice may be treated as a weak perturbation on the free electron motion. Using the two-band model, we showed that electrons experience the trembling motion (Zitterbewegung, ZB) in the absence of external fields, similar to that for free relativistic electrons in vacuum. The frequency of the ZB and its amplitude were derived. The frequency is $\omega \approx E_g/\hbar$ where E_g is the energy gap between the two bands. The amplitude λ_Z depends on the strength of the periodic potential and the lattice period. For typical parameters λ_Z can be of the order of 10–100 Å, that is 10^4–10^5 times larger than in a vacuum. The trembling motion is also considered for nearly-free electrons represented by wavepackets; it is shown that the amplitude is not strongly dependent on the packet's width. The Foldy–Wouthuysen type of unitary transformation, known from relativistic quantum mechanics, is used to separate the energy bands. The consequences of the Foldy–Wouthuysen transformation are investigated. It is demonstrated that if one uses a one-band description the electrons do not experience the trembling motion but they should be treated as particles having size λ_Z. Tightly-bound electrons are considered as well to provide the opposite case to nearly-free electrons. Within the two-band model the trembling motion is obtained, demonstrating that in this case as well the ZB phenomenon is not related to a specific theoretical approach. It is concluded that the trembling motion is directly related to the effect of the periodic potential on the electron and, as such, it should occur in many situations in solids.

Acknowledgment

This work was supported in part by the Polish Ministry of Sciences, grant no PBZ-MIN-008/P03/2003.

Appendix

First, we prove some properties of $\hat{H}_\Delta$ of (12). The eigen-values of $\hat{H}_\Delta$ are $\pm E_\Delta$. If $|1\rangle$ and $|2\rangle$ are eigen-states of $\hat{H}_\Delta$, then $\hat{P}_i = |i\rangle\langle i|$, $(i = 1, 2)$ are two projection operators. It follows that $\hat{P}_1 + \hat{P}_2 = 1$ and $\hat{H}_\Delta = E_\Delta(\hat{P}_1 - \hat{P}_2)$. Accordingly

$$(\hat{P}_1 - \hat{P}_2) = \frac{\hat{H}_\Delta}{E_\Delta}. \tag{A.1}$$

Since $\hat{H}_\Delta^{-1} = (1/E_\Delta)(\hat{P}_1 - \hat{P}_2)$, we have $\hat{H}_\Delta^{-1} = \hat{H}_\Delta/{E_\Delta}^2$. Then $\hat{H}_\Delta^{-2} = \hat{H}_\Delta^{-1}\hat{H}_\Delta^{-1} = 1/{E_\Delta}^2$ because $\hat{H}_\Delta^2 = {E_\Delta}^2$. For a real b there is

$$\exp(\mathrm{i}\hat{H}_\Delta b) = \exp(\mathrm{i}E_\Delta b)\hat{P}_1 + \exp(-\mathrm{i}E_\Delta b)\hat{P}_2. \tag{A.2}$$

Because $\exp(\pm\mathrm{i}E_\Delta b) = \cos(E_\Delta b) \pm \mathrm{i}\sin(E_\Delta b)$ we have

$$\exp(\mathrm{i}\hat{H}_\Delta b) = [\cos(E_\Delta b) + \mathrm{i}\sin(E_\Delta b)]\hat{P}_1 + [\cos(E_\Delta b) - \mathrm{i}\sin(E_\Delta b)]\hat{P}_2. \tag{A.3}$$

Grouping the terms with cosine and sine functions we get

$$\begin{aligned}\exp(\mathrm{i}\hat{H}_\Delta b) &= \cos(E_\Delta b)(\hat{P}_1 + \hat{P}_2) + \mathrm{i}\sin(E_\Delta b)(\hat{P}_1 - \hat{P}_2)\\ &= \cos(E_\Delta b) + \mathrm{i}\frac{\hat{H}_\Delta}{E_\Delta}\sin(E_\Delta b).\end{aligned} \tag{A.4}$$

This identity is used in (25).

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