HEAT CAPACITY OF ONE-DIMENSIONAL KANE OSCILLATOR

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We investigate the one-dimensional Kane oscillator in a thermal bath. We found that the heat capacity is four times greater than the heat capacity of the one-dimensional harmonic oscillator for higher temperatures.

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PACs: 71.24.+q, 73.22.Fg, 73.61.Ey.

1. INTRODUCTION

It is well known that the exact energy eigenvalues of the bound state play an important role in quantum mechanics. The non-relativistic harmonic oscillator remains the most typical example of these solvable systems and several authors have attempted to formulate for it an analogous relativistic extension.
This has led to the construction of the so-called Dirac oscillator, as initially introduced by Ito et al.[1] and later revived by Moshinsky and Szczepaniak.[2]. They gave it the name Dirac oscillator because it reduces to the standard harmonic oscillator with a strong spin-orbit coupling in the non-relativistic limit. The parabolic confining potential can be introduced through the so-called minimal substitution [2]:

$$\vec{p} = \vec{p} - i\beta\omega\vec{r} \tag{1}$$

where β is the diagonal matrix with the elements ±1. Here, we applied the above approach in deriving the oscillatory equation from the Kane 6-band Hamiltonian, in which the interaction between the valence and conduction bands is considered through a single matrix element of the Kane parameter P [3]. We referred to the obtained equation as the Kane oscillator by analogy with the Dirac oscillator. In the case Dirac equation, we do not include a harmonic potential in the usual way, as we do for the non-relativistic quantum mechanical harmonic oscillator. Instead, we start postulating a rather odd form for vector potential.
The energy spectrum of electrons in narrow-gap semiconductors (NGS) is analogous to that of relativistic electrons in a vacuum [4]. The energy spectrum and wave functions of the Kane oscillator were determined in the paper [5].
The paper [6] proposed a class of exactly solvable relativistic systems and found that the generalized (1 + 1)- dimensional Dirac oscillator in an electric field. In the paper **[7] authors** were considering the thermal properties of one-dimensional Dirac in the framework of the theory of superstatistics. The paper [8] analyzed the one-dimensional Dirac oscillator in a thermal bath and found that the heat capacity is two times greater than the heat capacity of the one-dimensional harmonic oscillator for higher temperatures.
Authors of the paper [9] studied (2+1)-dimensional Dirac oscillator in the presence of a transverse external magnetic field by defining suitable creation and annihilation operators in terms of properly chosen canonical pairs of coordinates and momenta.

2. THEORY

The non-relativistic harmonic oscillator potential is used for describing the confinement of quantum dots [10]. In this paper, we analyze the thermodynamic properties of a one-dimensional Kane oscillator. The Kane equations described the spectra of carriers in A_3B_5 type semiconductors. In the three-band Hamiltonian, the valence and conduction bands interaction is taken into account via the only matrix element. Let us consider the case in plane wave vector $k_x = k_y = 0$. For these states, the Kane Hamiltonian has the form [3,5]:

$$H = \begin{pmatrix} E_g - E & 0 & 0 & \sqrt{\frac{2}{3}}Pk_z & 0 & 0 \\ 0 & E_g - E & 0 & 0 & \sqrt{\frac{2}{3}}Pk_z & 0 \\ 0 & 0 & -E & 0 & 0 & 0 \\ \sqrt{\frac{2}{3}}Pk_z & 0 & 0 & -E & 0 & 0 \\ 0 & \sqrt{\frac{2}{3}}Pk_z & 0 & 0 & -E & 0 \\ 0 & 0 & 0 & 0 & 0 & -E \end{pmatrix} \tag{2}$$

Here P is the Kane parameter, E_g the band gap energy $k_z = -i\partial_z$. The zero energy is chosen at the bottom of the conduction band. Replacing operator

$$k_z \to k_z + i\beta \frac{m_e\omega}{\hbar} z \tag{3}$$

where

$$\beta_{11} = \beta_{22} = 1, \beta_{33} = \beta_{44} = \beta_{55} = \beta_{66} = -1 \tag{4}$$

The wavefunctions of the Hamiltonian in equation (2) can be expressed as a four-spinor wavefunction $\Psi = (\Phi_1, \Phi_2, \Phi_3, \Phi_4, \Phi_5, \Phi_6)^T$. By solving the Kane equation $(H - E)\Psi = 0$, we obtain the following two equations for heavy holes, electrons, and light holes:

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$E_{hh}=0$

$$\left(E_g - E + \frac{2}{3}\frac{P^2}{E}\left(k + i\frac{m_e\omega}{\hbar}z\right)\left(k - i\frac{m_e\omega}{\hbar}z\right)\right)\Phi_{1,2} = 0$$

The energy spectrum of the Kane oscillator is 2 times fold degenerate. Taking into account relationships [5]

$$\frac{2P^2}{3E_g} = \frac{\hbar^2}{2m_e} \tag{5}$$

we obtain

$$\left(\frac{(E_g - E)E}{E_g} + \left(\frac{P_z^2}{2m_e} + \frac{m_e\omega^2}{2}z^2 - \frac{\hbar\omega}{2}\right)\right)\Phi_{1,2} = 0 \tag{6}$$

This equation is similar to the Schrödinger equation for a one -dimensional harmonic oscillator, whose eigenvalues are given by

$$\frac{(-E_g + E)E}{E_g} + \frac{\hbar\omega}{2} = \hbar\omega\left(n + \frac{1}{2}\right) \tag{7}$$

From Eq. (7) we get

$$\frac{(-E_g + E)E}{E_g} = \hbar\omega n \tag{8}$$

If we choose zero of energy in the middle of the energy gap $E \to E + E_g/2$, the energy levels of electrons and light holes

$$E_{e,lh} = \pm\sqrt{\frac{E_g^2}{4} + n\hbar\omega E_g} \tag{9}$$

Given the energy spectrum of electrons, we can define the partition function as a sum of all possible states of the system

$$Z = \sum_{n\sigma} e^{-\beta E_{n\sigma}} = 2\sum_n e^{-\beta\sqrt{\frac{E_g^2}{4} + \hbar\omega E_g n}} \tag{10}$$

where $\beta = \frac{1}{k_B T}$, k_B is the Boltzmann constant and T is the thermodynamic equilibrium temperature, and factor 2 considers degeneracy for the spin. To evaluate this function, we use the Euler-MacLaurin formula defined as follows [11]:

$$\sum_{n=0}^{\infty} f(n) = \frac{1}{2}f(0) + \int_0^{\infty} f(x)dx - \sum_{p=1} \frac{1}{(2p)!}B_{2p} f^{(2p-1)}(0) \tag{11}$$

where are the B_{2p} Bernoulli numbers, $f^{(2p-1)}$ is the derivative of order (2p − 1). As a result, for the Kane oscillator statistical sum, we get:

$$Z = 2e^{-\beta\sqrt{b}}\left(\frac{1}{2} + \frac{2}{a\beta^2} + \frac{2\sqrt{b}}{a\beta} + \left(\frac{a}{24\sqrt{b}} - \frac{a^3}{1920b^{5/2}}\right)\beta - \frac{a^3}{1920b^2}\beta^2 - \frac{a^3\beta^3}{1920b^{3/2}}\right) \tag{12}$$

where $a = \hbar\omega E_g, b = \frac{E_g^2}{4}$. The heat capacity can be determined from the partition function [12],

$$C = k_B\beta^2 \frac{\partial^2 \ln Z}{\partial\beta^2} \tag{13}$$

The numerical values of the reduced specific heat $\frac{C}{k_B}$ of the one-dimensional Kane oscillator as a function of the reduced temperature are displayed in Fig. 1, $\frac{E_g}{4\hbar\omega} = 1$.

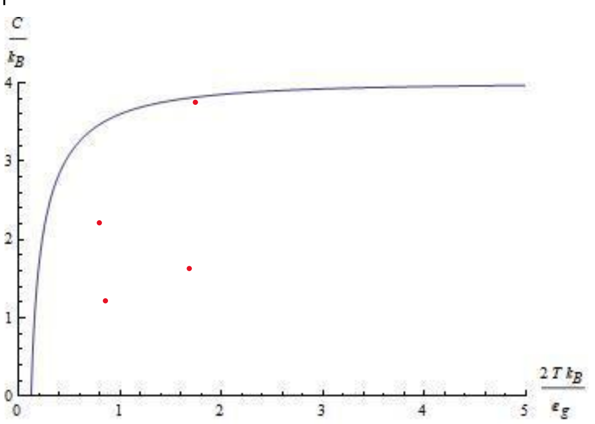

Fig.1. The reduced specific heat $\frac{C}{k_B}$ of the one-dimensional Kane oscillator as a function of the reduced temperature $\frac{2k_BT}{E_g}$ and $\frac{E_g}{4\hbar\omega} = 1$.

.From Fig. 1 it is also seen that the heat capacity for the Kane oscillator is forth times greater than the heat capacity for the harmonic oscillator, result that was anticipated by the analytical calculations presented above. Since the energy spectrum of the Kane oscillator is 2 folds degenerate, the specific heat of Kane electrons is 4 times the specific heat of harmonic oscillators. For high temperatures regime $\beta << 1$, the partition functions become

$$Z = 2e^{-\beta\sqrt{b}}\left(\frac{2}{a\beta^2}\right) \quad (14)$$

Using the partition function (14), the heat capacity for the Kane case can be written as:

$$C = 4k_B \quad (15)$$

In this work, we analyzed the Kane harmonic oscillator for electrons in one dimension. The heat capacity of Kane oscillators is investigated by employing the Euler-MacLaurin approximation.

3. CONCLUSIONS

In the present paper, we have found the complete energy spectrum of the Kane oscillator in one spatial dimension. It is shown that the specific heat of Kane electrons is 4 times greater than the specific heat of harmonic oscillators.

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[1] *M. Moshinsky and A. Szczepaniak*, J. Phys. A: Math. Gen. 22, L817, 1989.

[2] D. Ito, K. Mori, E. Carriere, Nuovo Cimento A 51, 1967, 1119.

[3] *T. Darnhofer and U. Rössler,* Phys. Rev. B 47 (23), 16020 (1993).

[4] *Wlodek Zawadzki1 and Tomasz M Rusin* J. Phys.: Condens. Matter 23, 2011, 143201 (19pp).

[5] *F. M. Gashimzade and A. M. Babaev,* Physics of the Solid State, Vol. 44, No. 1, 2002, pp. 162–163. Translated from Fizika Tverdogo Tela, Vol. 44, No. 1, 2002, pp. 155–156.

[6] *H.P. Laba1 and V.M. Tkachuk*, Eur. Phys. J. Plus (2018) 133: 279

[7] *Abdelmalek Boumali, Fadila Serdouk, Samia Dilmi,* Physica A: Statistical Mechanics and its Applications 553, 2020, 124207

[8] *M.H. Pacheco, R.R. Landim, C.A.S. Almeida,* Physics Letters A 311 (2003)

[9] *Bhabani Prasad Mandal, Shweta Verma,* Physics Letters A,374, 8, 2010, Pages 1021-1023

[10] *N. E. Kaputkina and Yu. E. Lozovik,* Fiz. Tverd. Tela (St. Petersburg) 40 (11), 1753 (1998) [Phys. Solid State 40, *1594 (1998)]*.

[11] *M.H. Pacheco, R.R. Landim, C.A.S. Almeida,* Physics Letters A 311 (2003) 93–96

[12] *T. Mishra, T.G. Sarkar, and J.N.Bandyopadhyay*, Phys. Rev E 89, 012103, 2014.