Вісник ХНУ, серія «Фізика», вип. 23, 2015. с. 16-21

PACS: 73.63.Fg Nanotubes;
73.21.Cd Superlattices;
УДК: 538.11

The magnetic response of a degenerate electron gas in nanotubes with superlattice

G.I. Rashba

Kharkiv National University named after V.N. Karazin
Sq. Svobody 4, Kharkiv, 61022, Ukraine
E-mail: georgiy.i.rashba@gmail.com

Within the framework of a simple model of the energy spectrum of electrons on the nanotube surface with a superlattice in a magnetic field, an analytical expression for the magnetic moment of a degenerate electron gas is obtained. It is shown that in the case of a large number of filled energy levels of the transverse motion of electrons there exist monotonous and oscillating contributions to the magnetic moment. The oscillation part demonstrates de Haas-van Alphen type of oscillation on electron density and Aharonov-Bohm like oscillations on longitudinal magnetic field.
Keywords: nanotube, superlattice, magnetic field, magnetic moment.

На основе модельного спектра энергии электронов на поверхности нанотрубки со сверхрешеткой в магнитном поле получено аналитическое выражение для магнитного момента вырожденного электронного газа. Показано, что в случае большого числа заполненных уровней энергии поперечного движения электронов существуют монотонные и осциллирующие вклады в магнитный момент. Последний испытывает осцилляции типа де Гааза-ван Альфена с изменением плотности электронов и осцилляции Ааронова-Бома с изменением магнитного потока через сечение трубки.
Ключевые слова: нанотрубка, сверхрешетка, магнитное поле, магнитный момент.

На основі модельного спектру енергії електронів на поверхні нанотрубки із надграткою у магнітному полі отримано аналітичний вираз для магнітного моменту виродженого електронного газу. Показано, що у випадку великої кількості заповнених рівнів енергії поперечного руху електронів існують монотонні та осцилюючі внески до магнітного моменту. Останній випробовує осциляції типу де Гааза-ван Альфена зі зміною густини електронів і осциляції Ааронова-Бома зі зміною магнітного потоку через перетин трубки.
Ключові слова: нанотрубка, надгратка, магнітне поле, магнітний момент.

Introduction

The study of the magnetic response in nanostructures with cylindrical geometry (nanotubes) provides us the important information about the electron energy spectrum and the potential of geometric confinement of electrons in such systems [1-6]. This is because the magnetic response of such nanostructures is mainly determined by the shape of the electron spectrum, which in turn depends on the geometry of the system.

Interest in carbon [1-3] and the semiconductor [4-6] nanotubes is caused by their unique characteristics – high strength and conductivity, magnetic, waveguide and optical properties. These systems are obtained by folding a sheet of graphene or two-dimensional heterostructures in a tube. Depending on the method of a folding the tube has a metal, semiconducting or dielectric properties.

Modern production methods allow one to create not only nanotubes, but also nanotubes with superlattices. Along with the flat superlattices [7-15] there exist the superlattices with cylindrical symmetry [16]. They are radial and longitudinal [16,17]. The radial superlattice represents a system of coaxial cylinders and the longitudinal superlattice is similar to the system of coaxial rings. The tubes with longitudinal superlattice are created by lithographic methods and by the introduction of fullerenes in a tube. In such a system there is a periodic potential acting on the electrons moving along the tube. The miniband appears in the energy spectrum of electrons. The density of electron states has a root singularities on the miniband boundaries [18].

It is important to note that the theoretical study of magnetic properties of nanotubes with a superlattice is quite a complex problem. The effect of one-dimensional superlattice on the magnetic moment of the semiconductor nanotubes is relatively little known. The theoretical research in this field is usually limited to numerical calculations.

The number of electrons, considered in these numerical studies, is little and such research methods can not be used for the study of nanostructures, containing hundreds or thousands of electrons. In addition, the most important thing is that the numerical methods do not always reveal the physical nature of the phenomena studied. In Ref. [19] the magnetic response of the electron gas on the surface of semiconductor nanotubes in a longitudinal magnetic field without the superlattice is considered. The Ref. [20] takes into account the effect of the superlattice on the magnetic moment. However the authors of [20] had obtained results which are expressed in terms of integrals. The authors Ref. [20] argue that these integrals are not expressed in terms of tabulated functions, and for this reason they are limited themselves to the numerical calculation.

The goals of this article are: to choose the suitable model for the description of the geometric confinement in nanotubes, to offer a convenient expression for the energy spectrum of electrons in the tube with superlattice, to obtain an analytical formula for the magnetic response of the electron system, to study the dependence of the magnetic moment on magnetic field and the surface curvature.

The electron energy spectrum

Equilibrium properties of the electron gas in nanosystems are determined by the electron energy spectrum, which is caused by the geometry of the system [19].

The energy of the electron with effective mass m_* on the nanotube cylindrical surface in a magnetic field $\vec{B}$ parallel to the tube axis was calculated by Kulik with taking into account the radial motion quantization of electrons in the tube of small thickness [21]:

$$\varepsilon_{mk} = \varepsilon_0 (m+\eta)^2 + \frac{\hbar^2 k^2}{2m_*}, \quad (1)$$

where $\hbar$ – quantum constant, $\hbar m$ and $\hbar k$ – the projection of the angular momentum and electron momentum on the axis of the tube, $\varepsilon_0 = \hbar^2 / 2m_* a^2$ – rotational quantum, a – the tube radius, $\eta = \Phi / \Phi_0$ – the ratio of the magnetic flux $\Phi = \pi a^2 B$ through the cross section of the tube to the flux quantum $\Phi_0 = 2\pi c\hbar / e$ [21]. Equation (1) describes a set of one-dimensional contiguous subzones, whose boundaries $\varepsilon_m = \varepsilon_0 (m+\eta)^2$ coincide with the quantized energy levels of the circular motion of the electrons on the tube in a magnetic field. The density of electron states has a root singularity at the subzone boundary. The simplest way to take into account the superlattice on the tube is to replace the longitudinal motion electron energy in the formula (1) by the expression

$$\varepsilon_k = \Delta(1-\cos kd), \quad (2)$$

where d – the period of the superlattice, 2Δ – the width of the energy spectrum band of the electron longitudinal motion. This expression (2) is borrowed from the theory of tight binding between the electrons and the lattice and it is often used in the theory of layered crystals and superlattices [20,22,23]. Thus, in the single-band approximation, the electron energy with an effective mass m_* and spin magnetic moment μ_B on the cylindrical nanotube surface with a longitudinal superlattice in the longitudinal magnetic field is

$$\varepsilon_{mk\sigma} = \varepsilon_0 (m+\eta)^2 + \Delta(1-\cos kd) + \sigma\mu_B B, \quad (3)$$

where $\sigma = \pm 1$ – spin quantum number. This band corresponds to the wave number values situated in the first Brillouin zone $-\pi/d \le k \le \pi/d$. The spectrum (3) describes a set of allowed electron energy region in intervals $\varepsilon_l \le \varepsilon \le \varepsilon_l + 2\Delta$, which separated by gaps. According to the analogy with the conventional superlattice theory these bands are called minibands.

Magnetic moment of the electron gas

Using the standard expression for the thermodynamic potential Ω [24], we obtain in considered case the following expression

$$\Omega = -\frac{k_B T L}{\pi} \sum_{m=-\infty}^{\infty} \sum_{\sigma} \int_0^{\pi/d} dk \ln\left[1 + \exp\left(\frac{\mu - \varepsilon_{mk\sigma}}{k_B T}\right)\right], \quad (4)$$

where L – the nanotubes length, k_B – Boltzmann constant, μ – chemical potential. Using formula (4) we find the magnetic moment according to the expression $M = -\left(\partial\Omega / \partial B\right)_{\mu,T}$. Then we get the expression

$$-\frac{M}{\mu_B} = \frac{L}{\pi}\frac{m_0}{m_*} \sum_{m=-\infty}^{\infty} \sum_{\sigma=-1}^{+1} \int_0^{\pi/d} dk \frac{m + \dfrac{\Phi}{\Phi_0} + \sigma\dfrac{m_*}{m_0}}{\exp\left(\dfrac{\varepsilon_{mk\sigma} - \mu}{k_B T}\right) + 1}, \quad (5)$$

where m_0 – the free electron mass. In Ref. [20] the spin is not taken into account but in this article it will be taken into account. The summation over m in the formula (5) is calculated using the Poisson summation formula:

$$\sum_{m=-\infty}^{\infty}\psi(m)=\sum_{l=-\infty}^{\infty}\int_{-\infty}^{\infty}dx\,\psi(x)e^{2\pi i l x}.$$

As a result of simple transformations, it turns out that the magnetic moment of the electron gas on the surface of the tube with a superlattice can be represented as the sum of three contributions $M=M_1+M_2+M_3$, where

$$-\frac{M_1}{\mu_B}=\sum_{\sigma}\frac{2L\sigma}{\pi}\int_0^{\pi/d}dk\int_0^{+\infty}dx'\,f(x'),\qquad(6)$$

$$-\frac{M_2}{\mu_B}=\sum_{\sigma}\frac{4Lm_0}{\pi m_*}\sum_{l=1}^{+\infty}\sin\left(2\pi l\frac{\Phi}{\Phi_0}\right)\int_0^{\pi/d}dk\int_0^{+\infty}dx'\,x'\sin(2\pi l x')\,f(x'),\qquad(7)$$

$$-\frac{M_3}{\mu_B}=\sum_{\sigma}\frac{4L\sigma}{\pi}\sum_{l=1}^{+\infty}\cos\left(2\pi l\frac{\Phi}{\Phi_0}\right)\int_0^{\pi/d}dk\int_0^{+\infty}dx'\cos(2\pi l x')\,f(x').\qquad(8)$$

The notation here we have used:

$$f(x')=\frac{1}{\exp\beta\left[\varepsilon_0 x'^2+\Delta(1-\cos kd)+\sigma\mu_B B-\mu\right]+1},$$

where $\beta=1/k_B T$ – the reverse temperature.

(From the formulas (6)-(8) it is seen that under $\sigma=0$ the only contribution M_2 is non-zero.)

Expressions (7) and (8) are the result of the expansion of Fourier series of the magnetic moment of nanotube with a superlattice:

$$-\frac{M_2}{\mu_B}=\sum_{\sigma}\sum_{l=1}^{+\infty}C_{2l}^{\sigma}(T)\sin\left(2\pi l\frac{\Phi}{\Phi_0}\right),\qquad -\frac{M_3}{\mu_B}=\sum_{\sigma}\sum_{l=1}^{+\infty}C_{3l}^{\sigma}(T)\cos\left(2\pi l\frac{\Phi}{\Phi_0}\right).\qquad(9)$$

Let us introduce the new variables $x=kd/2$, $2\pi x'=z$ and notation $\beta'=\beta 2\Delta$,

$$b_{\sigma}(z)=\frac{\mu_{\sigma}}{2\Delta}-\frac{\varepsilon_0 z^2}{8\pi^2\Delta},$$

where $\mu_{\sigma}=\mu_0-\sigma\mu_B B$, μ_0 – the chemical potential at zero temperature. Also we take into account that there is an identity $\Delta(1-\cos 2x)=2\Delta\sin^2 x$. As a result, we obtain the following expressions for the Fourier coefficients:

$$C_{2l}^{\sigma}=\frac{2m_0 L}{\pi^3 m_* d}\int_0^{+\infty}dz\,z\sin lz\int_0^{\pi/2}dx\frac{1}{e^{\beta'\left(\sin^2 x-b_{\sigma}\right)}+1},\qquad(10)$$

$$C_{3l}^{\sigma}=\frac{4L\sigma}{\pi^2 d}\int_0^{+\infty}dz\,\cos lz\int_0^{\pi/2}dx\frac{1}{e^{\beta'\left(\sin^2 x-b_{\sigma}\right)}+1}.\qquad(11)$$

It follows from (9)-(11), the magnetic moment of the semiconductor nanotubes is an oscillating function of magnetic flux with a period equal to the flux quantum.

Following the authors Ref. [20], with the goal of qualitative research nature of the dependence of the magnetic moment of the magnetic flux, one considers the case $T=0$. Then in the $\int dx$ integrand takes the formula $\Theta\left(\sin^2 x-b_\sigma\right)$, where $\Theta(x)$ – the Heaviside theta function. Next, you need to consider the following case, when $\mu_\sigma>2\Delta$.

In that case there exist the contributions for the magnetic moment:

$$-\frac{M_2}{\mu_B}=\frac{2m_0L}{\pi^3 m_* d}\sum_{l=1}^{+\infty}\sin\left(2\pi l\frac{\Phi}{\Phi_0}\right)\sum_\sigma\left[\frac{\pi}{2}\int_0^{2\pi\sqrt{\frac{\mu_\sigma-2\Delta}{\varepsilon_0}}}dz\,z\sin lz+\int_{2\pi\sqrt{\frac{\mu_\sigma-2\Delta}{\varepsilon_0}}}^{2\pi\sqrt{\frac{\mu_\sigma}{\varepsilon_0}}}dz\,z\sin lz\arcsin\sqrt{b_\sigma(z)}\right], \quad (12)$$

$$-\frac{M_1+M_3}{\mu_B}=\frac{2L}{\pi^2 d}\sum_\sigma\sigma\left[\frac{\pi}{2}\int_0^{2\pi\sqrt{\frac{\mu_\sigma-2\Delta}{\varepsilon_0}}}dz+\int_{2\pi\sqrt{\frac{\mu_\sigma-2\Delta}{\varepsilon_0}}}^{2\pi\sqrt{\frac{\mu_\sigma}{\varepsilon_0}}}dz\,\arcsin\sqrt{b_\sigma(z)}\right]\times$$
$$\times\left[1+2\sum_{l=1}^{+\infty}\cos\left(2\pi l\frac{\Phi}{\Phi_0}\right)\cos lz\right]. \quad (13)$$

Further analysis of the magnetic moment dependence of the magnetic flux is performed using the values of typical parameters $GaAs$, which are commonly used in experiments [16,20]: $m_*=0.07\cdot m_0$ (m_0 – free electron mass), $a=10^{-7}\,cm$, $\mu_0/\varepsilon_0=10$, $L=10\,\mu m$, $\Delta=0.01\,\text{eV}$, $d=3500\,\overset{0}{\text{A}}$. Provided you use inequalities $\mu_\sigma\gg 2\Delta$, $\mu_\sigma\gg\varepsilon_0$ it can be represented (12) in the form

$$-\frac{M_2}{\mu_B}=\frac{2m_0L}{m_* d}\sum_{l=1}^{+\infty}\sum_\sigma\left[\frac{\Delta}{\varepsilon_0}\sin\left(2\pi l\sqrt{\frac{\mu_\sigma}{\varepsilon_0}}\right)-\frac{1}{\pi l}\sqrt{\frac{\mu_\sigma}{\varepsilon_0}}\cos\left(2\pi l\sqrt{\frac{\mu_\sigma}{\varepsilon_0}}\right)\right]\sin\left(2\pi l\frac{\Phi}{\Phi_0}\right). \quad (14)$$

If we consider the inequality $\Delta\ll\varepsilon_0$, we can neglect the first term in brackets in (14). The second term in brackets in formula (13) contains the integral of the form $B_l^\sigma=\int_{z_{\min}}^{z_{\max}}dz\arcsin\sqrt{b_\sigma(z)}\cos lz$.

Proceeding in this integral to a new variable u according to the formula $z=\sqrt{\frac{8\pi^2\Delta}{\varepsilon_0}}\sqrt{\frac{\mu_\sigma}{2\Delta}-u^2}$,

followed by an approximate calculation under condition $\mu_\sigma\gg 2\Delta$ it gives

$$B_l^\sigma\approx\frac{\pi^2}{2}\frac{\Delta}{\sqrt{\varepsilon_0\mu_\sigma}}\cos\left(2\pi l\sqrt{\frac{\mu_\sigma}{\varepsilon_0}}\right). \quad (15)$$

As a result the contributions were obtained:

$$-\frac{M_1+M_3}{\mu_B}=\frac{2L}{d}\sum_\sigma\sigma\sqrt{\frac{\mu_\sigma}{\varepsilon_0}}\left[1+\frac{\Delta}{2\mu_\sigma}+\frac{\Delta}{\mu_\sigma}\sum_{l=1}^{+\infty}\cos\left(2\pi l\sqrt{\frac{\mu_\sigma}{\varepsilon_0}}\right)\cos\left(2\pi l\frac{\Phi}{\Phi_0}\right)\right]. \quad (16)$$

It is important to note, that the integral

$$B_0^\sigma = \sqrt{\frac{8\pi^2\Delta}{\varepsilon_0}} \int_0^1 du \frac{u}{\sqrt{\frac{\mu_\sigma}{2\Delta} - u^2}} \arcsin u$$

can be calculated exactly. As a result of the integration by parts it is equal to:

$$B_0^\sigma = -\sqrt{\frac{8\pi^2\Delta}{\varepsilon_0}} \left[\frac{\pi}{2}\sqrt{\frac{\mu_\sigma}{2\Delta} - 1} - \sqrt{\frac{\mu_\sigma}{2\Delta}} E\left(\sqrt{\frac{2\Delta}{\mu_\sigma}}\right) \right],$$

where $E(k) = E\left(\pi/2, k\right)$ – the complete elliptic integral of the second kind [25]:

$$E(\varphi, k) = \int_0^\varphi d\alpha \sqrt{1 - k^2 \sin^2 \alpha}$$

– elliptic integral of the second kind, k – its module. Performing expansion in the $E\left(\sqrt{2\Delta/\mu_\sigma}\right)$ over small parameter $2\Delta \ll \mu_\sigma$ we obtain the result that is consistent with (15) at $l = 0$.

The formula (14) and (16) undergoes Aharonov-Bohm oscillations under variation of magnetic flux through the tube cross-section. The oscillation period is equal to the flux quantum Φ_0. Also there exist the oscillations looking like de Haas-van Alphen ones. They are caused by transition of root singularities of electron density of states at the miniband boundaries through Fermi boundary due to the tube radius variation or changing the electron density n. The latter is related with the Fermi energy under $\mu \gg 2\Delta$ as follows [26]

$$\mu = \frac{1}{8m_*}\left(\pi\hbar dn\right)^2.$$

In addition, we neglect the weak spin levels splitting. Analyzing the dependence of oscillations in (14) and (16) on $\left(adn\right)^{1/2}$ we obtain the period

$$\tau = \left(\frac{1}{\pi a\sqrt{m_*\Delta}}\right)^{1/2}. \qquad (17)$$

Conclusions

The increasing interest in electron properties of carbon and semiconductor nanotubes is due to several reasons. They are functional elements of various instruments and devices. The existence of an additional parameter – the curvature of the nanostructure – increases the number of ways to control the properties of these systems. Modern production methods allow us to create the superlattice on the tubes. Nanotubes with a superlattice are characterized by additional parameters – the period and amplitude of modulating potential. As a result, the physical properties of the electron gas on the surface of the tube with a superlattice become richer.

Observation of the magnetic moment oscillations of de Haas-van Alphen type allow us to determine the electron effective mass m_*, Fermi momentum, rotational quantum ε_0 and the superlattice parameters d and Δ. These values determine the amplitude (14), (16) and period (17) of magnetic response of the nanotube. The magnetic field results in Aharonov-Bohm oscillations of the magnetic moment caused by nonconnectivity of the area occupied by electrons.

1. S. Iijima. Nature (London), 354, 56 (1991).
2. R. Saito, G. Dresselhaus, M. Dresselhaus. Physical Properties of Carbon Nanotubes, World Scientific Publ., London (1998), 346 pp.
3. M. Dresselhaus, G. Dresselhaus, P. Avouris. Carbon Nanotubes. Synthesis, structure, properties and applications, Springer-Verlag, Berlin (2001), 420 pp.
4. V. Prinz, A. Chehovskiy, V. Preobrazhenski, B. Semyagin and A. Gutakovsky. Nanotechnology, 13, 231 (2002).
5. I. Chun, V. Verma. Journ. of Cryst. Growth., 310, 235 (2008).
6. L.I. Magarill, A.V. Chaplik, M.V. Entin. Uspehi Fiz. Nauk, 175, 995 (2005).
7. L.V. Keldysh. Fizika Tverd. Tela, 4, 2265 (1962).
8. L. Esaki, R. Tsu. IBM J. Res. Develop., 14, 61 (1970).
9. A. Fetter. Ann. Phys., 88, 1 (1974).
10. D. Sarma, J. Quinn. Phys. Rev., B 25, 7603 (1982).
11. A. Tselis, J. Quinn. Phys. Rev. B, 29, 2021 (1984).
12. A. Tselis, J. Quinn. Phys. Rev. B, 29, 3318 (1984).
13. M. Herman. Semiconductor Superlattices, Akademie-Verlag, Berlin (1986), 240 p.
14. W.-M. Que, G. Kirczenov. Phys. Rev. B 36, 6596 (1987).
15. K. Golden, G. Kalman. Phys. Rev., B 52, 14719 (1995).
16. V. Dragunov, I. Neizvestnyi, V. Gridchin. Fundamentals of Nanoelectronics, Logos, Moscow (2006), 258 pp.
17. C. Yannouleas, E. Bogachek, U. Landman. Phys. Rev., B 53, 10225 (1996).
18. A.M. Ermolaev, G.I. Rashba, M.A. Solyanik. Fizika Nizk. Temp., 37, 1033 (2011).
19. V.A. Geiler, V.A. Margulis, A.V. Shorohov. JETP, 115, 1450 (1999).
20. O.P. Volosnikova, D.V. Zavyalov, S.V. Kruchkov. Proceedings of the XVII International Workshop "Radiational Solid state physics" 645, Sevastopol', 7 (2007).
21. I.O. Kulik. JETP letters, 11, 407 (1970).
22. F.G. Bass, A.A. Bulgakov, A.P. Tetervov. High-frequency properties of the semiconductor superlattice, Nauka,

Moscow (1989), 288 pp.

23. E.A. Pashitskiy, Yu.M. Malozovskiy, A.V. Semenov. Ukr. Fizich. Journ., 36, 889 (1991).
24. L.D. Landau, E.M. Lifshits. Statistical Physics, Nauka, Moscow (1995), 568 pp.
25. H. Bateman, A. Erdelyi. Higher Transcendental Functions, v. 2, Mc Graw-Hill Book Comp., New York (1953), 296 pp.
26. N.V. Gleizer, A.M. Ermolaev, G.I. Rashba and M.A. Solyanik. Visnik KhNU, ser. “Physics”, № 962, vip. 15, 15 (2011).