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

2008 J. Phys.: Condens. Matter 20 454208

(http://iopscience.iop.org/0953-8984/20/45/454208)

J. Phys.: Condens. Matter **20** (2008) 454208 (5pp) doi:10.1088/0953-8984/20/45/454208

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

W Zawadzki[1] **and T M Rusin**[2]

[1] Institute of Physics, Polish Academy of Sciences, 02-668 Warsaw, Poland
[2] PTK Centertel Sp. z o.o., 01-230 Warsaw, Poland

E-mail: zawad@ifpan.edu.pl

Received 3 May 2008, in final form 7 July 2008
Published 23 October 2008
Online at stacks.iop.org/JPhysCM/20/454208

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 $\omega = 2m_0c^2/\hbar$ 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 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 $\dot{\hat{v}}_j = 1/(\mathrm{i}\hbar)[\hat{v}_j, \hat{H}] = 0$. This means that $\hat{v}_j(t) = \mathrm{const}$, 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 $\mathrm{d}\hat{v}_j/\mathrm{d}t$ 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 Γ_6 (conduction), Γ_8 (light and heavy hole) and Γ_7 (split-off) bands and it is represented by an 8×8 operator matrix. Assuming the spin–orbit energy $\Delta \gg \mathcal{E}_g$, 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

$$\hat{H} = u\hat{\alpha}_3\hat{p}_z + \tfrac{1}{2}\mathcal{E}_g\hat{\beta}, \tag{1}$$

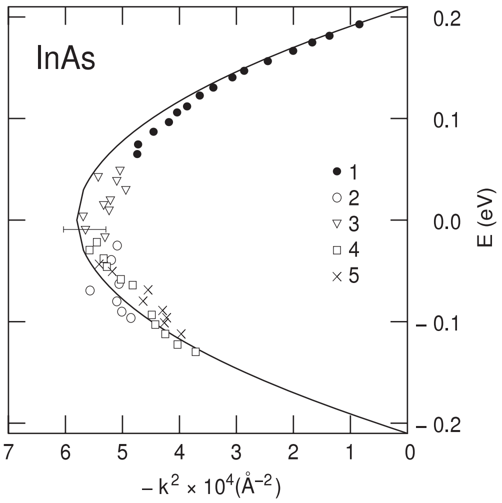

Figure 1. Energy-wavevector dependence in the forbidden gap of InAs. Various symbols show the experimental data of Parker and Mead [17]. The solid line is a theoretical fit. The determined parameters are $\lambda_Z = 41.5$ Å and $u = 1.33 \times 10^8$ cm s^{-1} (after [4]).

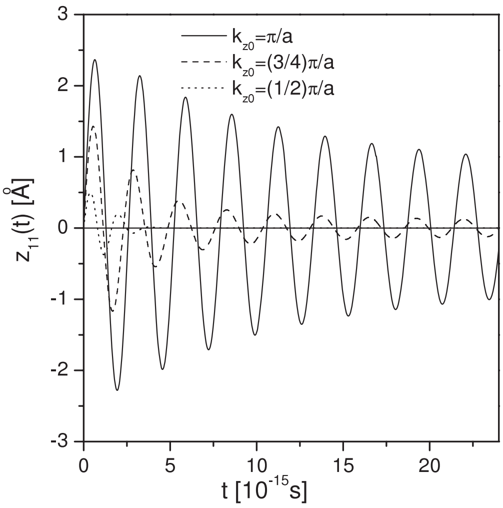

Figure 2. Transient Zitterbewegung oscillations of nearly free electrons versus time, calculated for a very narrow wavepacket centered at various k_{z0} values. The band parameters correspond to GaAs.

where $\hat{\alpha}_3$ and $\hat{\beta}$ are the well known 4×4 Dirac matrices and $u = (\mathcal{E}_g/2m_0^*)^{1/2} \approx 1 \times 10^8$ cm s^{-1} is the maximum velocity. Hamiltonian (1) has the form appearing in the Dirac equation. The electron velocity is $\dot{\hat{z}} = (1/\mathrm{i}\hbar)[\hat{z}, \hat{H}] = u\hat{\alpha}_3$. To determine $\hat{\alpha}_3(t)$ one calculates the commutator of $\hat{\alpha}_3$ with $\hat{H}$ and integrates the result with respect to time. This gives $\dot{\hat{z}}(t)$, and $\hat{z}(t)$ is calculated integrating again. The result is

$$\hat{z}(t) = \hat{z}(0) + \frac{u^2\hat{p}_z}{\hat{H}} + \frac{\mathrm{i}\hbar u}{2\hat{H}}\hat{A}_0\left[\exp\left(\frac{-2\mathrm{i}\hat{H}t}{\hbar}\right) - 1\right], \quad (2)$$

where $\hat{A}_0 = \hat{\alpha}(0) - u\hat{p}_z/\hat{H}$. The first two terms represent the classical motion. The third term describes time-dependent oscillations with the frequency $\omega_Z \approx \mathcal{E}_g/\hbar$. Since $\hat{A}_0 \approx 1$, the amplitude of oscillations is $\hbar u/\hat{H} \approx \hbar/(m_0^* u) = \lambda_Z$. Here

$$\lambda_Z = \frac{\hbar}{m_0^* u} \quad (3)$$

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 λ_Z can be measured directly. The energy for electrons in NGS can be written in a 'semi-relativistic' form (see [15]) $E = \pm\hbar u(\lambda_Z^{-2} + k^2)^{1/2}$. 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 ($m_0^* \approx 0.024m_0$). Similar data for GaAs give λ_Z between 10 and 13 Å [16], again in good agreement with the theoretical predictions ($m_0^* \approx 0.066m_0$).

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 $V(\boldsymbol{r})$ is treated as a perturbation (see [10]). Near the Brillouin zone boundary the Hamiltonian has, to a good approximation, a 2×2 form

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

where $V_q^* = V_{-q}$ are the Fourier coefficients in the expansion of $V(\boldsymbol{r})$, and $\epsilon_k = \hbar^2 k_z^2/2m_0$ is the free-electron energy. The 2×2 quantum velocity $\hat{v}_z$ can now be calculated and the acceleration $\dot{\hat{v}}_z$ 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

$$\psi(z) = \frac{1}{\sqrt{2\pi}}\frac{d^{1/2}}{\pi^{1/4}}\int_{\infty}^{\infty} \exp\left(-\tfrac{1}{2}d^2(k_z - k_{z0})^2\right) \times \exp(\mathrm{i}k_z z)\,\mathrm{d}k_z \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (5)$$

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 $\omega_Z = \mathcal{E}_g/\hbar$, where $\mathcal{E}_g = 2|V_q|$.

Now we turn to interesting and intensively studied materials: bilayer and monolayer graphene and carbon

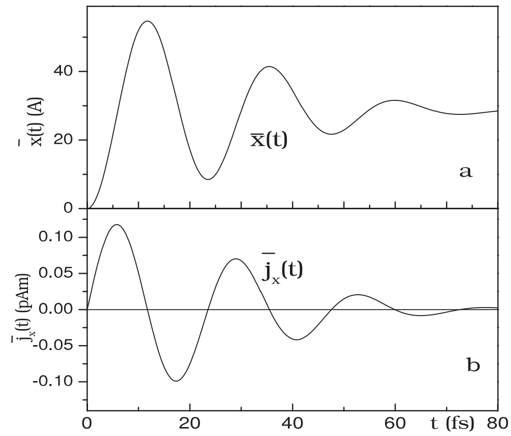

Figure 3. Zitterbewegung of a charge carrier in bilayer graphene versus time, calculated for a Gaussian wavepacket width $d = 300$ Å and $k_{0y} = 3.5 \times 10^8$ m^{-1}: (a) displacement, (b) electric current. The decay time is about $\Gamma_Z^{-1} = 40$ fs (after [11]).

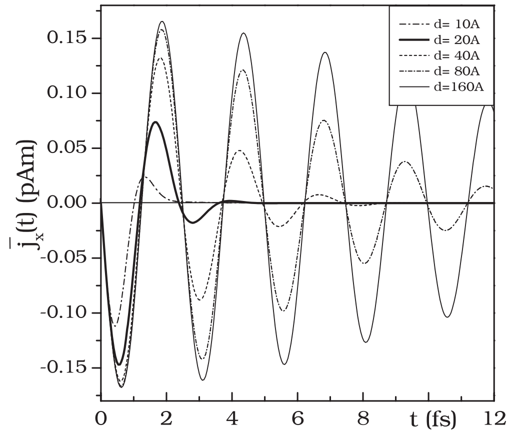

Figure 4. Oscillatory electric current in the x direction caused by ZB in monolayer graphene versus time, calculated for a Gaussian wavepacket with $k_{0y} = 1.2 \times 10^9$ m^{-1} and various packet widths d (after [11]).

nanotubes (CNT), see [8, 11, 20]. The two-dimensional Hamiltonian for bilayer graphene is well approximated by [21]

$$\hat{H}_B = -\frac{1}{2m^*}\begin{pmatrix} 0 & (\hat{p}_x - i\hat{p}_y)^2 \\ (\hat{p}_x + i\hat{p}_y)^2 & 0 \end{pmatrix}. \tag{6}$$

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

$$x_{11}(t) = x(0) + \frac{k_y}{k^2}\left[1 - \cos\left(\frac{\hbar k^2 t}{m^*}\right)\right], \tag{7}$$

where $k^2 = k_x^2 + k_y^2$. The third term represents Zitterbewegung with the frequency $\hbar\omega_Z = 2\hbar^2k^2/2m^*$, 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 $v = \hbar k_{0y}t/2m^*$, where $\hbar k_{0y}$ is the initial value of momentum. The relative velocity is $v^{\text{rel}} = \hbar k_{0y}t/m^*$. Each of these packets has an initial width d and it spreads (slowly) in time. After a time $\Gamma_Z^{-1} = d/v^{\text{rel}}$ 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 spacial 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]

$$\hat{H}_M = u\begin{pmatrix} 0 & \hat{p}_x - i\hat{p}_y \\ \hat{p}_x + i\hat{p}_y & 0 \end{pmatrix}, \tag{8}$$

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 $\hat{v}_j = \partial\hat{H}_M/\partial\hat{p}_j$, 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

$$v_x^{(11)} = u\frac{k_y}{k}\sin(2ukt). \tag{9}$$

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 $\hbar k_y$. The results for the current $\bar{j}_x = e\bar{v}_x$ 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 ω_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 $\hat{p}_x$ is quantized and takes discrete values $\hbar k_x = \hbar k_{n\nu}$, where $k_{n\nu} = (2\pi/L)(n - \nu/3)$, $n = 0, \pm1, \ldots$, $\nu = \pm1$, 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 $\nu = \pm1$ there *always* exists a non-vanishing value of the quantized momentum $\hbar k_{n\nu}$. Second, for

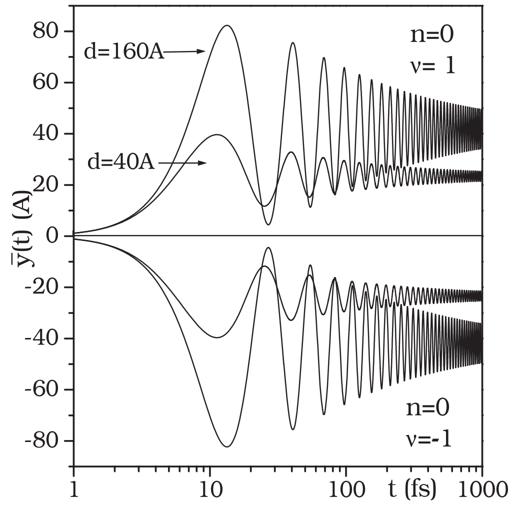

Figure 5. Zitterbewegung of charge carriers in the ground subband of a single carbon nanotube of $L = 200$ Å versus time (logarithmic scale), calculated for Gaussian wavepackets of two different widths d and $k_{0y} = 0$. After the ZB disappears a constant shift remains. The two carriers are described by different quantum numbers ν (after [11]).

each value of $k_{n\nu}$ there exists $k_{-n,-\nu} = -k_{n\nu}$ resulting in the same subband energy $\mathcal{E} = \pm E$, where $E = \hbar u\sqrt{k_{n\nu}^2 + k_y^2}$.

The time-dependent velocity $\hat{v}_y(t)$ 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_y the ZB frequency is $\hbar\omega_Z = E_g$, where $E_g = 2\hbar u k_{n\nu}$. The ZB amplitude is $\lambda_Z \approx 1/k_{n\nu}$. However, we are again interested in the displacement $\bar{y}(t)$ 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_x 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 $\boldsymbol{B} \parallel z$, 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 $E_{ns} = s\hbar\omega\sqrt{n}$, 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 $1/L = (eB/\hbar)^{1/2}$. 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 trembling motion. Its frequency ω_Z is about $\hbar\omega_Z \approx \Delta\mathcal{E}$, where $\Delta\mathcal{E}$ is the energy separation between the interacting 'positive' and 'negative' states. If the real energy gap $\mathcal{E}_g$ exists, there is $\Delta\mathcal{E} = \mathcal{E}_g$; if $\mathcal{E}_g = 0$ the energy separation $\Delta\mathcal{E}$ is caused by the non-vanishing value of momentum. The amplitude λ_Z goes as $\lambda_Z \propto 1/\Delta\mathcal{E}$. 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].

Acknowledgments

One of us (WZ) acknowledges many years of friendship and collaboration with Guenther Bauer. We are both pleased and honored to be able to contribute to the Festschrift celebrating the 65th birthday of Professor Bauer.

References

[1] Schroedinger E 1930 *Sitzungsber. Preuss. Akad. Wiss. Phys. Math. Kl.* **24** 418
Schroedinger's derivation is reproduced in Barut A O and Bracken A J 1981 *Phys. Rev.* D **23** 2454

[2] Strange P 1998 *Relativistic Quantum Mechanics* (Cambridge: Cambridge University Press)
[3] Ferrari L and Russo G 1990 *Phys. Rev.* B **42** 7454
[4] Zawadzki W 2005 *Phys. Rev.* B **72** 085217
[5] Schliemann J, Loss D and Westervelt R M 2005 *Phys. Rev. Lett.* **94** 206801
[6] Katsnelson M I 2006 *Eur. Phys. J.* B **51** 157
[7] Cserti J and David G 2006 *Phys. Rev.* B **74** 172305
[8] Zawadzki W 2006 *Phys. Rev.* B **74** 205439
[9] Winkler R, Zulicke U and Bolte J 2007 *Phys. Rev.* B **75** 205314
[10] Rusin T M and Zawadzki W 2007 *J. Phys.: Condens. Matter* **19** 136219
[11] Rusin T M and Zawadzki W 2007 *Phys. Rev.* B **76** 195439
[12] Rusin T M and Zawadzki W 2007 *Preprint* 0712.3590 [cond-mat]
[13] Zuelicke U, Bolte J and Winkler R 2007 *New J. Phys.* **9** 355
[14] Schliemann J 2008 *New J. Phys.* **10** 034024
[15] Zawadzki W and Lax B 1966 *Phys. Rev. Lett.* **16** 1001
[16] Pfeffer P and Zawadzki W 1990 *Phys. Rev.* B **41** 1561
[17] Parker G H and Mead C A 1968 *Phys. Rev. Lett.* **21** 605
[18] Lock J A 1979 *Am. J. Phys.* **47** 797
[19] Garraway B M and Suominen K A 1995 *Rep. Prog. Phys.* **58** 365
[20] Novoselov K S, Geim A K, Morozov S V, Jiang D, Zhang Y, Dubonos S V, Grigorieva I V and Firsov A A 2004 *Science* **306** 666
[21] McCann E and Fal'ko V I 2006 *Phys. Rev. Lett.* **96** 086805
[22] McClure J W 1956 *Phys. Rev.* **104** 666
[23] Ajiki H and Ando T 1993 *J. Phys. Soc. Japan* **62** 2470
[24] Thaller B 2004 *Preprint* quant-ph/0409079
[25] Zawadzki W 1997 *High Magnetic Fields in the Physics of Semiconductors II* ed G Landwehr and W Ossau (Singapore: World Scientific) p 755
[26] Vaishnav J Y and Clark C W 2008 *Phys. Rev. Lett.* **100** 153002
[27] Zhang X 2008 *Phys. Rev. Lett.* **100** 113903
[28] Bermudez A, Martin-Delgado M A and Luis A 2008 *Phys. Rev.* A **77** 033832
[29] LeRoy B J 2003 *J. Phys.: Condens. Matter* **15** R1835
[30] Topinka M A, LeRoy B J, Shaw S E J, Heller E J, Westervelt R M, Maranowski K D and Gossard A C 2000 *Science* **289** 2323
[31] Zhang X and Liu Z 2008 *Preprint* 0804.1978 [cond-mat]