CONFERENCES AND SYMPOSIA

PACS number: 01.10.Fv

Joint scientific session of the Physical Sciences Division of the Russian Academy of Sciences and the Joint Physical Society of the Russian Federation "Electrons in curved structures" (20 April 2005)

A joint scientific session of the Physical Sciences Division of the Russian Academy of Sciences (RAS) and the Joint Physical Society of the Russian Federation was held on April 20, 2005 in the conference hall of the P N Lebedev Physics Institute, RAS under the name "Electrons in curvilinear structures". The following reports were presented at the session:

(1) Magarill L I, Chaplik A V, Entin M V (Institute of Semiconductor Physics, Siberian Branch (SB) of the RAS, Novosibirsk) "Spectrum and kinetics of electrons in curved nanostructures";

(2) Romanenko A I, Okotrub A V (Institute of Inorganic Chemistry, SB RAS, Novosibirsk), Kuznetsov V L (G K Boreskov Institute of Catalysis, SB RAS, Novosibirsk), Kotosonov A S (Federal State Unitary Enterprise 'Scientific Research Institute for Graphite-based Construction Materials' — NIIgrafit, Moscow), Obraztsov A N (Moscow State University, Moscow) "Heterogeneous electronic states in carbon nanostructures with different dimensionalities and curvatures of the constituent graphene layers";

(3) Belov V V (Moscow State Institute of Electronics and Mathematics, Moscow), Dobrokhotov S Yu, Maslov V P, Tudorovskii T Ya (Institute of Problems of Mechanics, Moscow) "A generalized adiabatic principle for electron dynamics in curved nanostructures".

An abridged version of the reports is given below.

PACS numbers:73.20. - r, 73.25. + i, 73.50. - h, 73.61. - r DOI: 10.1070/PU2005v048n09ABEH005730

Spectrum and kinetics of electrons in curved nanostructures

L I Magarill, A V Chaplik, M V Entin

1. Introduction

Rapid technological progress has recently made possible various low-dimensional systems of complex geometrical shape [1, 2], such as scrolls, rings, spirals, goffers, and so on. This has led to renewed interest in the theoretical study of curved low-dimensional systems.

Uspekhi Fizicheskikh Nauk **175** (9) 995–1010 (2005) Translated by D V Belyaev; edited by A Radzig Many works have been devoted to the derivation of the general Hamiltonian of curved low-dimensional systems. The electronic states of curved low-dimensional systems have been studied both theoretically [3-6] and experimentally [7, 8].

The reduction of system dimensionality due to the constraint of electron motion along one or several coordinates results in transverse quantization of the electronic states. In a heterogeneous system, the transverse energy levels begin to depend on the longitudinal coordinate. This description is adequate provided that the characteristic size of heterogeneity is large in comparison with the thickness of a layer or a quantum wire. Such adiabatic quantization may be applied to curved low-dimensional systems. By these systems we mean those that locally coincide with the corresponding plane two-dimensional or rectilinear one-dimensional systems. The 'equal-width' quantizing when the system is described by the same confining potential at every section, is a simple (but not the only possible!) situation.

If the electron moved strictly over a surface or along a curve, it would be possible to describe its motion by an appropriate transformation of the two-dimensional or onedimensional Schrödinger equation for a free particle to the curvilinear coordinates. Taking the finite thickness of a surface layer or a quantum wire into account significantly complicates the effective Hamiltonian. First of all, the quantization of the transverse states gives rise to large contributions to the energy, proportional to $1/d^2$. These contributions grow as the thickness of d tends to zero, while the kinetic energy of the longitudinal motion may remain finite. However, provided that the transverse characteristics of the confining potential and the states across the surface are uniform, these contributions are also constant and may be subtracted out by an energy shift. The presence of a curvature gives rise to the additional energy contributions that, on the one hand, remain small in comparison with the quantum energy, but prove to be comparable to the longitudinal kinetic energy. The best-known contribution is the geometric potential independent of the transverse potential characteristic and the transverse state structure. Since this quantity is local, it is determined by only local geometric characteristics of the curved system. The geometric potential has to have the dimensionality proportional to the second degree of curvature of the system.

If the longitudinal kinetic energy of the electron is small in comparison with the transverse quantizing intervals, the geometric potential is mainly determined by the system's curvature. Whenever the electron kinetic energy compares with or exceeds the above intervals, then another factor may play a role: the centrifugal displacement of the electron toward the outer side of a quantum wall contributes to the energy, proportional to the curvature, the kinetic energy, and the layer thickness.

The difference between one-dimensional and two-dimensional curved systems lies in the necessity to consider their transverse geometry — that is, the shapes of the sections. Since the cross section may undergo a turn along the wire, the local one-dimensional Hamiltonian of the system has to be determined both by the local system's curvature and the axial wire torsion. Torsion and curvature also influence the spin degree of freedom, thus contributing extra to spin – orbit (SO) interaction in curved low-dimensional systems. The subjects mentioned above constitute the contents of the present report.

2. The Hamiltonian of a curved surface

The effective Hamiltonian for electrons on a curved surface in the absence of SO coupling has been derived in Refs [3, 4]. We will extend the approach utilized in those works to the case of asymmetric confinement across the surface layer, based on the Schrödinger equation for an electron with a quadratic non-degenerate spectrum:

$$\left(-\frac{1}{2m}\,\Delta + U(\mathbf{r})\right)\Psi = E\,\Psi\,.\tag{1}$$

Hereinafter we assume $\hbar = 1$; *m* is the effective mass.

Let $\mathbf{a}(q_1, q_2)$ parametrically determine a surface in a 3D space. Parameters q_1 and q_2 can be considered as curvilinear coordinates on the surface. In a finite layer enclosing the surface, any point is defined as

$$\mathbf{r}(q_1, q_2, q_3) = \mathbf{a}(q_1, q_2) + q_3 \mathbf{n}, \quad |q_3| \le \delta,$$
 (2)

where $\mathbf{n} = \partial_1 \mathbf{a} \times \partial_2 \mathbf{a} / |\partial_1 \mathbf{a} \times \partial_2 \mathbf{a}|$ is a unit vector transverse to the surface, $\partial_i \equiv \partial/\partial q_i$, and the layer thickness δ is assumed to be small relative to the radius of the surface curvature. The triad $\{q_1, q_2, q_3\}$ constitutes a coordinates system in a 3D space.

The problem is to derive the effective Hamiltonian for an electron motion across the surface. The bottom of the well, $q_3 = 0$, is assumed to form an equipotential surface, and the potential depends only on q_3 . We also assume that the characteristic geometric lengths of the $q_3 = 0$ surface, in particular, curvature radii, exceed the width of the surface well. Such a potential well is locally plane, therefore the electron states may be described in the adiabatic approximation. According to this approximation, the wave function Ψ may be represented as a series expansion of functions $\phi_n(q_3)$ relating to the transverse motion in the well:

$$\Psi = \frac{1}{\sqrt{f}} \sum_{n} \psi_n(q_1, q_2) \phi_n(q_3),$$

$$\left(\frac{\mathbf{p}_3^2}{2m} + U\right) \phi_n = E_n \phi_n,$$
 (3)

where E_n is the transverse state energy, and the function $f = \sqrt{\det(G_{ij})/\det(g_{ij})}$ is determined by the ratio of determinants of the three-dimensional and surface metric tensors, G_{ij} and g_{ij} , respectively. Using the adiabatization procedure, we find the effective Hamiltonian of electrons in an *n*-th

subband:

$$\hat{H} = -\frac{1}{2m}\,\hat{D}_0 + V_{\rm g}\,(q_1, q_2) + \hat{H}_{\rm c}\,,\quad \hat{H}_{\rm c} = -\frac{1}{2m}\,(q_3)_{nn}\,\hat{D}_1\,,\tag{4}$$

where

$$\hat{D}_0 = \frac{1}{\sqrt{g}} \sum_{i,j=1}^2 \partial_i \sqrt{g} g_{ij} \partial_j; \qquad (5)$$

$$\hat{D}_{1} = -\{\hat{D}_{0}, \operatorname{Sp}(\hat{\beta})\} -\frac{1}{\sqrt{g}} \partial_{i}\sqrt{g} \left[2(\hat{h}^{-1})_{ij} \operatorname{det}(\hat{\beta}) + g^{ij} \operatorname{Sp}(\hat{\beta})\right] \partial_{j}, \qquad (6)$$

 $(q_3)_{nn} = \langle \phi_n | q_3 | \phi_n \rangle, \ \hat{\beta} = -(\hat{h}\hat{g}^{-1}), \text{ and } h_{ij} = h_{ji} = -\partial_i \mathbf{a} \partial_j \mathbf{n}$ are the coefficients of the second fundamental form; the appearance of braces mean that the operator product is symmetrized.

The \hat{D}_0 operator stands for the purely surface part of the Laplacian. In other words, $-\hat{D}_0/2m$ is the longitudinal part of the kinetic energy. When passing to the classical limit with respect to longitudinal motion, this Hamiltonian gives rise to particle motion along the geodetic lines.

The geometric potential V_g can be expressed through the principal surface curvatures $\varkappa_{1,2}$ [4]:

$$V_{\rm g}(q_1, q_2) = -\frac{1}{8m} \left[(\operatorname{Tr} \hat{\beta})^2 - 4 \det \hat{\beta} \right] \equiv -\frac{\hbar^2}{8m} (\varkappa_1 - \varkappa_2)^2 \,.$$
(7)

As seen from formula (7), V_g does not depend on the structure of the confinement potential. The geometric potential contains the Planck constant, and in the classical approximation it becomes zero.

The quantity \hat{H}_c is related to the centrifugal force: an electron moving along a curved surface displaces toward the outer side of a potential well; in an asymmetric potential well, its potential energy changes proportionally to the centrifugal force. In the simplest cases of a sphere and round cylinder we get

$$\hat{H}_{\rm c} = -\frac{(q_3)_{nn}}{mR^3} \hat{\mathbf{I}}^2 \quad (\text{sphere}) \,, \tag{8}$$

$$\hat{H}_{c} = -\frac{(q_{3})_{mn}}{mR^{3}}\hat{l}_{z}^{2}$$
 (cylinder), (9)

where \hat{l} , \hat{l}_z are the operators of the angular momentum and its projection onto the cylinder axis.

Thus, \hat{H}_c accounts for the effective mass renormalization of the relative order δ/R , where δ is the mean value of the transverse coordinate, i.e., the effective layer thickness; naturally, only the azimuth mass component is renormalized for a cylinder.

3. The Hamiltonian for a curved quantum wire

Let us consider the motion of electrons having a quadratic and isotropic spectrum within curved and/or twisted quantum wire. Neglecting its thickness, such wire is defined by the equation

$$\mathbf{r} = \mathbf{a} \left(q_3 \right). \tag{10}$$

Here, q_3 is the arc length along this curve. To consider the wire's shape, however, this one-dimensional description is not enough. Taking the thickness finiteness into account, equation (10) gives only some center line inside the wire, going along it.

The system in question can be regarded as a homogeneous and initially straight wire with an arbitrary section shape, which was twisted and/or bent along the wire axis arbitrarily with respect to q_3 . Mathematically, the wire can be given as a locus formed by a planar figure moving along a curve, provided that:

(1) the figure plane remains normal to the curve at their intersection points;

(2) the curve crosses the figure at the same point of the figure.

In general, we constrain the electron motion across the wire by an arbitrary and not necessarily hard potential $U(\mathbf{r})$. The potential adequate for our premises has to be equally dependent on local coordinates transverse to the curve in any section, correct to the rotation of the coordinate system around the tangent to the curve. Let us choose a (curvilinear) coordinate system where the potential does not depend upon q_3 . We introduce a moving 3-hedron of the curve comprising a tangent $\mathbf{t}(q_3) = \partial_3 \mathbf{a}$, a normal $\mathbf{n}(q_3) = \partial_3 \mathbf{t}/|\partial_3 \mathbf{t}|$, and a binormal $\mathbf{b}(q_3) = \mathbf{t} \times \mathbf{n}$, as well as their related vectors

$$\mathbf{n}_1 = \mathbf{n}\cos\phi - \mathbf{b}\sin\phi, \quad \mathbf{n}_2 = \mathbf{n}\sin\phi + \mathbf{b}\cos\phi. \tag{11}$$

Here, $\phi(q_3)$ is the angle of rotation of a cross section around **t**. We define the new coordinates by the relationship

$$\mathbf{r}(\mathbf{q}) = \mathbf{a}(q_3) + q_1 \mathbf{n}_1 + q_2 \mathbf{n}_2.$$
(12)

In q_i coordinates, the transverse potential takes the form $U = U(\mathbf{q}_{\perp})$, where $\mathbf{q}_{\perp} = (q_1, q_2)$.

We consider the wire thickness to be small relative to its radius of curvature. In addition, we will regard the product of the wire's internal torsion $\omega \equiv \partial_3 \phi$ and of thickness to be small as well. These parameters define the adiabatic conditions of the electron motion in the wire: when moving along the wire electrons retain the number of the transverse quantization subband.

We expand the wave function

$$\Phi(\mathbf{q}) = \frac{1}{(G)^{1/4}} \sum_{n} \phi_n(\mathbf{q}_\perp) \psi_n(q_3)$$
(13)

in terms of the transverse states $\phi_n(\mathbf{q}_{\perp})$ in the wire, which satisfy the equation

$$\left(\frac{\hat{\mathbf{p}}_{\perp}^{2}}{2\mu}+U\right)\psi_{n}=E_{n}\psi_{n}\,,\tag{14}$$

where E_n is the energy of a transverse state in the wire.

Consider a nondegenerate spectrum of the transverse states. We search for the states resulting from some transverse state *n*, all other $\psi_{n'}$ with $n' \neq n$ being small relative to ψ_n . In doing so, we arrive at

$$\left[\frac{\hat{p}_{3}^{2}}{2m} - \frac{\varkappa^{2}(q)}{8m} + \frac{1}{2m}\beta_{n}\zeta^{2}(q) + \frac{1}{m}\{\varkappa\mathbf{l}, \ \hat{p}_{3}^{2}\}(\mathbf{q}_{\perp})_{nn}\right]\psi_{n} \\
= (E - E_{n})\psi_{n}.$$
(15)

Here, $\beta_n = (\hat{l}_z^2)_{nn}$, $\zeta = \tau + \omega$, and τ is a geometric torsion of the curve.

The second term in square brackets in equation (15) is the well-known [3, 4] geometric potential brought about exclusively by a wire curvature and independent of its internal structure. The third term in square brackets is determined by inner and geometric torsion of a wire. It depends, via the matrix element $(\hat{l}_z^2)_{nn}$, on the shape of the transverse potential and on the transverse wave functions. Finally, the fourth term comprises the diagonal matrix element $(\mathbf{q}_{\perp})_{nn}$ of the transverse vortex coordinate. For potentials $U(\mathbf{q}_{\perp})$ symmetric with respect to rotations around the axis 3 through angles $2\pi/N$, N = 2, 3..., which also include potentials axially symmetric about this axis, the matrix elements $(\mathbf{q}_{\perp})_{nn} = 0$ at all *n*. In particular, the parabolic potentials, as well as quantum wires of the square cross-section with rigid walls, possess such symmetry.

In the more general case of a quantum wire with an asymmetric potential, the fourth term in the left part of Eqn (15) remains. It is of centrifugal origin: an electron moving along a curved wire is being pressed to the outer side of the bent wire by a centrifugal force, and thus its potential energy in the asymmetric well potential changes, too. This contribution depending on the electron longitudinal momentum is a small addition to its kinetic energy and corresponds to the mass re-normalization.

For a round spiral of radius *R*, pitch *D*, and centrally symmetric cross-section without internal torsion ($\omega = 0$), the effective Hamiltonian takes the form (the energy is measured from the bottom of the *n*-th subband)

$$\hat{H} = \frac{\hat{p}_3^2}{2m} - \frac{\varkappa^2}{8m} + \frac{\beta\tau^2}{2m} \,, \tag{16}$$

where $\varkappa = 4\pi^2 R/(4\pi^2 R^2 + D^2)$, and $|\tau| = 2\pi D/(4\pi^2 R^2 + D^2)$; for the lower subband in the wire of rectangular section one has $\beta = \pi^2/6 - 1$.

4. Spin – orbit interaction

4.1 Two-dimensional case (curved quantum well)

In the $q_{1,2,3}$ coordinates introduced above, the initial SO coupling operator is given by

$$\hat{\mathcal{H}}_{so} = i\alpha \frac{1}{\sqrt{G}} \left(\hat{\partial}_3 U \right) \epsilon^{ij} \left(\sigma(\hat{\partial}_i \mathbf{r}) \right) \hat{\partial}_j, \qquad (17)$$

where ϵ^{ij} is the Levi-Civita symbol, $\epsilon^{11} = \epsilon^{22} = 0$, $\epsilon^{12} = -\epsilon^{21} = 1$, and α is an SO coupling constant in the bulk material.

We will derive the effective two-dimensional SO Hamiltonian using the smallness of the parameter δ/R . The rather cumbersome computations result in the following conclusion. The SO coupling operator comprises two contributions that are proportional to the transverse T_n and the longitudinal L_n kinetic energies of a particle in a given subband, respectively. The first contribution comes from the across-layer gradient of the layer-tangential electron velocities, whereas the second one is a consequence of the centripetal force turning the particle along the curved surface (in moving coordinate system, this force contributes to the effective magnetic field). When the wavelength of longitudinal motion is small relative to the radius of curvature, the surface may be considered locally plane. In this case, as follows from formula (17):

$$\hat{H}_{so} = -2\alpha \Big[T_n(\sigma_x \hat{p}_y \varkappa_y - \sigma_y \hat{p}_x \varkappa_x) \\ -\frac{1}{2m} (\varkappa_x \hat{p}_x^2 + \varkappa_y \hat{p}_y^2) (\sigma_x \hat{p}_y - \sigma_y \hat{p}_x) \Big].$$
(18)

An illustrative example is the result for the spectrum of electrons on a cylindrical surface of radius *R*:

$$\varepsilon_{np_{z}j_{z}} = \frac{1}{2mR^{2}} \left\{ k^{2} + j_{z}^{2} + \frac{1}{4} - \frac{\bar{\alpha}}{2} \left(\frac{1}{4} + 3j_{z}^{2} - t_{n} \right) \\ \pm \sqrt{j_{z}^{2} \left[1 + \bar{\alpha}t_{n} - \bar{\alpha} \left(j_{z}^{2} + \frac{3}{4} \right) \right]^{2} + \bar{\alpha}^{2}k^{2} \left(j_{z}^{2} + \frac{1}{4} \right)^{2}} \right\}.$$
(19)

Here, $\bar{\alpha} = 2\alpha/R^2$, $t_n = 2mR^2T_n$, and $k = p_zR$; p_z and j_z are the momentum along the cylinder axis and the angular momentum about the cylinder axis, respectively.

4.2 A one-dimensional case

(a bent and twisted quantum wire)

In q coordinates (see Section 3), we have

$$\mathcal{H}_{\rm so} = \alpha \epsilon^{ijk} \frac{1}{G^{1/4}} \,\bar{\sigma}_j(\partial_k U) \,\hat{p}_i \,\frac{1}{G^{1/4}}, \quad \bar{\sigma}_j = (\partial_j r_i) \,\sigma_i \,. \tag{20}$$

Let us expand this formula in terms of powers of $q_{1,2}$ and average it over the functions of the transverse motion in the *n*-th subband. In general, the averaged SO Hamiltonian is linear with respect to the longitudinal momentum and includes both the contribution proportional to the wire curvature and the contribution proportional to the wire torsion. The contribution due to torsion reduces to zero if $U(\mathbf{q}_{\perp})$ has a symmetry center. So, we get the dispersion law for a round wire spiraled with radius *R* and constant pitch *D*:

$$\varepsilon_n^{\pm} - \varepsilon_{\min}^{(n)} = \frac{1}{2m} \left[p^2 \pm |p| \sqrt{4(m\alpha \varkappa E_n)^2 + 4(m\alpha \varkappa E_n) \varkappa + \frac{\varkappa}{R}} \right], (21)$$

where $\varepsilon_{\min}^{(n)}$ is the constant *n*-th subband shift dependent on the spiral curvature and torsion.

5. Possible applications

Consider a bent quantum wire (the same is obviously true for a quantum well in the shape of a cylindrical surface). Let it look like two straight lines matched with a circular arc ('open book') (Fig. 1). The geometric potential of such a structure is represented by a rectangular well $1/8mR^2$ deep and $R\theta$ wide,



Figure 1. A single quantum well in a bent wire.

where *R* is the radius of circle, and θ is the angle between the straight lines ($\theta \le \pi$). This well has one and only one bound state. At $m = 0.07m_0$ (GaAs), R = 100 Å, and $\theta = \pi$, the binding energy W_0 is about 4 K; for $\theta = \pi/2$, one finds $W_0 \approx 3$ K. Since the geometric potential is also a well for holes, one can expect exciton condensation in the vicinity of the wire bend. In this case, we deal with bosons whose spectrum, in addition to the continuous part of positive energy, possesses one negative level. When the exciton concentration exceeds some temperature-dependent critical value, the particles begin accumulating in the bound state. For the above parameters, the critical exciton concentration is of the order of 10^5 cm⁻¹ at T = 1 K.

For a curved wire with a single point of maximal curvature, $q_3 = q_0$ (parabola, hyperbola), provided that $a^* \ll R$, where a^* is the effective exciton radius, the potential may be considered quadratic with respect to small displacements $(q_3 - q_0)^2$. Since $V_g \propto 1/m$, then the internal motion within an exciton and the motion of its center of gravity can be resolved, when the masses of the electron and the hole are equal, $m_e = m_h$. In this hypothetical case, the probability *P* of exciton formation depends on the quantum number *N* of the oscillator describing the mass center motion:

$$P_{2N} \propto \frac{(2N)!}{2^{2N}(N!)^2}, \quad P_{2N+1} \equiv 0, \quad N = 0, 1, 2, \dots$$
 (22)

Thus, the exciton absorption (and luminescence) line acquires a kind of fine structure on a scale of order $1/mR^2$. When the masses are unequal, $m_e \neq m_h$, the separation of the degrees of freedom is not possible and the spectrum gets more complex, although its fine structure is still retained (in the case of a straight wire or a flat quantum well, a single line corresponding to a zero value of the total exciton momentum would be present).

Next, consider a so-called Π element (Fig. 2). Two identical potential wells correspond to it, being *a* apart. The resonance level splitting gives a two-level system, all characteristic parameters of which are regulated during its manufacture (a mechanical q-bit). A meander type Π -element chain (Fig. 3) is a combination of q-bits; communication among them may take place by, for example, the exchange of phonons of a surface acoustic wave (SAW) of an appropriate frequency. By applying mechanical force to the substrate whereupon the wire is placed one can deform the particular meander links, resulting in shifts of the energy levels in wells and making possible the tuning of the chain elements in or out of resonance with the SAW. The building of three-dimensional structures of mechanical q-bits is obviously possible as well.



Figure 2. A two-level system in a Π element.



Figure 3. A q-bit chain (a meander).



Figure 4. A mechanical electron interferometer.

Yet another variant of the connection between mechanical and electronic degrees of freedom is illustrated in Fig. 4. This is a mechanical electron interferometer. By bending one of its arms we create a geometric potential in it, resulting in the phase shift of the wave function of electrons passing through the bent arm. For $k_F R \ge 1$, the phase shift $\Delta \Phi$ may be estimated as $\Delta \Phi \sim \theta/8k_F R$, where θ is the bending angle, and k_F is the Fermi electron wavenumber. In the opposite limiting case, when $k_F R \le 1$, the result is quite simple: $\Delta \Phi = \theta/2$.

In conclusion, consider an example of a 2D-electron system on a surface with two significantly different principal curvatures. Here, we are dealing with a bent nanotube (NT). Introducing the NT axial arc length *s* and azimuth angle φ in its sectional plane as a coordinate system, we get the Hamiltonian

$$\hat{H} = -\frac{1}{2m} \left[\frac{1}{ah} \frac{\partial}{\partial \varphi} \left(\frac{h}{a} \frac{\partial}{\partial \varphi} \right) + \frac{1}{h} \frac{\partial}{\partial s} \left(\frac{1}{h} \frac{\partial}{\partial s} \right) \right] -\frac{1}{8m} \left[\frac{1}{a} - \frac{\cos \varphi}{R(s) + a \cos \varphi} \right]^2, \quad h = 1 + \frac{a \cos \varphi}{R(s)}. \quad (23)$$

Here, *a* is the NT radius, and R(s) is the radius of curvature of its axis at a point *s*.

The NT bend removes the energy level degeneracy with respect to the sign of the azimuth quantum number M. The situation is analogous to Λ -doubling in a spectrum of diatomic molecules: the splitting of the $\pm M$ states is achieved in the 2M-th order of the perturbation theory. The small parameter is the ratio a/R. Approximating a bent NT by an arc of torus measuring L in length, we get for $M = \pm 1$:

$$|E_{+1,n} - E_{-1,n}| = \frac{1}{2mR^2} \left(Q_k^4 a^4 + \frac{3}{4} Q_k^2 a^2 - \frac{3}{16} \right), \quad (24)$$

where $Q_k = k\pi/L$, k = 1, 2, ... The line of an intra- or interband optical transition, in which subband with |M| = 1 participates, splits accordingly.

The second consequence of the NT bend is a change in its ballistic conductance, for the bend area acts as an electron scatterer. More exactly, the transmission factor of a bent NT differs from unity even in the absence of impurities or defects. Consider the NT asymptotically straight — that is, $R(s) \rightarrow \infty$ as $s \rightarrow \pm \infty$, and, besides that, $dR/ds \ll 1$, so that the bend is smooth enough. This enables an adiabatic approximation to

smooth enough. This enables an adiabatic approximation to be applied, with φ being the fast variable, and *s* the slow one. The wave function is sought for as the expansion $\sum c_i(s) \chi_i(\varphi, s)$, where χ_i are the instantaneous eigenfunctions of the Hamiltonian (23), in which *s* is considered a parameter. The interesting peculiarity of this problem is the dependence of the coefficient of the slow part of the NT Hamiltonian (with d/ds derivatives) on the fast variable: *h* depends on φ . Therefore, even in the zero-th adiabatic approximation $(\partial \chi_i/\partial s = \partial^2 \chi_i/\partial s^2 = 0)$, the set of equations for the slow amplitudes $c_i(s)$ is not uncoupled as usually takes place in other adiabatic problems. In this case, the effective mass actually becomes a matrix (dependent on *s*, of course):

$$-\frac{1}{2}\sum_{j}\left\langle\frac{1}{m}\right\rangle_{ij}\frac{\partial^{2}c_{j}}{\partial s^{2}}+\epsilon_{i}(s)c_{i}(s)=Ec_{i}(s),$$
$$\left\langle\frac{1}{m}\right\rangle_{ij}=\frac{1}{m}\int\chi_{i}^{*}h^{-2}(\varphi,s)\chi_{j}\,\mathrm{d}\varphi,\qquad(25)$$

where $\epsilon_i(s)$ are the instantaneous terms. Thus, the bend brings about not only electron wave reflection, but also intersubband transitions, while the energy is conserved.

In an ideal straight NT, the transmission factor equals unity at any energy value exceeding the subband bottom level, and the dependence of the longitudinal conductance on the Fermi level $G(E_F)$ is given by the well-known step function with discontinuities at the subband edge points, $E = BM^2$, where $B = 1/2ma^2$ is a rotational quantum.

The analysis of equations (25) leads us to the following conclusions. For $E_{\rm F} < B$, when only the subband M = 0 is populated, the transmission factor is T(E) = E/(E+C), C being dependent on the bend shape and not on the particle energy. Thus, at small $E_{\rm F}$ the conductance $G(E_{\rm F})$ is 'turned on' linearly. The following steps in $G(E_{\rm F})$ are smeared as $\sqrt{E_{\rm F} - BM^2}$, (|M| = 1, 2, ...), corresponding to passing over the potential wall at small energy excess (a slow particle in a finite state). This contribution comes from the intersubband transitions and is a principle one in the threshold range $0 < E_{\rm F} - BM^2 \ll aB/R$.

This report is based on our publications [9-13].

The work has been supported by RFBR grant No. 05-02-16939, the Support Program for Scientific Schools NSh-593.2003.2, as well as by the RAS and the RF Ministry of Science and Technology programs.

References

- 1. Prinz V Ya et al. Physica E 6 828 (2000); Nanotechnology 12 399 (2001)
- 2. Schmidt O G, Eberl K Nature 410 168 (2001)
- 3. Jensen H, Koppe H Ann. Phys. (New York) 63 586 (1971)
- 4. da Costa R C T Phys. Rev. A 23 1982 (1981)
- 5. Ogawa N, Fujii K, Kobushukin A Prog. Theor. Phys. 83 894 (1990)
- Magarill L I, Romanov D A, Chaplik A V Zh. Eksp. Teor. Fiz. 110 669 (1996); 113 1411 (1998) [JETP 83 361 (1996); 86 771 (1998)]; Magarill L I, Chaplik A V Zh. Eksp. Teor. Fiz. 115 1478 (1999) [JETP 88 815 (1999)]
- Leadbeater M L et al. J. Phys.: Condens. Matter 7 L307 (1995); Phys. Rev. B 52 R8629 (1995)

- Bykov A A et al. Pis'ma Zh. Eksp. Teor. Fiz. 74 182 (2001) [JETP Lett. 74 164 (2001)]
- 9. Entin M V, Magarill L I Phys. Rev. B 64 085330 (2001)
- 10. Entin M V, Magarill L I Phys. Rev. B 66 205308 (2002)
- Magarill L I, Éntin M V Zh. Eksp. Teor. Fiz. 123 867 (2003) [JETP 96 766 (2003)]
- 12. Chaplik A V, Blick R H New J. Phys. 6 33 (2004)
- Chaplik A V Pis'ma Zh. Eksp. Teor Fiz. 80 140 (2004) [JETP Lett. 80 130 (2004)]

PACS numbers: 72.15.Gd, 72.15.Rn, **73.63.-b**, 73.63.Bd, 73.63.Fg DOI: 10.1070/PU2005v048n09ABEH005733

Heterogeneous electronic states in carbon nanostructures with different dimensionalities and curvatures of the constituent graphene layers

A I Romanenko, A V Okotrub, V L Kuznetsov, A S Kotosonov, A N Obraztsov

1. Introduction

Production of skeleton carbon nanostructures is always accompanied by curving the constituent graphene layers. New properties result that are not characteristic of the graphite composed of the plane graphene layers. The most brightest display of graphene layer-curvature is the existence of a superconducting state in the bundles of single-layer carbon nanotubes 10 Å in diameter (with the radius of curvature r = 5 Å) at the temperature $T_c \sim 1$ K [1], and the presence of superconductivity in nanotubes 4 Å in diameter (r = 2 Å) at $T_c = 16 \text{ K}$ [2], whereas no superconducting transition is observed in graphite. None the less, Y Kopelevich et al. [3] stated that superconductivity in an ideal graphite must show itself and that in real graphite samples superconductivity was not observed due to omnipresent defects. It is our belief that superconducting state in skeleton carbon nanostructures is related to curvatures of graphene layers forming them.

In addition, the crystal structures of nanocrystallites, for instance, nano-onions, not only have curved surfaces but also have one-dimensional fibres of various lengths and curvatures [4]. This results in reduced dimensionalities of motion of charge carriers in such structures.

This report is concerned with experimental determination of the electron–electron interaction constant λ_c in carbon nanostructures based on curved graphene layers, and with the peculiarities of motion of charge carriers in systems composed of curved surfaces and one-dimensional fibres.

2. Methods of investigation

The general method of studying the electron-electron interaction constant has been a combined analysis of the quantum corrections to the electrical conduction, magnetic conductance and magnetic susceptibility of the investigated samples. All graphene-layer-based skeleton nanostructures usually possess structural defects resulting in charge carrier diffusion at low temperatures. The quantum corrections to kinetic and thermodynamic quantities due to quantum interference are therefore observed in them at a low enough temperature. For single-particle processes (localization effects, LEs [5, 6]), this is the interference of wave functions of an electron proceeding along the closed trajectories in opposite directions (for path lengths *l* smaller than the phase interruption length $L_{\varphi}(T) = (D\tau_{\varphi})^{1/2}$, where *D* is the diffusion coefficient, and τ_{φ} is the phase interruption time). As a consequence, the full conductance decrease: when the temperature decreases, $L_{\varphi}(T)$ grows and the conductance goes down.

In a magnetic field, the additional phase shift of various signs are added, depending on the direction round of closed trajectory. The interference is therefore suppressed provided that $L_B = (\hbar c/2eB)^{1/2} < L_{\varphi}$, resulting in a negative magnetoresistance (NMR) - that is, the conductance increases in a magnetic field. Electron - electron interaction effects (IE) [7] also produce quantum corrections. In this case, at a repeat interaction of two electrons at distances less than the interference length $L_{\text{int}} = (D\hbar/k_{\text{B}}T)^{1/2} (L_{\text{int}} \text{ is the distance})$ through which information about the electron phase change in the course of previous interaction have not yet lost), the repeat interaction will depend on their previous one. The effective density of states $v_{\rm F}$ on the Fermi surface therefore proves to be renormalized. The interaction effects contribute not only to electrical conduction, but also to the thermodynamic quantities dependent on $v_{\rm F}$, namely, the magnetic susceptibility γ , and the heat capacity. Contrary to corrections to electrical conduction and magnetoresistance, the corrections to thermodynamic quantities are due to EC effects only.

To determine the effective dimensionality of motion of the charge carriers, we have used combined analysis of temperature dependences of electrical conduction and magnetoresistance in the conditions of variable range hopping conduction.

3. Arc-produced multiwall carbon nanotubes

A distinguishing feature of multiwall carbon nanotubes (MWNTs) that were produced at the Institute of Inorganic Chemistry, SB RAS [8, 9] with an electric-arc technology is the presence of nanotube bundles preferentially oriented in a plane perpendicular to the electric arc axis, therefore the MWNT-based bulk samples possess an anisotropy of electrical conductivity: $\sigma_{||}/\sigma_{\perp} \sim 100$ [8, 9], where $\sigma_{||}$ is the electrical conductivity in the plane of the preferred orientation of nanotube bundles, and σ_{\perp} is the electrical conductivity in the direction normal to this plane. The mean diameter of a single nanotube is $d \sim 140$ Å. According to the electron paramagnetic resonance data, our samples contain less than $10^{-6}\%$ of paramagnetic impurities, thus excluding the impurity contribution to the susceptibility observed. Bromination of MWNTs in bromine vapors at room temperature [9] produces a sample of CBr_{0.06} chemical composition and results in a conductivity increase due to the higher concentration of hole (p-type) charge carriers. The corrections to orbital susceptibility $\delta \chi_{orb}$ in the Cooper channel were theoretically predicted [7] to be the main contributors to quantum corrections to magnetic susceptibility $\chi(T, B)$ in the magnetic fields below $B_{\rm c} = (\pi k_{\rm B} T/g\mu_{\rm B})^{1/2} (B_{\rm c} = 9.8 \text{ T})^{1/2}$ at T = 4.2 K). These corrections are determined by the value and sign of the electron – electron interaction constant λ_c and are proportional to the diamagnetic susceptibility χ_{orb} of electrons. Since the diamagnetic susceptibility of graphites and multiwall carbon nanotubes is greater than that of any