Physics Letters A 374 (2010) 4057–4060

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Electrical current in nanoelectronic devices

Andrea Sacchetti

Faculty of Sciences, University of Modena e Reggio Emilia, Via Campi 213/B, I-41100 Modena, Italy

ARTICLE INFO

Article history:
Received 14 July 2010
Accepted 1 August 2010
Available online 4 August 2010
Communicated by V.M. Agranovich

Keywords:
Electrical density current
Acceleration theorem

ABSTRACT

In ultra-small electronic devices of the next generations the semiclassical model of electron motion in a periodical lattice between collisions turns out to be inadequate because the electron spread has magnitude order of the size of the ultra-small electronic device. In this Letter we consider the basic conceptual framework regarding how the length scale of the electrical device influences the transport behavior of the electrons between collisions and the electrical current. By taking into account the interference effects we obtain a very basic model for electrons transport, where the density current peak is given as function on the ratio between the thermal de Broglie wavelength and the lattice period. This result could be also useful in order to understand the basic effect of the insulator/metal transition.

Let us consider one of the most popular electric devices: the field effect transistor, which is basically a resistor consisting of a region called the channel with two conductive contacts at its two ends called the source and the drain. The electrical current generated in the channel depends on the voltage applied to a third terminal called the gate. At present, most of the researches are addressed to the understanding of the contribution to the device performance from effects like interaction between electrons, impurities, granularity of the dopant, and so on [1]. In fact, power consumption and heat problems are two of the most actual relevant problems for nanoscale electronic devices.

Consider that we are now in the so-called 45 nm transistor generation, then a typical transistor has a channel length of order of 50 nm, which amounts to a few hundred of atoms. At this scale length the transport behavior along the direction of the channel is still of ballistic kind and typical quantum effects like interference are not considered [2]. Within the next five years, or so, it is expected that device lengths will reduce to 16 nm or less [3]. Hence, the spread of electrons is going to be comparable with this channel length; for instance, at room temperature the thermal de Broglie wavelength λ for electrons in Silicon is of order of 5 nm. Therefore, we expect that in the next generations of ultra-small transistors quantum mechanics issues like *quantum localization*, that is how small can be the minimum area in which a single electron can be localized, will play a crucial role since the effective size of the electron would be of the order of the lattice period; if not, the electron wave-function will spread over the whole channel and the drain and source contacts giving raise to questions of coexistence of classical apparatus (the two contacts) and quantum environment (the channel) [4].

Up to now, an approach to the understanding of the transport problem from large macroscopic conductors to small atomic scale conductors has been adopted. Typically, in this approach the models are based on the semiclassical acceleration theorem (3) and on the associated Boltzmann transport equation for macroscopic semiconductors [5,6], then quantum confinement effects arising at small atomic scale have been treated by means of some effective potentials [4,7].

On the other hand, bottom–up approaches including quantum effects have been recently found to be more suitable for the understanding of the electrons transport in ultra-small devices [2]. Following this kind of approach here we include in our model, from the very first steps, also the quantum interference effect.

To this end we introduce a very basic model by neglecting the motion along the plane perpendicular to the channel direction, we thus only consider the motion of an electron with charge e in a one-dimensional periodical lattice under the effect of an homogeneous external field E. When the external field is small enough, then it is a well-know fact [8–10] that an electron initially prepared in the first bands remains confined in a finite region for a long time much larger than the Bloch period T_B given below, and finally it escapes because of the tunneling effect. Such a confined motion is a periodical-like motion, usually named Bloch Oscillators, with period

$$T_B = \frac{2\pi\hbar}{|F|d} \tag{1}$$

where $F = -Ee$ is the strength of the external homogeneous force and where d is the period of the one-dimensional periodical lattice.

Indeed, for macroscopic devices and in the bullet-like regime it is expected that when the quantum particle is initially prepared on one energy band of the periodical lattice, then the semiclassi-

E-mail address: Andrea.Sacchetti@unimore.it.

0375-9601/$ – see front matter
doi:10.1016/j.physleta.2010.08.001

cal picture associates the band dispersion relation $\mathcal{E}(k)$ with the electron velocity in the position space

$$v(k) = \frac{1}{\hbar}\frac{d\mathcal{E}(k)}{dk}, \tag{2}$$

where k denotes the quasimomentum variable belonging to the Brillouin zone (or reciprocal lattice) $\mathcal{B} = (-\frac{\pi}{d}, +\frac{\pi}{d}]$. On the other hand, because of the spatially uniform applied force F, the electron moves in the quasimomentum space according to the "Newton's law in the k space" [11–16] (also called "semiclassical acceleration theorem")

$$\hbar\frac{dk}{dt} = F. \tag{3}$$

Then the dynamics of the electron in the quasimomentum space is given by

$$k(t) = \frac{1}{\hbar}Ft + k_0, \tag{4}$$

k_0 is the value of the quasimomentum at the initial instant $t = 0$. From this law and from the Bragg's reflection process in the Brillouin zone, the electron motion is periodic with period given by Eq. (1).

When scattering processes interrupt this oscillatory behavior, then the electron changes its quasimomentum k restoring the thermal equilibrium, and the scattered electron will be found close to the minimum energy at $k_0 = 0$. If the average scattering time is much smaller than $T_B/2$ then the electron will remain in the range where its velocity $v(k)$ takes positive values, and thus an increase of F will generate a larger density current; in contrast, for scattering time larger than $T_B/2$, the electron current density can be expected to drop with the field [17,18].

We may remark that the rather simple argument given above has two serious limits as pointed out by, respectively, [19,20]:

1) It treats the electron wave-function as a pure Bloch state, for which the acceleration theorem holds true in the semiclassical form (3); that is, it reduces the initial distribution of electron momentum to a Dirac δ-function in wavevector space neglecting the thermal broadening of this distribution at finite temperatures.
2) This semiclassical picture describes the dynamics of the wave-packet when the channel length is much more greater than the spread of the wave-packet of the electron, which in turn is much larger than the lattice constant.

Therefore, in nanoscale devices, where lengths are typically in a range about ten nanometers or less, the wave nature of electrons cannot be anymore neglected and the electron wave-functions should spread over only few lattice periodical sites or less, then *the electron wave-packet cannot be treated as a pure Bloch state and it has a given not zero standard deviation in the k-space*. In such a case, the group velocity formula (2) and the semiclassical acceleration theorem (3) hold true in the mean value sense. More precisely Eq. (3) should replaced by (see, e.g., [21])

$$\hbar\frac{d\langle k\rangle^t}{dt} = F, \tag{5}$$

where $\langle k\rangle^t$ denotes the centroid of the wave-packet in the quasimomentum representation at time t, and (2) should be replaced by (see, e.g., [22])

$$\langle v\rangle^t = \frac{1}{\hbar}\left[\frac{d\mathcal{E}(k + Ft/\hbar)}{dk}\right], \tag{6}$$

where $\langle v\rangle^t$ denotes the group velocity of the wave-packet in the position representation at time t. Here, $[g] = \int_{\mathcal{B}} g(k)|a(k)|^2\,dk$ denotes the expectation value of an observable $g(k)$ on the initial wave-packet $a(k)$ in the k-space.

By means of (6) we compute the particle current density. To this end we assume that the electron is prepared in the first band and, as in [4], that the initial wave-packet $a(k - k_0; \lambda)$ has a Gaussian-like shape with center k_0, where $a(k, \lambda)$ is the following Gaussian-like function periodically arranged on the Brillouin zone:

$$a(k, \lambda) = ce^{-\lambda^2 k^2/4\pi}, \quad k \in \mathcal{B}, \tag{7}$$

where c is the normalization numerical pre-factor given by

$$c = \left[\sqrt{2\pi}\,\mathrm{erf}(\sqrt{\pi}\lambda/\sqrt{2}d)\right]^{-1/2},$$

and where λ is the thermal de Broglie wavelength given by

$$\lambda = \sqrt{\frac{2\pi\hbar^2}{m^\star k_B T}}$$

where $m^\star$ is the electron effective mass and T is the temperature. The effective size of the electron particle is of order λ.

If, as usual, we assume that the dispersion relation of the first band is simply given by

$$\mathcal{E}(k) = \frac{1}{2}\delta\big[1 - \cos(kd)\big],$$

where δ is the amplitude of the band, then, from (6), it follows that the mean velocity of an electron with initial wave-packet $a(k - k_0; \lambda)$ is given by

$$\begin{aligned}\langle v\rangle^t(k_0; \lambda) &= \frac{1}{\hbar}\int_{\mathcal{B}} \frac{d\mathcal{E}(k + Ft/\hbar)}{dk}\big|a(k - k_0; \lambda)\big|^2\,dk \\ &= \frac{1}{\hbar}\int_{\mathcal{B}} \frac{d\mathcal{E}(k + k_0 + Ft/\hbar)}{dk}\big|a(k; \lambda)\big|^2\,dk \\ &= v_{\max}(\lambda)\sin\big[dk(t)\big]\end{aligned} \tag{8}$$

where $k(t)$ is the law given in Eq. (4), and

$$v_{\max}(\lambda) = \frac{d\delta}{2\hbar}m(\lambda) \tag{9}$$

where a straightforward calculation gives that

$$m(\lambda) = \frac{\Re[\mathrm{erf}((\lambda^2/d^2 + i)d/2\lambda\sqrt{2\pi})]}{e^{\pi d^2/2\lambda^2}\,\mathrm{erf}(\sqrt{\pi}\lambda/\sqrt{2}d)}$$

is a real-valued function which takes values within the interval $[0, 1]$, depending on the ratio between the thermal de Broglie wavelength and the lattice period.

We may remark that the spatial amplitude of this oscillation is given by

$$x_{\max}(\lambda) = \frac{\hbar}{F}v_{\max}(\lambda) = \frac{d\delta}{2F}m(\lambda)$$

and that in the limit of large thermal de Broglie wavelength we obtain again

$$\lim_{\lambda\to+\infty} v_{\max}(\lambda) = \frac{d\delta}{2\hbar} \tag{10}$$

in agreement with Eq. (33) by [18].

In the limit of an electron scattering frequency negligibly small with respect to the Bloch frequency, then any electron would eventually become randomly distributed throughout the Brillouin zone

with given distribution function $f(k_0)$, where k_0 denotes the centroid of the electron wave-packet in the k-space. Such a distribution function is normalized as follows

$$\int_{\mathcal{B}} f(k_0)\,dk_0 = \frac{Nd}{2\pi}$$

where N is the total number of electrons per unit length. Even if this distribution function can always be expanded into a Fourier series [23], here we restrict ourselves to a basic simplified model where

$$f(k_0) = \frac{Nd}{2\pi}\big[1+\cos(dk_0)\big] \tag{11}$$

is an even function with minimum value in correspondence of the bottom of the dispersion relation $\mathcal{E}(k)$ at $k=0$. Here, we adopt this continuous distribution, rather than using the thermal-equilibrium limit (which essentially corresponds to $f(k_0)=\delta(k_0)$ where $\delta(k_0)$ is the Dirac's delta at $k_0=0$); however, our qualitative conclusions will be independent of this choice.

Given a distribution function $f(k_0)$ of the form (11), and drawing on the velocity relation, we obtain the *particle current density* at time t:

$$j^t(\lambda) = \int_{\mathcal{B}} \langle v\rangle^t(k_0;\lambda)\,f(k_0)\,dk_0. \tag{12}$$

If we insert (8) in (12) we finally get the explicit expression for the particle current density

$$\begin{aligned} j^t(\lambda) &= v_{\max}(\lambda)\int_{\mathcal{B}} \sin\big[d(k_0+Ft/\hbar)\big]f(k_0)\,dk_0 \\ &= j_{\max}(\lambda)\sin(dtF/\hbar) \end{aligned} \tag{13}$$

where the maximum value of the particle current density is given by

$$j_{\max}(\lambda) = \frac{1}{2}N v_{\max}(\lambda). \tag{14}$$

From relation (9) then we obtain that the maximum value of the particle current density will depend on the thermal de Broglie wavelength λ as follows

$$j_{\max}(\lambda) = Jm(\lambda) \tag{15}$$

where

$$J = \frac{Nd\delta}{4\hbar}$$

is the well-known particle current density for macroscopic devices, for which λ is much larger than the period d of the periodical lattice and where $m(\lambda)\approx 1$. We may remark that the peak current J divided by the lattice period linearly depends on the band width in agreement with experiment and numerical results (see, e.g., [24, Fig. 3-Top]).

In Eq. (15), the peak current J is modulated by means of the term $m(\lambda)$ which monotically increases with respect to the ratio between the thermal de Broglie wavelength and the lattice period. In Fig. 1 we plot the graph of the maximum value of the particle current density (15) as function of the thermal de Broglie wavelength λ, where d is the period lattice. Hence, for λ of the order of the lattice period d then we expect to observe a strong damping effect on the peak current. In particular, the maximum value of the particle current density decreases when the wave-packet is sharply localized in the position space, and this value goes to zero when the wave-packet initially coincides with a Wannier function, which corresponds to a constant wave-function in the k-space (that is, for $\lambda\to 0$). On the other side, the peak current is not damped when the thermal de Broglie wavelength is of the order of about ten times the lattice period.

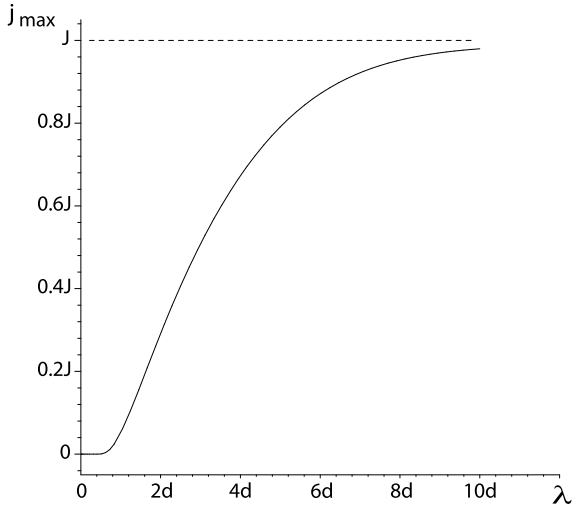

Fig. 1. Maximum value of the particle current density versus the thermal de Broglie wavelength λ, where d is the period lattice. $J = Nd\delta/4\hbar$, where N denotes the total number of electrons for unit length and δ denotes the energy width of the band.

Table 1
Numerical constants for some semiconductors at $T=300$ K [25]; λ represents the thermal de Broglie wavelength and the value $m(\lambda)$ represents the modulation factor of the particle current density peak.

	$m^\star$	λ (nm)	d (nm)	λ/d	$m(\lambda)$
Si	$0.98m_0$	4.35	0.5431	8.00	0.9524
GaAs	$0.07m_0$	16.26	0.5653	28.77	0.9981
InP	$0.073m_0$	15.92	0.5868	27.14	0.9979
GaSb	$0.049m_0$	19.44	0.6094	31.89	0.9985
InAs	$0.023m_0$	26.18	0.6059	43.22	0.9992
InSb	$0.013m_0$	37.73	0.6479	57.16	0.9995

Table 2
Metal/insulator transition for Nb-doped $SrTi_xNb_{1-x}O_3$ with concentration below and beyond the critical concentration value $x=0.25$.

	$m^\star$	λ (nm)	d (nm)	λ/d	$m(\lambda)$
$x<0.25$	$8m_0$	1.52	0.3905	3.90	0.6577
$x>0.25$	$0.2m_0$	9.62	0.3905	24.64	0.9974

In Table 1 we consider different semiconductors, where we compute the thermal de Broglie wave-functions at $T=300$ K and we see that for these materials the modulation factor is close to 1; only for Silicon we expect to see a small damping effect on the current peak since the modulation factor is about 0.95.

We close our Letter remarking that Eq. (15) could also explain some basic effects of the metal/insulator transition. Indeed, it is a well-known fact that the *qualitative* difference between crystalline insulators and metals depends on the position of the Fermi level: insulator behavior corresponds to filled band, while partially filled band corresponds to metallic behavior [26]. However, how pointed out in [27], the detailed understanding of this most basic electronic transition, i.e. the transformation of metal to insulator, is still far from complete; in this sense our research could be useful in order to *quantitative* understand the difference between crystalline insulators and metals. For instance, let us consider the metal-to-insulator transition of Nb-doped $SrTi_{1-x}Nb_xO_3$ bulk, where for Nb concentration beyond the critical transition value $x=0.25$ the effective mass drops from $m^\star/m_0>8$ to $m^\star/m_0>0.2$ [28]. Indeed, in Table 2 we compare the modulation factor for Nb-doped insulator $SrTiO_3$. For small concentration we observe a very severe damping factor; in contrast, for concentration larger than the critical con-

centration value $x = 0.25$ the modulation factor is practically 1 and we don't see damping effect in agreement with numerical analysis [28].

References

[1] D.K. Ferry, et al., Int. J. High Speed Electr. Syst. 17 (2007) 445.
[2] S. Datta, Nanoelectronic devices: A unified view, in: A.V. Narlikar, Y.Y. Fu (Eds.), Oxford Handbook in Nanosciences and Nanotechnology: Basic Aspets, vol. I, 2010.
[3] H. Iwai, MicroElectr. Eng. 86 (2009) 1520.
[4] D.K. Ferry, Superlatt. Microstruc. 27 (2000) 61.
[5] J.J. Duderstadt, W.R. Martin, Transport Theory, Wiley, 1979.
[6] A. Jüngel, Transport Equations for Semiconductors, Springer, 2009.
[7] S.M. Ramey, D.K. Ferry, Semicond. Sci. Technol. 19 (2004) S238.
[8] E.O. Kane, J. Phys. Chem. Solids 12 (1959) 181.
[9] V. Grecchi, A. Sacchetti, Phys. Rev. Lett. 78 (1997) 4474.
[10] M. Glück, A.R. Kolosky, H.J. Korsch, Phys. Rep. 366 (2002) 103.
[11] H.V. Houston, Phys. Rev. 57 (1940) 184.
[12] K. Kroemer, Proc. IEEE 63 (1975) 988.
[13] K. Kroemer, Am. J. Phys. 54 (1986) 177.
[14] A. Manohar, Phys. Rev. B 34 (1986) 1287.
[15] C. Kittel, Quantum Theory of Solids, 2nd ed., Wiley, 1987.
[16] K. Schönhammer, Phys. Rev. B 63 (2001) 245102.
[17] L. Esaki, R. Tsu, IBM J. Res. Develop. 14 (1970) 61.
[18] A. Wacker, Phys. Rep. 357 (2002) 1.
[19] A. Sibille, Miniband transport, in: E.T. Grahn, et al. (Eds.), Semiconductor Superlattices. Growth and Electronic Properties, World Scientific, 1995.
[20] N.W. Ashcroft, N.D. Mermin, Solid State Physics, Saunders College Publ., 1976.
[21] J. Callaway, Quantum Theory of the Solid State, Academic, 1974.
[22] V. Grecchi, A. Sacchetti, Phys. Rev. B 63 (2001) 212303.
[23] H. Kroemer, Large-amplitude oscillation dynamics and domain suppression in a superlattice Block oscillator, arXiv:cond-mat/0009311, 2000.
[24] A. Sibille, J.F. Palmier, H. Wang, F. Mollot, Phys. Rev. Lett. 64 (1990) 52.
[25] A. Sasaki, Phys. Rev. B 30 (1984) 7016.
[26] R. Resta, J. Phys.: Condens. Matter 14 (2002) R625.
[27] P.P. Edwards, et al., Philos. Trans. R. Soc. London A 356 (1998) 5.
[28] W. Wunderlich, H. Ohta, K. Koumoto, Physica B: Condens. Matter 404 (2009) 2202.