HEAT CAPACITY 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 are investigated. It is shown that for high temperatures the specific heat of Kane electrons on the surface of a nanotube is 4 times greater than the specific heat of the semiconductor nanotube with parabolic dispersion laws and for low temperatures the specific capacity is equal to $2k_B$.

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Recently, low-dimensional semiconductor systems have become the object of great interest due to their wide application in technology. Scientists are increasingly interested in semiconductor heterostructures with curved surfaces, quantum dots, and nanotubes.

The extraordinary electrical properties of nanotubes make them one of the main materials of nanoelectronics [1,2]. Nanometer-sized electronic devices are created based on nanotubes. Thermodynamic properties of the electron gas on the surface of a nanotube have been studied in Ref. [3]. 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].

In the work [4], authors utilized the Dirac equation to find the energy of electrons on the nanotube surface in the presence of a magnetic field. Using this energy spectrum, the thermodynamic functions of the nanotube at low and high temperatures were calculated. Rubens R.S. et al [5] calculated the thermodynamic properties of the quantum ring according to the solutions of both Dirac and Schrödinger equations. Ref. [6] Ermolaev studied the thermodynamic properties of degenerate and non-degenerate electron gas on the semiconductor nanotube surface in a magnetic field.

The heat capacity and magnetic properties of electrons in superlattices on the surface of the nanotube in a magnetic field orientated along the axis of the nanotube were studied in [7]. In paper [8], the energy spectrum of the one-dimensional Kane oscillator was found, and it was found that the heat capacity is four times larger than the heat capacity of the one-dimensional harmonic oscillator at high temperatures.

Ref. [9] studied the heat capacity and magnetic moment of a lattice of non-interacting nanotubes in a magnetic field.

In this paper, the standard tube model is used: a sheet of non-interacting 2D electron gas is twisted into a tube shape. This model allows us to obtain the energy spectrum of electrons on the nanotube surface. In this study, we used the Kane model, which takes into account the interaction of the conduction and the valence bands. Kane's model allows us to express the energy spectra of electrons, light holes, and spin-orbital splitting holes on the surface of the nanotube. Using the energy spectrum of carriers on the surface of a tube calculated the heat capacity of non-degenerate electrons in a Kane-type semiconductor tube. The study of the heat capacity of objects is very important in physics since the specific heat depends on the internal state of the substance and the movement of its constituent particles.

We consider a non-interacting two-dimensional electron gas on the nanotube surface out of Kane type semiconductor. The Kane equations has the form [10]:

$$-EC_1-\frac{Pk_-}{\sqrt{2}}C_3+\sqrt{\frac{2}{3}}Pk_zC_4+\frac{Pk_+}{\sqrt{6}}C_5+\sqrt{\frac{1}{3}}Pk_zC_7+\frac{Pk_+}{\sqrt{3}}C_8=0 \quad (1)$$

$$-EC_2-\frac{Pk_-}{\sqrt{6}}C_4+\sqrt{\frac{2}{3}}Pk_zC_5+\frac{Pk_+}{\sqrt{2}}C_6+\frac{Pk_-}{\sqrt{3}}C_7-\sqrt{\frac{1}{3}}Pk_zC_8=0 \quad (2)$$

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

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

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

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

$$\frac{Pk_+}{\sqrt{3}}C_2+\sqrt{\frac{1}{3}}Pk_zC_1-\left(E+E_g+\Delta\right)C_7=0 \tag{7}$$

$$\frac{Pk_-}{\sqrt{3}}C_1-\sqrt{\frac{1}{3}}Pk_zC_2-\left(E+E_g+\Delta\right)C_8=0 \tag{8}$$

The parameter P characterizes the interaction between the conduction and valence bands. E_g the band gap energy, Δ the value of spin–orbital splitting, and $k_\pm=k_x\pm ik_y$ $\vec{k}=i\vec{\nabla}$, C_i are envelope functions. Substituting expressions (3)–(8) into formulas (1) and (2) we obtain

$$\left\{-E-\frac{P^2}{3}\left[\frac{2}{E+E_g}+\frac{1}{E+E_g+\Delta}\right]\Delta_3\right\}C_{1,2}=0 \tag{9}$$

where Δ_3 is the three-dimensional Laplacian. In cylindrical coordinates the eigenfunctions

$$C_{1,2}=A\exp(im\varphi+ik_zz)Q_{1,2} \tag{10}$$

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

$$\left(\frac{3}{P^2}\frac{E(E+E_g)(E+E_g+\Delta)}{(3E+3E_g+2\Delta)}-\left(\frac{m^2}{\rho^2}+k_z^2\right)\right)^2=0 \tag{11}$$

As can be seen from the formula (11), the energy spectra of charge carriers are doubly degenerate.
For the strong spin-orbit approximation $\Delta\to\infty$ Eq. (11) transforms as

$$E(E+E_g)=\frac{2P^2}{3}\left(\frac{m^2}{\rho^2}+k_z^2\right) \tag{12}$$

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

$$\frac{2P^2}{3E_g}=\frac{\hbar^2}{2m_n} \tag{13}$$

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

$$E=\pm\sqrt{\frac{E_g^2}{4}+\frac{\hbar^2E_g}{2m_n}\left(\frac{m^2}{\rho^2}+k_z^2\right)} \tag{14}$$

The expression inside the square root is the sum of the square of the energy of the motion of the electron along the axis of the tube and the square of the energy of the charged rotator in the magnetic field. The canonical partition function is defined as

$$z=\sum_{mk_z} e^{-\beta E_{mk_z}} \tag{15}$$

$\beta=(k_B T)^{-1}$, k_B −is the Boltzmann constant. The summation over k_z can be transformed into integral as:

$$z=\sum_{mk_z} e^{-\beta E_{m\sigma k_z}}=\frac{L}{2\pi}\sum_m \int_0^\infty dk_z e^{-\beta\sqrt{\frac{\hbar^2 E_g}{2m_n}k_z^2+u_m^2}} \tag{16}$$

where

$$u_m=\sqrt{\frac{E_g^2}{4}+\frac{\hbar^2 E_g}{2m_n\rho^2}} \tag{17}$$

The integral over k_z can be calculated by substituting

$$k_z=\left(\frac{\hbar^2 E_g}{2m_n}\right)^{-\frac{1}{2}} u_{m\sigma} sh\theta \tag{18}$$

By using the following formula [11]

$$K_\nu(x)=\int_0^\infty d\theta ch(\nu\theta) e^{-xch\theta} \tag{19}$$

we find the partition function as

$$z=\frac{L}{2\pi}\left(\frac{\hbar^2 E_g}{2m_n}\right)^{-\frac{1}{2}}\sum_m u_m K_1(\beta u_m) \tag{20}$$

If we ignore the quantization of the circular motion and go from summation to integration for the quantum number m, we get

$$\sum_{m=-\infty}^{\infty}\to\int_{-\infty}^{\infty} dt \tag{21}$$

where

$$t=\sqrt{\left(u^2-\frac{E_g^2}{4}\right)\left(\frac{\hbar^2 E_g}{2m_n\rho^2}\right)^{-1}} \tag{22}$$

We use the following formula [12]

$$\int_a^\infty x^{1\pm\nu}\left(x^2-a^2\right)^{\beta-1}K_\nu(cx)dx=2^{\beta-1}c^{-\beta}\Gamma(\beta)K_{\nu\pm\beta}(ac) \tag{23}$$

We have the partition function as

$$z=\frac{L}{\pi\rho}\left(\frac{\hbar^2}{2m_n\rho^2}\right)^{-1}2^{-\frac{1}{2}}\left(\frac{E_g}{2}\right)^{\frac{1}{2}}\Gamma\left(\frac{1}{2}\right)\beta^{-\frac{1}{2}}K_{3/2}\left(\beta\frac{E_g}{2}\right) \tag{24}$$

The heat capacity is defined as

$$C=k_B\beta^2\frac{\partial^2}{\partial\beta^2}\ln z \tag{25}$$

If $\beta\frac{E_g}{2}$ <<1, we should use [11]

$$K_\nu(x)\approx\frac{1}{2}\Gamma(\nu)\left(\frac{x}{2}\right)^{-\nu} \tag{26}$$

From (25) we find $C=2k_B$ at $T\to\infty$. Since the energy spectrum of the Kane electrons is 2-fold degenerate, the specific heat of Kane electrons is 4 times greater than the specific heat of the semiconductor nanotube with parabolic dispersion laws [9]. If $\beta \frac{E_g}{2}$ >>1 we can use the asymptotic formula

$$K_\nu\left(x\right) \approx \sqrt{\frac{\pi}{2x}} e^{-x}\left(1+\frac{4\nu^2-1}{8x}\right) \qquad (27)$$

The heat capacity is now reduced $C = k_B$. Unlike tubes with a parabolic dispersion law, the specific heat of electrons in Kane tubes is 2 k_B at low temperatures.

CONCLUSIONS

In this work, the energy spectrum and heat capacities of electrons on the surface of Kane-type semiconductor tubes are calculated, taking into account the nonparabolicity energy spectrum of electrons. it is shown that the heat capacity is equal to 4 kB at high temperatures and 2 kB at low temperatures.

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