Thermal Broadening of the Density of States of the Quasi-Two-Dimensional Electron Gas With Non-Parabolicity of Energy Spectrum

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Abstract
In letter the analyses of the density of states in quasi two dimensional electron gas with of energy spectrum non-parabolicity are presented. It is shown that with increasing temperature due to thermal broadening of an abrupt change in the density of states and smoothed at high temperatures is completely blurred.

Keywords: *Quasi-two-electron gas, Density of states, Non-parabolicity of energy spectrum, hermal broadening.*

I. INTRODUCTION

Studying the behaviour of carriers in low dimensional systems such as quantum wells, wires and dots are extremely important [1]. It is known, that in such structures macroscopic characteristics associated density of states – is depend of the size of the structure, and these relationships are oscillatory in nature. It is now known that the oscillation characteristics of such systems depending on the size associated with the effects of size quantization. As the size of the structure increased the oscillation is decreased, and the structure behaves as a bulk material. Generally, the effects associated with the quantization of the energy spectrum of the charge carriers are observed in materials with high carrier mobility at low temperatures.

It is also known that the presence of crystal inhomogeneities, the electron-electron and electron-phonon interactions density of states (DOS) of the gas has difficult character, it can depend on the temperature $N(E,T)$ [2]. Only in the approximation of an ideal gas at low temperatures DOS has known energy dependence $N(E,0) \sim \sqrt{E}$

In [3] it is shown that the temperature dependence of DOS can be described by series expansion $N(E,T)$ in *GN*-function (defined as energy derived probability of filling the energy levels). In [4] study the DOS using a series expansion in *GN*-functions able to explain the temperature dependence of the DOS in quantizing magnetic fields.

The purpose of this work - is study of the temperature dependence of DOS of a quasi-two dimensional electron gas with non-parabolicity of energy spectrum. It will be shown that with increasing temperature, an abrupt change in the DOS gradually eroded, nonparabolicity of dispersion law manifests itself in a wide range of temperatures.

II. THE DENSITY OF STATES

According to the band theory of solids, the energy spectrum and the wave functions of the carriers in the two-dimensional semiconductor heterostructures are the solution of the stationary Schrödinger equation in the effective mass approximation [1]. The wave vector of electrons in a 2D-well can written the following relation

$$k^2 = k_\perp^2 + k_n^2, \quad k_\perp^2 = k_x^2 + k_y^2, \quad k_n = \frac{\pi n}{L}, \quad E_n = \frac{\hbar^2 \pi^2 n^2}{2m(0)L^2} = E_1 n^2 \tag{1}$$

There $m(0)$ - electron effective mass at the bottom of the conduction band, L - width of the well, $k_\perp$ - a module of the wave vector of the electron in the plane x, y; k_n is a z- component of the wave vector. Nonparabolicity of electron energy spectrum will be approximated by the following expression [5]

$$\chi(E) = E(1+\alpha E+\beta E^2) = \frac{\hbar^2 k^2}{2m(0)} = \frac{\hbar^2 \left(k_\perp^2 + k_n^2\right)}{2m(0)} \tag{2}$$

There α, β - nonparabolicity parameters. To find an expression for the density of states (DOS) of the gas we use the equation for the number of particles. It has the form (here $s = 2$, spin of electrons)

$$N = s\frac{L_x L_y}{(2\pi)^2}\sum_{n=1}^{\infty}\int dk_x dk_y\, f(E) = s\frac{L_x L_y}{2\pi}\sum_{n=1}^{\infty}\int_0^{\infty} kdk\, f(E) = s\frac{L_x L_y}{4\pi}\sum_{n=1}^{\infty}\int_0^{\infty} dk_{\perp}^2 f(E) =$$

$$= s\frac{L_x L_y}{4\pi}\frac{2m(0)}{\hbar^2}\sum_{n=1}^{\infty}\int_0^{\infty} d\left(\frac{\hbar^2 k_{\perp}^2}{2m(0)}\right) f(E) = \frac{L_x L_y}{\pi}\frac{m(0)}{\hbar^2}\sum_{n=1}^{\infty}\int_0^{\infty}\frac{\partial\chi(E)}{\partial E} f(E)\Theta[\chi(E)-E_n]\, dE \quad (3)$$

or

$$= \frac{L_x L_y}{\pi}\frac{m(0)}{\hbar^2}\sum_{n=1}^{\infty}\int_{\overline{E}_n}^{\infty}\frac{\partial\chi(E)}{\partial E} f(E) dE\,, \qquad \overline{E}_n \in \chi(E) \geq E_n\ . \quad (4)$$

Here, $f(E)$ is the Fermi-Dirac distribution function

$$f(E) = \frac{1}{e^{\frac{E-\mu}{T}}+1} \quad (5)$$

Let's express concentration of electrons through the DOS. Then from (3) we find

$$n_{3D} = \frac{N}{L_x L_y L} = \frac{m(0)}{\pi\hbar^2 L}\sum_{n=1}^{\infty}\int_0^{\infty}\frac{\partial\chi(E)}{\partial E} f(E)\Theta[\chi(E)-E_n]\, dE = \int_0^{\infty} N(E) f(E) dE$$

Hence we obtain the formula for DOS

$$N(E) = N_0\sum_{n=1}^{\infty}\frac{\partial\chi(E)}{\partial E}\Theta[\chi(E)-E_n], \qquad N_0 = \frac{m(0)}{\pi\hbar^2 L} \quad (7)$$

$$\frac{\partial\chi(E)}{\partial E} = 1 + 2\alpha E + 3\beta E^2, \quad (8)$$

$$N(E) = N_0\sum_{n=1}^{\infty}(1+2\alpha E+3\beta E^2)\Theta[E(1+\alpha E+\beta E^2)-E_n] \quad (9)$$

In the particular case, when $\alpha = \beta = 0$ we obtain the known formula corresponding parabolic dispersion [1]

$$N(E) = N_0\sum_{n=1}^{\infty}\Theta(E-E_n)\,. \quad (10)$$

We construct graphics of function $N(E)/N_0$ by formula (9) at $E_1 = 0.01\,\mathrm{eV}$, $\beta = 0,\quad \alpha = -0.1,\ 0,\ 0.1\,\mathrm{eV}^{-1}$.

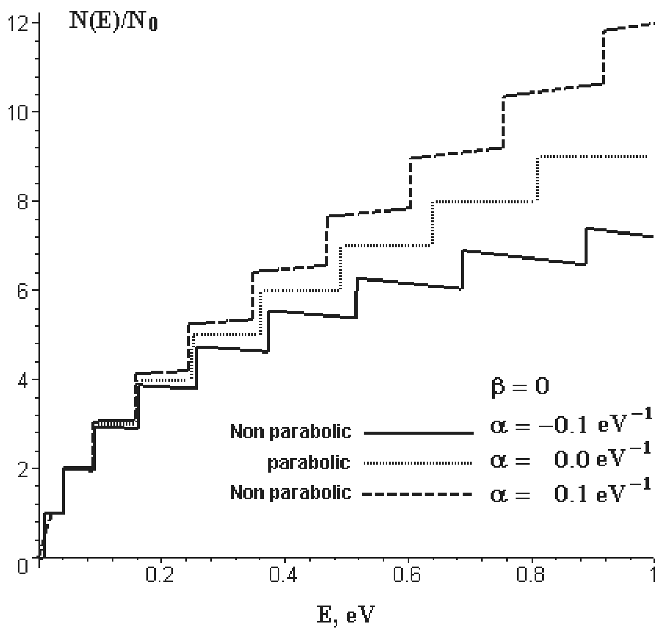

Fig.1. Energy Dependence of DOS for $E_1 = 0.01$ **eV,** $\beta = 0, \quad \alpha = -0.1,\ 0,\ 0.1\,\mathrm{eV}^{-1}$.

As can be seen from Fig.1 the DOS of a two-dimensional electron gas is highly dependent on the energy spectrum nonparabolicity. For negative values of the coefficient of nonparabolicity the DOS of two-dimensional electron gas is decreased in comparison with the parabolic case. Steps changes of DOS shifts toward higher energies. And this shift decreases monotonically with increasing energy. The horizontal sections steps leans toward smaller substations, the more nonparabolicity, the greater the slope.

With the disappearance of nonparabolicity slope disappears and the step becomes strictly horizontal position. At the positive values of α DOS increases with increasing energy. Thus, nonparabolicity strongly influences the position of the steps when α growing - step up and shifted towards lower energies.

III. THERMAL BROADENING

To account for the dependence of the DOS (9) with temperature is decomposed $N(E,T)$ into a series of derivative functions of the Fermi-Dirac energy $\partial f / \partial E$

$$N(E,T) = \int_0^\infty N(E',0)\frac{\partial f(E',E,T)}{\partial E}dE' \tag{11}$$

here

$$f = \frac{1}{\exp((E'-E)/T)+1}.$$

In this formula, $f(E)$ it is the probability of filling a discrete level E. At thermodynamic equilibrium $f(E)$ corresponds to the Fermi-Dirac function. When the system is non-equilibrium, it is determined by the form Shokley-Reed-Hall statistics and $\partial f / \partial E$ corresponds to GN function [3,4]

$$N(E,T) = \int_0^\infty N(E',0)GN(E',E,T)dE', \qquad GN(E',E,T) = \frac{1}{T}\exp\left[\frac{E'-E}{T} - \exp\left(\frac{E'-E}{T}\right)\right] \tag{12}$$

If conditions close to thermodynamic equilibrium filling of the energy levels is determined by the Fermi-Dirac function. The derivative of this function with respect to energy $\partial f/\partial E$ is a symmetric function of energy near μ.

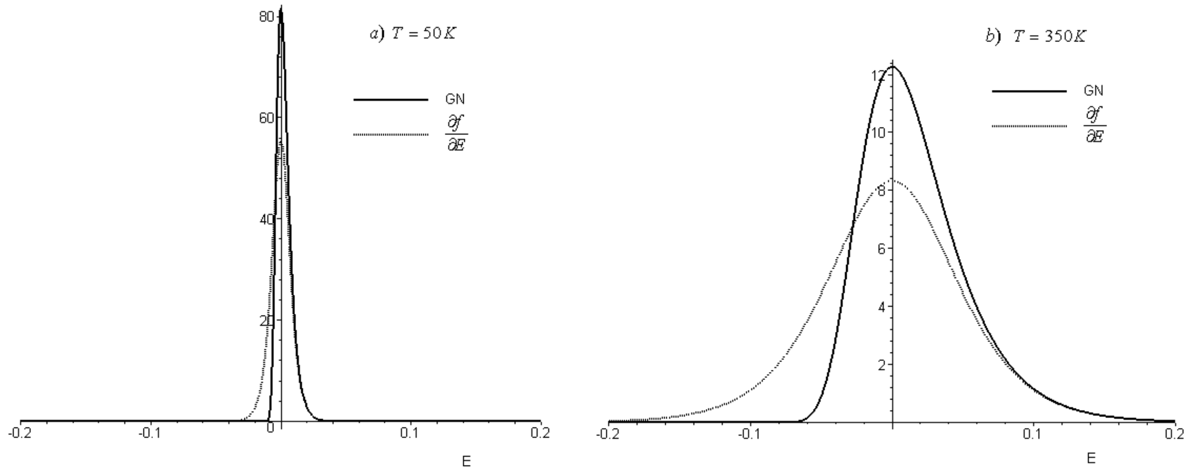

Fig.2. Graphs of GN And $\partial f/\partial E$ For Temperatures: A) $T=50K$, and B) $T=350K$

Substituting (9) into (11) we have

$$N(E,T)=N_0\sum_{n=1}^{\infty}\int_0^{\infty}(1+2\alpha E'+3\beta E'^2)\Theta[E'(1+\alpha E'+\beta E'^2)-E_n]\frac{\partial f(E',E,T)}{\partial E}dE' \qquad (13)$$

For the analysis (13), consider the simple case when $\beta=0$. Then, the Heaviside function $\Theta[E'(1+\alpha E')-E_n]$ cuts the lower bound is integral to a point

$$\overline{E_n}=\frac{\sqrt{1+4\alpha E_n}-1}{2\alpha}.$$

Rewrite (13) as a

$$N(E,T)=N_0\sum_{n=1}^{\infty}\int_{\overline{E_n}}^{\infty}(1+2\alpha E')\frac{\partial f(E',E,T)}{\partial E}dE'=-N_0\sum_{n=1}^{\infty}\int_{\overline{E_n}}^{\infty}(1+2\alpha E')\frac{\partial f(E',E,T)}{\partial E'}dE' \qquad (14)$$

Integrating (14) by parts we have

$$\int_{\overline{E_n}}^{\infty}(1+2\alpha E')\frac{\partial f(E',E,T)}{\partial E'}dE'=(1+2\alpha E')f(E',E,T)\Big|_{\overline{E_n}}^{\infty}-2\alpha\int_{\overline{E_n}}^{\infty}f(E',E,T)dE'=$$
$$=-(1+2\alpha\overline{E_n})f(\overline{E_n},E,T)-2\alpha\int_{\overline{E_n}}^{\infty}f(E',E,T)dE'=-\frac{(1+2\alpha\overline{E_n})}{e^{\frac{\overline{E_n}-E}{T}}+1}-2\alpha T\ln\left(1+e^{\frac{E-\overline{E_n}}{T}}\right) \qquad (15)$$

Substituting (15) into (14) we finally obtain

$$\frac{N(E,T)}{N_0}=\sum_{n=1}^{\infty}\left[\frac{(1+2\alpha\overline{E}_n)}{e^{\frac{\overline{E}_n-E}{T}}+1}+2\alpha T\ln\left(1+e^{\frac{E-\overline{E}_n}{T}}\right)\right] \tag{16}$$

For a parabolic dispersion relation (16) takes the simple form

$$\frac{N(E,T)}{N_0}=\sum_{n=1}^{\infty}\frac{1}{e^{\frac{E_n-E}{T}}+1}.$$

We construct graphics of $N(E)/N_0$ by formula (16) at $E_1=0.01\,\text{eV}$, $\alpha=-0.1,\ 0001,\ 0.1\,\text{eV}^{-1}$ for two temperatures: $T=23\,K,\quad 230\,K$.

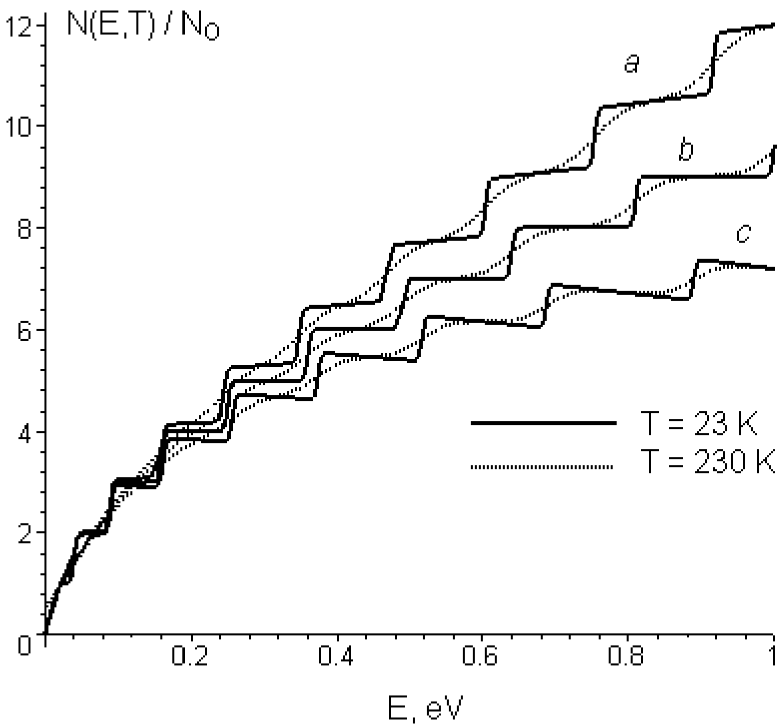

Figure 3. Energy Dependence of the DOS (16), With $E_1=0.01\,$**Ev,** $a)\ \alpha=0.1\,\text{eV}^{-1}$, $b)\ \alpha=0.0001\,\text{eV}^{-1}$, $c)\ \alpha=-0.1\,\text{eV}^{-1}$ **And At T = 23 K And T = 230 K**

Let's result also function $N(E,T)/N_0$ calculated on the basis of function GN (12)

$$N(E,T)=N_0\sum_{n=1}^{\infty}\int_0^{\infty}(1+2\alpha E'+3\beta E'^2)\Theta[E'(1+\alpha E'+\beta E'^2)-E_n]GN(E',E,T)dE' \tag{17}$$

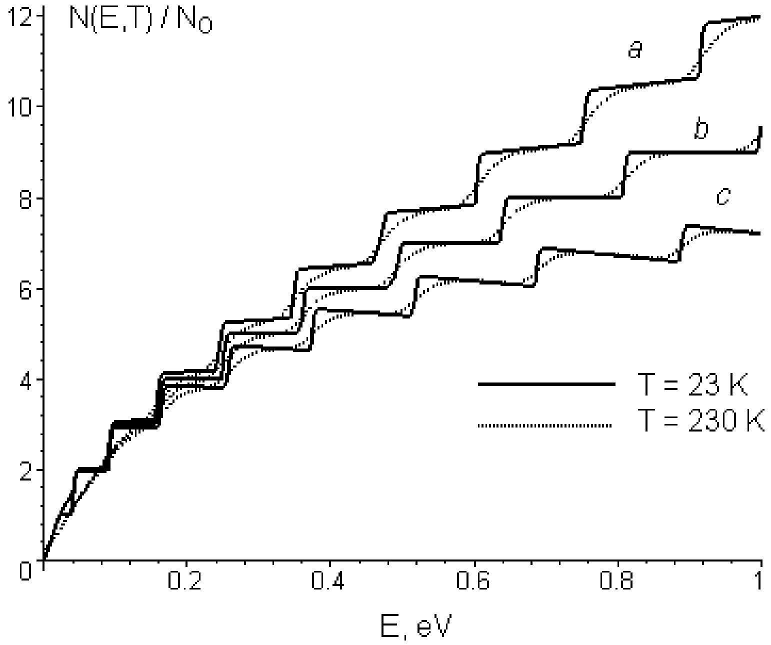

Figure 4. Energy Dependence of the DOS (17), with $E_1 = 0.01\,\text{eV}$, $a)\ \alpha = 0.1\,\text{eV}^{-1}$, $b)\ \alpha = 0.0001\,\text{eV}^{-1}$, $c)\ \alpha = -0.1\,\text{eV}^{-1}$ **and at T = 23 K and T = 230 K**

As seen from Fig.3,4, temperature greatly affects the shape depending on the temperature dependence of $N(E,T)$. DOS is caused by thermal generation of electrons from discrete energy states to conduction band states E_n. The degree of filling of the energy states E_n is determined by Shockley-Read-Hall statistics [3].

At low temperatures, the thermal generation from the energy states E_n is weak and it does not lead to a strong broadening of the energy levels and the DOS has sharply stepped shape. At the same angles of steps slightly smoothed (Fig.3,4). There dependency nonparabolicity dispersion law remains the same as Fig.1. The low temperature has smaller effect on the shape of DOS.

With further increase in temperature the thermal generation from energy levels is increased. This leads to a strong broadening thermodynamic DOS. It significantly changes its shape. On Fig.3,4 is shown the thermodynamic DOS at $T = 230K$. In this case, the thermal broadening almost washed away a step change in the DOS and the steps have become a growing smoothly smooth curve.

At low energies, the steps disappear completely. With increasing energy is weak deviations consistent with the provisions of the former steps of the respective discrete levels. With further increase of the temperature the thermodynamic DOS transformed into a smooth curve. With the growth coefficient of nonparabolicity α the DOS curve increases monotonically. As can be seen from Ris.3,4 nonparabolicity dispersion law greatly increases the DOS for positive values and decreases with negative values of α.

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