THERMODYNAMIC FUNCTIONS OF ELECTRONS IN KANE TYPE SEMICONDUCTOR TUBE

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The energy spectrum and heat capacity of Kane electrons on the surface of a nanotube in a longitudinal magnetic field are investigated for degenerate electron gas. It was shown, that at low temperatures, the specific heat of electrons on the surface of the tube varies linearly with temperature.

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Low-dimensional systems based on semiconductors have been the object of great interest for many years since there are numerous applications in technology based on these systems. The interest of scientists in semiconducting heterostructures, quantum dots [1,2], and nanosystems on curved surfaces increases.

In the paper, Ermolaev [3] thermodynamic functions have been calculated in the effective mass approximation for degenerate and nondegenerate electron gases on the semiconductor cylindrical nanotube surface in a longitudinal magnetic field.

An analytical expression for the energy of a relativistic electron on a nanotube in an external magnetic field was obtained using the Dirac equation in [4]. Using this energy spectrum, the thermodynamic functions of the nanotube at low and high temperatures were calculated. The thermodynamic and magnetic properties of electrons in superlattices on the surface of a nanotube in a longitudinal magnetic field are investigated in Ref. [5].

A standard nanotube model is used: a sheet of 2D electron gas rolled into a cylinder with metallic conductivity. The peculiarity of this model system is that it allows us to obtain an exact solution to the problem of the electron energy spectrum.

In this work, using a three-band Kane's model including the conduction band, light, and spin–orbital hole bands, the energy spectrum of carriers on the surface of a tube in a vertical magnetic field is derived.

In the three-band Kane's Hamiltonian, the valence and conduction bands interaction is taken into account via the only matrix element P (the so-called Kane's parameter). The system of Kane equations including the nondispersional heavy hole bands has the form [6]:

$$-EC_1-\frac{Pk_-}{\sqrt{2}}C_3+\sqrt{\frac{2}{3}}Pk_zC_4+\frac{Pk_+}{\sqrt{6}}C_5+\frac{Pk_z}{\sqrt{3}}C_7+\frac{Pk_+}{\sqrt{3}}C_8=0 \tag{1}$$

$$-EC_2-\frac{Pk_-}{\sqrt{6}}C_4+\sqrt{\frac{2}{3}}Pk_zC_5+\frac{Pk_+}{\sqrt{2}}C_6+\frac{Pk_-}{\sqrt{3}}C_7-\frac{Pk_z}{\sqrt{3}}C_8=0 \tag{2}$$

$$-\frac{Pk_+}{\sqrt{2}}C_1-(E+E_g)C_3=0 \tag{3}$$

$$\sqrt{\frac{2}{3}}Pk_zC_1-\frac{Pk_+}{\sqrt{6}}C_2-(E+E_g)C_4=0 \tag{4}$$

$$\sqrt{\frac{2}{3}}Pk_zC_2+\frac{Pk_-}{\sqrt{6}}C_1-(E+E_g)C_5=0 \tag{5}$$

$$\frac{Pk_-}{\sqrt{2}}C_2-(E+E_g)C_6=0 \tag{6}$$

$$\frac{Pk_z}{\sqrt{3}}C_1+\frac{Pk_+}{\sqrt{3}}C_2-(\Delta+E+E_g)C_7=0 \tag{7}$$

$$\frac{Pk_-}{\sqrt{3}}C_1-\frac{Pk_z}{\sqrt{3}}C_2-(\Delta+E+E_g)C_8=0 \tag{8}$$

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Here P is the Kane parameter, E_g the band gap energy, Δ the value of spin–orbital splitting, and $k_{\pm} = k_x \pm ik_y$, C_i are envelope functions. The zero of energy is chosen at the bottom of the conduction band. For a uniform magnetic field H directed along the z-axis, the vector potential may be chosen in the form

$$\vec{A} = \left(-\frac{H.y}{2}, \frac{H.x}{2}, 0 \right) \tag{9}$$

$k_{\pm}$ have the forms

$$k_{\pm} \to k_{\pm} \pm i\frac{1}{2}\lambda_H r_{\pm} \tag{10}$$

where

$$r_{\pm} = x \pm iy, \quad \lambda_H = \frac{eH}{\hbar c} \tag{11}$$

Substituting expressions (3)–(8) into formulas (1) and (2), and using relations (9), (10) we obtain two coupled equations for the spin-up and the spin-down conduction band:

$$\begin{pmatrix} -E + \frac{P^2}{3}\left(\frac{2}{E+E_g} + \frac{1}{E+E_g+\Delta}\right)\left(-\nabla^2 + \lambda_H L_z + \frac{1}{4}\lambda_H^2\rho^2\right) \\ \pm \frac{P^2\lambda_H}{3}\left(\frac{1}{E+E_g} - \frac{1}{E+E_g+\Delta}\right) \end{pmatrix} C_{1,2} = 0 \tag{12}$$

where L_z z component of angular momentum operator and $\rho^2 = x^2 + y^2$, ∇^2 is the three-dimensional Laplacian. In cylindrical coordinates the eigenfunctions

$$C_{1,2} = A\exp(im\varphi + ik_z z)\,Q_{1,2} \tag{13}$$

where A is a normalization factor and the energy spectrum of carriers in a Kane-type semiconductor tube is satisfies

$$\frac{3}{P^2}\frac{E\left(E+E_g\right)\left(E+E_g+\Delta\right)}{3E+3E_g+2\Delta} = \frac{\left(m+\frac{1}{2}\lambda_H\rho^2\right)^2}{\rho^2} + k_z^2 \pm \lambda_H \frac{\Delta}{3E_1+3E_g+2\Delta} \tag{14}$$

Here the magnetic quantum number m has the values $m = 0, \pm1, \pm2, \ldots$.For the strong spin-orbit approximation, $\Delta \to \infty$ Eq. (14) transforms as

$$E(E+E_g) = \frac{2P^2}{3}\left(\frac{1}{\rho^2}\left(m + \frac{1}{2}\lambda_H\rho^2\right)^2 + k_z^2 \pm \lambda_H \frac{1}{2} \right) \tag{15}$$

The matrix element P^2 is expressed in terms of the effective mass of electrons m_n as

$$\frac{2P^2}{3E_g} = \frac{\hbar^2}{2m_n} \tag{16}$$

If we choose zero of energy in the middle of the energy gap $E \to E - \frac{E_g}{2}$ we find the energy levels of electrons (sign +) and light holes

$$E = \pm\sqrt{\frac{E_g^2}{4} + \frac{\hbar^2 E_g}{2m_n\rho^2}\left[\left(m+f\right)^2 \pm f + k_z^2\rho^2\right]} \tag{17}$$

The energy spectrum is a sequence of one-dimensional subbands with the number m.
where

$$f = \frac{\rho^2 \lambda_H}{2} = \frac{\Phi}{\Phi_0} \qquad (18)$$

$\Phi = \pi\rho^2 H$ is the magnetic flux and $\Phi_0 = \frac{2\pi\hbar}{e}$ is the flux quantum. As seen from Eq. (17) the energy spectrum of electrons in the surface tube is not additive. Under the radical is the square of the energy of the longitudinal motion of the Kane electron in the tube and the square of the energy of a charged rotator in a magnetic field.

For the energy spectrum (17) the density of states of a Kane-type nanotube can be written as

$$g(E) = \sum_{lk_z\sigma} \delta\left(E - E_{lk_z\sigma}\right) = \frac{LE}{\pi}\sqrt{\frac{2m_n}{\hbar^2 E_g}}\sum_{m\sigma}\frac{\Theta(E-u_{m\sigma})}{\sqrt{E^2-u_{m\sigma}^2}} \qquad (19)$$

where $\Theta(x)$ is the Heaviside function and

$$u_{m\sigma} = \sqrt{\frac{\hbar^2 E_g}{2m_n\rho^2}\left[\left(m+f\right)^2+\sigma f\right]+\frac{E_g^2}{4}};\sigma=\pm1 \qquad (20)$$

As seen from Eq.(19) the density of states has a singularity, when energy coincides with $u_{m\sigma}$ it is convergent to infinity. Using the density of states (19) we can calculate the number of electrons N, their energy E, chemical potential, and heat capacity C. We consider degenerate electron gas at the surface in Kane type of semiconductor nanotube. The total number of electrons can be found as follows.

$$N = \sum_{mk_z\sigma} f\left(E\right) = \frac{L}{2\pi}\sum_{mk_z\sigma}\int_{-\infty}^{\infty} f\left(E\right)\frac{dk_z}{dE}dE = \int_{u_{m\sigma}}^{\infty} f(\mathrm{E})g\left(E\right)dE \qquad (21)$$

where f(E) Fermi-Dirac distribution functions. The total energy of electrons

$$U = \int_0^\infty Eg(E)f(E)dE \qquad (22)$$

At zero temperature the number of electrons

$$N = \int_u^\mu g(\mathrm{E})dE \qquad (23)$$

After integration we get

$$N = \frac{L}{\pi}\sqrt{\frac{2m_n}{\hbar^2 E_g}}\sum_{m\sigma}\sqrt{\mu^2-u_{m\sigma}^2} \qquad (24)$$

the energy of electrons in Kane type nanotube according to (22)

$$U = \frac{L}{\pi}\sqrt{\frac{2m_n}{\hbar^2 E_g}}\sum_{m\sigma}\left(\frac{1}{2}\mu\sqrt{\mu^2-u_{m\sigma}^2}+u_{m\sigma}^2 Arcch\frac{\mu}{u_{m\sigma}}\right) \qquad (25)$$

By using the Sommerfeld method [7] we find temperature correction of the energy of electrons in nanotube

$$\delta E(\mathrm{T}) \approx \frac{\pi^2 k_B^2 T^2}{6}\left(\mu g'(\mu)+\mathrm{g}(\mu)\right) \qquad (26)$$

Expressing μ in (26) using the zero-order approximation $\mu = \mu_0$. İf μ lies far from the borders of the subzones the specific heat of electrons at the surface nanotube is

$$C = \frac{2\pi^2 k_B^2 T}{3} g(\mu) \quad (27)$$

From these formulas, it is seen that with the change in the magnetic field, every time the u_m coincides with the Fermi boundary the heat capacity experiences a sharp jump, i.e. has a peculiarity.

CONCLUSIONS

The thermodynamic functions of degenerate electrons on the surface of Kane-type semiconductor nanotubes in a longitudinal quantizing magnetic field are calculated. It has been observed that the specific heat and density of states oscillates as the magnetic field varies.

[1] *R. Saito, G. Dresselhaus, M.S. Dresselhaus.* Physical Properties of Carbon Nanotubes, Imperial College Press, London, 1998.

[2] *P.N. Dyachkov.* Electronic Properties and Application of Nanotubes, Binom. Laboratory of Knowledge, Moscow, 2012.

[3] *A.M. Ermolaev and G.I. Rashba.* J. Phys. Condens. Matter 20, 175212 (2008)

[4] *N.V. Gleizer, A.M. Ermolaev and G.I. Rashba.* International Journal of Modern Physics B Vol. 33, № 22 (2019) 1950253

[5] *A.M. Babanlı.* Low Temperature Physics, Fizika Nizkikh Temperatur, 2023, Vol. 49, № 2, pp. 220–224

[6] *F.M. Gashimzade, A.M. Babayev, S. Çakmak, Ş. Çakmaktepe.* Physica- E 23, Issues 1–2, June 2004, Pages 177-182

[7] *B.M. Askerov, S. Figarova.* Thermodynamic, Gibbs Method and Statistical Physics of Electron. Berlin: Springer Verlag, 2010, 374 p.

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