Bloch oscillations in carbon nanotubes

2009 J. Phys.: Condens. Matter 21 212202

(http://iopscience.iop.org/0953-8984/21/21/212202)

IOP FTC

IOP Publishing | Journal of Physics: Condensed Matter

J. Phys.: Condens. Matter **21** (2009) 212202 (5pp) doi:10.1088/0953-8984/21/21/212202

FAST TRACK COMMUNICATION

Bloch oscillations in carbon nanotubes

Esther Jódar[1], Antonio Pérez-Garrido[1] and Fernando Rojas[2]

[1] Departamento Física Aplicada, Antiguo Hospital de Marina Campus Muralla del Mar, UPCT, Cartagena 30202 Murcia, Spain

[2] Centro de Nanociencias y Nanotecnologia-UNAM, Apartado Postal 356, Ensenada, Baja California 22800, Mexico

E-mail: ejodar@upct.es

Received 3 March 2009, in final form 8 April 2009

Published 30 April 2009

Online at stacks.iop.org/JPhysCM/21/212202

Abstract

Bloch oscillations arise when electrons are in a one-dimensional linear chain of atoms under a constant electric field. In this paper we show numerically that electrons in different types of carbon nanotubes show oscillations with a Bloch frequency proportional to the constant electric field applied along the nanotube axis. We show these oscillations, calculating the quadratic displacement as a function of the electric field. Because of the double periodicity of the nanotubes' geometry (the lattice constant and the lines of atoms) two frequencies appear, one twice the value of the other. These frequencies coincide perfectly with those predicted for a linear chain of atoms, taking into account the periodicity considered in each case.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Carbon nanotubes (CNTs) can behave as metallic or semiconducting depending on their chirality, as has been well known since they were discovered by Iijima in 1991 [1]. Thus, CNTs are a great test bed for experiments with a large impact on semiconductor physics (see [2, 3] for a general review). Much effort has been dedicated to investigate junctions made of different kinds of CNTs [4–9], mechanical properties and even structural or mechanical deformations [10, 11]. Recent experiments show that CNTs could be used as nanoelectronic devices [12–16] and show other important quantum properties, e.g. quantum dot behaviour [17, 11, 18–21].

Bloch oscillations of the electronic wavepacket take place when an electron is under the influence of an electric field in a periodic potential (a crystal) [22, 23]. These oscillations are due to the Bragg reflections at the edges of the Brillouin regions. Although they were predicted in 1934, those oscillations were not observed until 1992 [27], thanks to advances in the fabrication of semiconductors. In addition, these Bloch oscillations have been observed experimentally in other physical systems, such as mechanical systems [24] cold atoms in optical lattices [25] and light pulses in photonic crystals [26].

The period and the amplitude of Bloch oscillations can be obtained with [28]:

$$T_{\mathrm{B}} = \frac{h}{eFd}, \tag{1}$$

$$A_{\mathrm{B}} = \frac{\delta}{eF}, \tag{2}$$

where d is the period of the potential (lattice constant), δ is the width of the energy band where the electron moves, and F is the applied electric field. This is equivalent to a Bloch frequency $\omega_{\mathrm{B}} = 2\pi eFd/h$, a linear relation with the electric field F.

The behaviour of the extended and localized waves under the influence of an electric field is quite different. In the latter case, the wave propagates along the system and comes back to its initial position after a time given by equation (1), but the wave propagates in such way that its centre does not move from the initial position. In the former case, extended waves, the centre of the wavepacket oscillates, with a period given by equation (1).

In this paper we investigate the temporal evolution of electrons in carbon nanotubes of type armchair and zig-zag under constant electric fields. We show that these molecules present Bloch oscillations, when an electric field is applied along the nanotube axis. We study the dynamics of these oscillations as a function of the electric field.

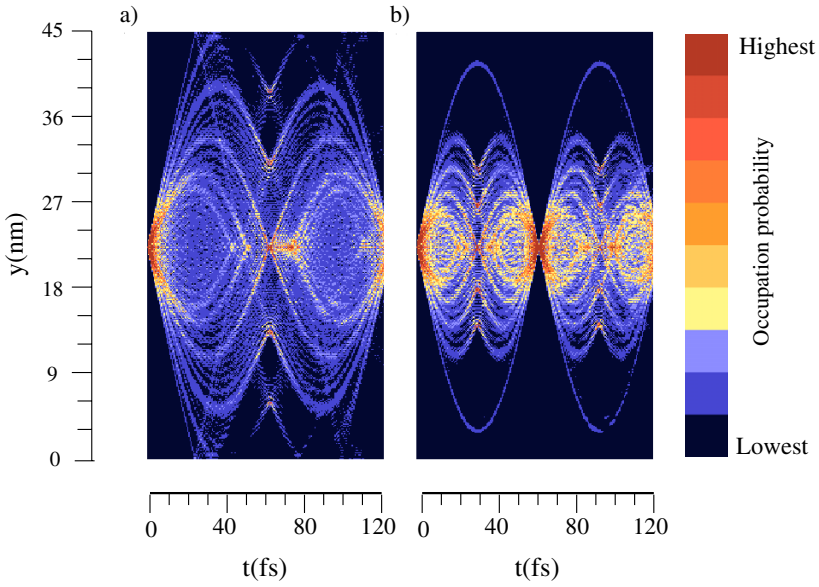

Figure 1. Occupation probability versus time (horizontal axis) for an armchair nanotube (6, 6) with 180 unit cells: (a) the results for 271 MV m^{-1}; (b) the results for 542 MV m^{-1}. The value of occupation probability increases from dark to light (from dark blue to red in the online version).

2. Model

We firstly obtain the stationary properties for a nanotube using a time independent tight-binding model. Then, we apply a constant electric field F simply by adding the electric energy in the diagonal elements of the Hamiltonian matrix. To construct the Hamiltonian, we are using a π-electron approximation; even though this is quite a simplistic model, it reproduces quite well the general features of the electronic transport [18]. Our Hamiltonian for localized Wannier functions is given by:

$$H = H_0 + H_t + H_F. \tag{3}$$

In this equation the first term H_0, the on-site energy is given by:

$$H_0 = \sum_i E_{0i} a_i^\dagger a_i, \tag{4}$$

where we set $E_{0i} = 0$. $a_i^\dagger$ and a_i terms represent creation and annihilation operators. The second term in equation (3) is the hopping term:

$$H_t = -t \sum_{\langle i,j \rangle} a_i^\dagger a_j + \text{c.c.}, \tag{5}$$

where c.c. is the complex conjugate. i and j are restricted to bonded atoms, and t is the overlap energy which is equal to 2.66 eV. Finally, H_F in equation (3) is obtained as:

$$H_F = \sum_i E_i a_i^\dagger a_i, \tag{6}$$

the applied electric field is taken into account through the calculation of the electric energy E_i:

$$E_i = neFy, \tag{7}$$

F being the applied electric field and y the coordinate of atom i, we place the nanotube axis parallel to the y axis. Temporal evolution of the electronic wavefunction is given as a linear combination of the stationary states of the system with the electric field. We denote these stationary eigenenergy terms and wavefunctions as U_j and $|\Phi_j\rangle$, respectively. Then, $|\Psi(t)\rangle$ can be written as:

$$|\Psi(t)\rangle = \sum_j C_j e^{-iU_j t/\hbar} |\Phi_j\rangle, \tag{8}$$

where the coefficients C_j are the occupation amplitude of the system in the state j. They can be calculated through the projection of the initial state over each state j of the Hamiltonian:

$$C_j = \langle \Phi_j | \Psi(t=0) \rangle. \tag{9}$$

Here we consider two kinds of initial conditions: localized or extended states. For the localized case, the electron is placed in a middle site of the nanotube and for the extended case, we use a nanotube eigenfunction in the absence of electric field $F = 0$.

The averaged quadratic displacement gives us a measure of the dispersion of the wavefunction in space which is obtained in the direction of propagation of the wavefunctions along the axis of the nanotube (y axis, as stated before):

$$\langle y^2(t) \rangle = \sum_i |\Psi(t)|^2 |y|^2. \tag{10}$$

3. Results and discussion

We study the dynamics of wavefunctions in the presence of a one-dimensional constant electric field using equation (8).

For our calculations we use different kinds of nanotubes for different chiralities and different conductive behaviours,

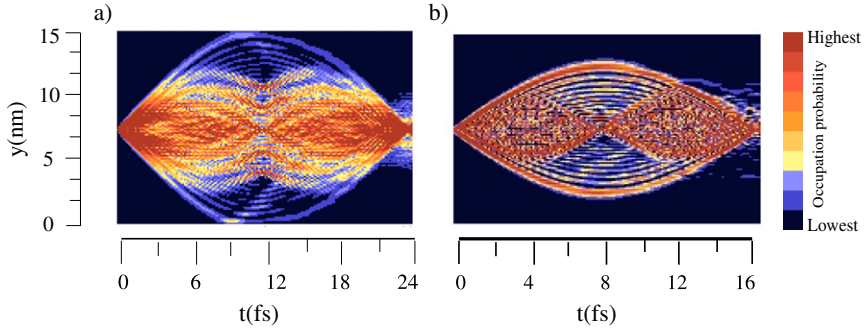

Figure 2. (a) Occupation probability versus time for a (6, 6) armchair nanotube with 60 unit cells. The applied electric field is $F = 1355$ MV m^{-1}. (b) Occupation probability versus time for a linear chain of atoms where the unit cell has two different atoms. The applied electric field in this case is $F = 2033$ MV m^{-1}. In both figures we can see that there are two frequencies for the oscillation, one twice the value of the other.

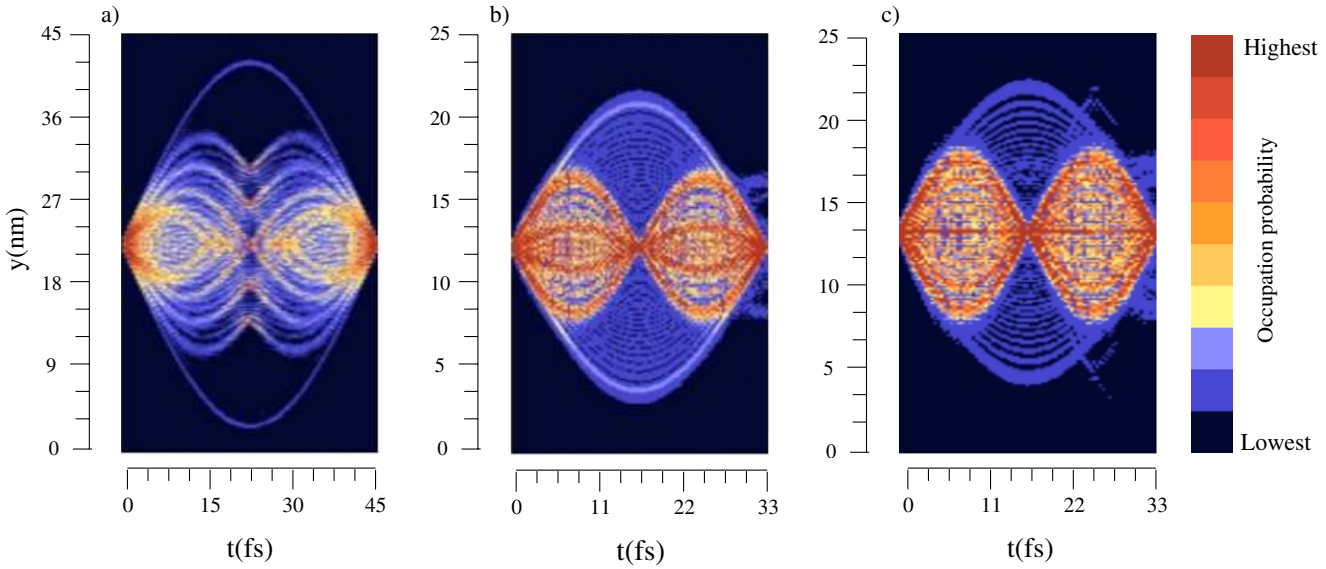

Figure 3. Occupation probability versus time for: (a) a (6, 6) metallic armchair nanotube for $F = 542$ MV m^{-1}, (b) a (9, 0) metallic zig-zag nanotube for $F = 1174$ MV m^{-1}, and (c) a (8, 0) semiconductor zig-zag nanotube for $F = 1174$ MV m^{-1}. The time intervals have been adjusted differently for (a)–(c) in order to show a full oscillation period.

characterized by the numbers (n, m): (6, 6) armchair metallic nanotube, (8, 0) semiconductor and (9, 0) metallic zig-zag nanotubes. The behaviour of extended and localized waves is significantly different. We describe the dynamics of the oscillations for initially localized waves, using Wannier states and also for initially extended electronic eigenfunctions. By initially, we mean the electronic state before applying the electric field.

For the (6, 6) armchair nanotube we obtain the occupation probability as a function of time, which we plot in figure 1. Figure 1(a) shows the results for the electric field $F = 271$ MV m^{-1}, where a is the lattice constant of bidimensional graphite $a = 2.46$ Å. Figure 1(b) shows the results for $F = 542$ MV m^{-1}. Different colours are used for different values of the occupation probability. More specifically, from dark to light (from dark blue colour to red colour in the online version) the value of occupation probability increases, as shown in figure 1. For the sake of clarity, contrast is automatically adjusted for each figure.

We obtain the period of oscillations, as well as their amplitude and check these results with equations (1) and (2) for a linear chain of atoms, with lattice constant $d = a$. As can be seen in figure 2(a), we have a mix of oscillations with two different frequencies ω_B and $\omega_B/2$, first one half then the other, which is related to the fact that armchair nanotubes have two lines of atoms in the unit cell. This is analogous to the behaviour of a linear chain of atoms with two different kinds of atoms, A and B, alternatively positioned with lattice constants $d = a$ and $d = a/2$. In this case we have a double periodicity too. A numerical simulation of this system can be seen in figure 2(b), whose behaviour is very similar to figure 2(a).

A similar behaviour to that of the metallic nanotube (6, 6) is obtained for other kinds of nanotubes with different conductive regimes and chirality, as can be seen in figure 3. In this figure we show the occupation probability versus time for metallic nanotubes (6, 6) (figure 3(a)) and (9, 0) (figure 3(b)), together with semiconductor nanotubes (8, 0) (figure 3(c)). The time intervals are different for each nanotube, as we

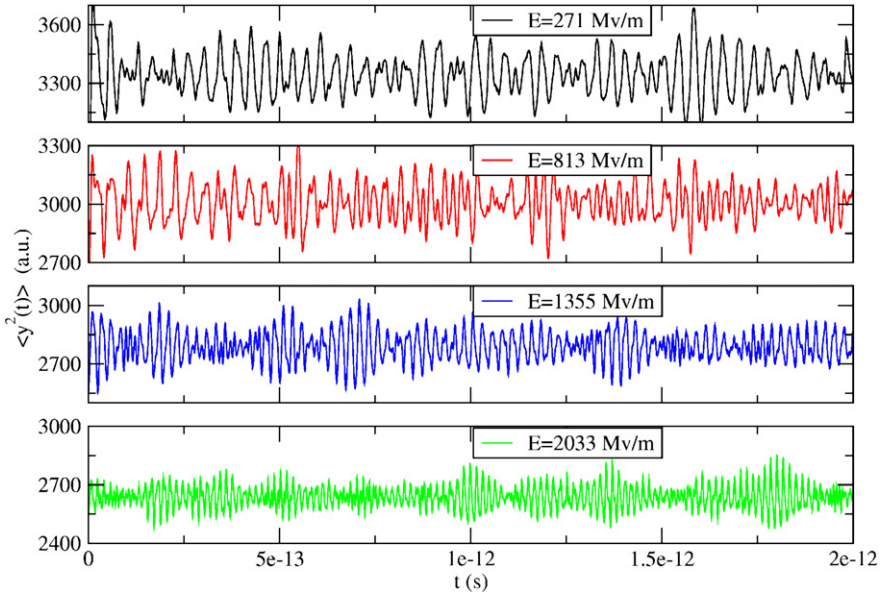

Figure 4. Averaged quadratic displacement as a function of time for a wavefunction in a nanotube (6, 6) of length $L = 60a$. We show the results obtained for different values of electric field F.

have modified the horizontal scale in these figures in order to see clearly the periodicity of each oscillation. The zig-zag nanotubes also present two oscillations, $\alpha\omega_B$, one of which is half the other, with $\alpha = \sqrt{3}/2 = 0.87$, which is explained below.

The averaged quadratic displacement is obtained through equation (10). As Bloch theory predicts, this function must show oscillations as well as the occupation probability does. In figure 4 we show the averaged quadratic displacement as a function of time for a nanotube (6, 6) of length $L = 60a$ for different values of the electric field. It is clear that the frequency is an increasing function of electric field and the amplitude decreases with electric field, these results are in agreement with equations (1) and (2), for the one-dimensional case.

Fourier transformation of the averaged quadratic displacement allows us to obtain the frequency of these oscillations. In figure 5 we show the largest frequency of the oscillation ω_B as a function of the electric field, for different lengths of the (6, 6) nanotube. The frequency does not depend on the length of the nanotube, as expected from theoretical expressions. This is clearly seen in the figure. One can check that the results are very similar for zig-zag nanotubes, in the sense that they present a linear relation of the Bloch frequency with the electric field. Nevertheless, the slopes for zig-zag nanotubes are slightly different. In the case of the nanotube (6, 6) a linear regression of the experimental data gives us a periodicity for $d = a$. In the case of zig-zag nanotubes the slope gives us a periodicity for $d = \alpha a$, being $\alpha = \cos(\phi - 30) = 0.87$, where ϕ is the chiral angle of any zig-zag nanotube. The theoretical line drawn in figure 5 has been obtained with equation (1) for the one-dimensional case.

As we have discussed earlier in this paper, in the case of extended waves the dynamics of Bloch oscillations shows different behaviour to that of localized states. The centre of

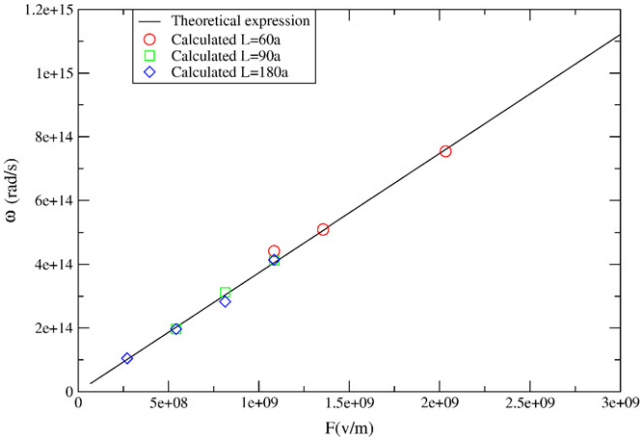

Figure 5. Frequency of the oscillation of averaged quadratic displacement as a function of the electric field. The continuous line corresponds to the theoretical expression (1). The points marked correspond to the results obtained with the numerical calculations. The figure shows the results for a nanotube (6, 6) of different lengths.

the wavepacket moves periodically for extended waves, which is not the case for the localized states. We also show the wavefunctions for the (6, 6) nanotube in figure 6, where the results have been obtained for a nanotube with 90 unit cells and different values of the electric field. In figure 6(a) there is no electric field $F = 0$, and in figure 6(b) an electric field $F = 90$ MV m^{-1} is applied, no Bloch oscillation has been formed due to border reflection. In figure 6(c) for an electric field $F = 406$ MV m^{-1}, a Bloch oscillation phenomenon takes place.

We also obtain the frequency of the oscillations for extended waves through the calculation of the Fourier transform of averaged quadratic displacement. Our numerical

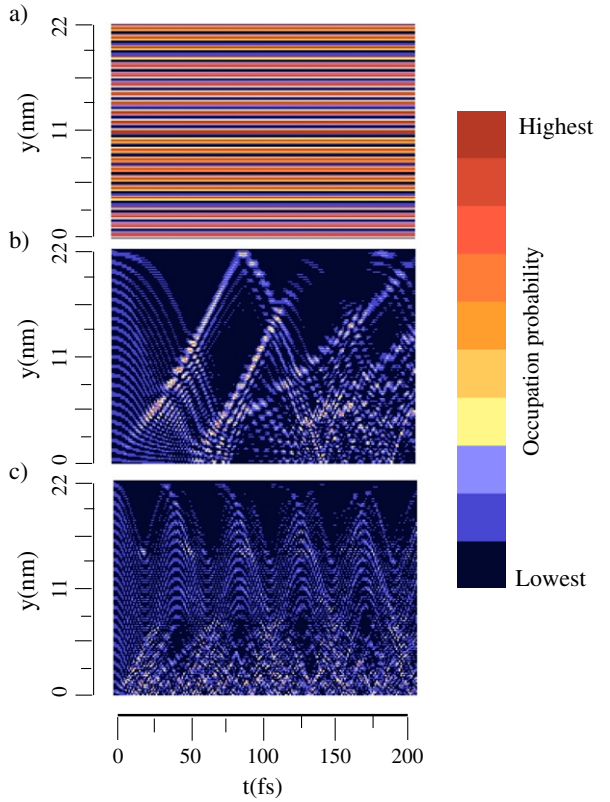

Figure 6. Occupation probability for a wavefunction versus time for a (6, 6) nanotube of length $L = 90a$ for extended states as initial condition: (a) the results for an electric field $F = 0$; (b) for $F = 90$ MV m^{-1}, where the wave is reflected at the borders of the system and Bloch oscillations cannot be formed; (c) for $F = 406$ MV m^{-1}, where Bloch oscillations are revealed.

results for nanotubes agree with theoretical predictions for a linear chain of atoms (equation (1)).

4. Conclusions

In summary, in this paper we have studied the behaviour of different kinds of carbon nanotubes under the influence of a constant electric field. We have shown that the dynamics of the electrons in this kind of structure show Bloch oscillations; the armchair shows the Bloch frequency $\omega_B = eFa/h$, with a the lattice constant of the bidimensional graphite. The frequency of these oscillations has been identified through the calculation of the Fourier transform and it fits quite well with the theoretical equations obtained for an electron in a linear chain of atoms. Both armchair and zig-zag present two oscillations with two frequencies one half the value of the other.

Acknowledgment

We are grateful for the financial support from Project PAPPIT IN110908, UNAM, México.

References

[1] Iijima S 1991 *Nature* **354** 56
[2] Saito R, Dresselhaus G and Dresselhaus M S 1998 *Physical Properties of Carbon Nanotubes* (London: Imperial College Press)
[3] Dresselhaus M S, Dresselhaus G and Avouris Ph (ed) 2001 *Carbon Nanotubes* (Berlin: Springer)
[4] Tamura R and Tsukada M 1994 *Phys. Rev.* B **49** 7697
[5] Chico L, Crespi V H, Benedict L X, Louie S G and Cohen M L 1996 *Phys. Rev. Lett.* **76** 971
[6] Kostyrko T, Bartkowiak M and Mahan G D 1999 *Phys. Rev.* B **59** 3241
[7] Treboux G, Lapstun P and Silverbrook K 1999 *J. Phys. Chem.* B **103** 1871
[8] Pérez-Garrido A and Urbina A 2002 *Carbon* **40** 1227
[9] Del Valle M, Tejedor C and Cuniberti G 2005 *Phys. Rev.* B **71** 125306
[10] Sammalkorpi M, Krasheninnikov A, Kuronen A, Nordlund K and Kaski K 2004 *Phys. Rev.* B **70** 245416
[11] Sim H S, Park C J and Chang K J 2001 *Phys. Rev.* B **63** 073402
[12] Collins P G, Zettl A, Bando H, Thess A and Smalley R E 1997 *Nature* **278** 100
[13] Saito R, Dresselhaus G and Dresselhaus M S 1996 *Phys. Rev.* B **53** 2044
[14] Bockrath M, Obden D H, McEuen P L, Chopra N G, Zettl A, Thess A and Smalley R E 1997 *Science* **275** 1922
[15] Tans S J, Verschueren A R M and Dekker C 1998 *Nature* **393** 49
[16] Yao Z, Postma H W Ch, Balents L and Dekker C 1999 *Nature* **402** 273
[17] Chico L, López Sancho M P and Muñoz M C 1998 *Phys. Rev. Lett.* **81** 1278
[18] Orlikowski D, Mehrez H, Taylor J, Guo H, Wang J and Roland C 2001 *Phys. Rev.* B **63** 155412
[19] Chico L and Jaskolski W 2004 *Phys. Rev.* B **69** 085406
[20] Jódar E, Pérez-Garrido A and Díaz-Sánchez A 2006 *Phys. Rev.* B **73** 205403
[21] Jódar E and Pérez-Garrido A 2007 *Phys. Status Solidi* **204** 1892
[22] Bloch F 1928 *Z. Phys.* **52** 555
[23] Zener C 1934 *Proc. R. Soc.* A **145** 1523
[24] Gutierrez L, Diaza-de Anda A, Flores J, Mendez-Sanchez R A, Mosivais G and Morales A 2006 *Phys. Rev. Lett.* **97** 114301
[25] Ben Dahan M, Peik E, Reichj J, Castin Y and Salomn C 1996 *Phys. Rev. Lett.* **76** 4508
[26] Pertsch T, Dannberg P, Elflein W, Brauer A and Ledeger F 1999 *Phys. Rev. Lett.* **83** 4752
[27] Feldmann J, Leo K, Shah J, Miller D A B, Cunningham J E, Meier T, von Plessen G, Schulze A, Thomas P and Schmitt-Rink S 1992 *Phys. Rev.* B **46** 7252
[28] Ashcroft N W and Mermin N D 1976 *Solid State Physics* (New York: Saunders)