

NAMANGAN DAVLAT
UNIVERSITETI
ILMIY AXBOROTNOMASI, [2026-9]
ISSN:2181-1458
ISSN:2181-0427



01.00.00-FIZIKA-MATEMATIKA
journal.namdu.uz
PHYSICS AND MATHEMATICS

DENSITY OF STATES CALCULATIONS IN A QUANTIZING MAGNETIC FIELD WITH A NONPARABOLIC DISPERSION LAW

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Abstract: The temperature dependence of the density of states of charge carriers in a quantizing magnetic field is studied for semiconductors with a nonparabolic (Kane-type) dispersion law, characteristic of narrow-gap $A_{III}B_V$ and $A_{II}B_{VI}$ compounds such as InSb. An analytical expression is derived for the thermodynamic density of states at absolute zero from the cubic dispersion equation, reducing to the parabolic result in the appropriate limit. Thermal broadening of the Landau levels is then incorporated via the energy derivative of the Fermi–Dirac function, yielding a temperature-dependent density of states. Numerical calculations for InSb show that sharp Landau peaks progressively broaden into a continuous spectrum as kT exceeds $\hbar\omega_c$, indicating that neglecting band nonparabolicity leads to an incorrect description of Landau-level positions and their thermal smoothing.

Keywords: density of states, quantizing magnetic field, Landau levels, nonparabolic dispersion law, Kane model, narrow-gap semiconductors.

NOPARABOLIK DISPERSIYA QONUNIGA EGA KVANTLOVCHI MAGNIT MAYDONDA ENERGETIK HOLATLAR ZICHLIGINI HISOBLASH

Annotatsiya: InSb kabi tor ta'qiqlangan zonali $A_{III}B_V$ va $A_{II}B_{VI}$ birikmalariga xos bo'lgan neparabolik (Keyn tipidagi) dispersiya qonuniga ega yarimo'tkazgichlar uchun kvantlovchi magnit maydonda zaryad tashuvchilarning holatlar zichligining haroratga bog'liqligi tadqiq etilgan. Kubik dispersiya tenglamasidan absolyut nol haroratdagi termodinamik holatlar zichligi uchun analitik ifoda keltirib chiqarilgan bo'lib, u tegishli chegaraviy holatda parabolik natijaga o'tadi. Landau sathlarining termik kengayishi Fermi–Dirak funksiyasining energiya bo'yicha hosilasi orqali hisobga olinib, natijada haroratga bog'liq holatlar zichligi olingan. InSb uchun bajarilgan sonli hisoblar shuni ko'rsatadiki, kT qiymati $\hbar\omega_c$ dan oshgan sari Landau sathlarining keskin cho'qqilari asta-sekin kengayib, uzluksiz spektrga aylanadi — bu esa zonaning neparabolikligini e'tiborga olmaslik Landau sathlari holatini va ularning termik silliqilanishini noto'g'ri tavsiflashga olib kelishini ko'rsatadi.

Kalit so'zlar: holatlar zichligi, kvantlovchi magnit maydon, Landau sathlari, neparabolik dispersiya qonuni, Keyn modeli, tor ta'qiqlangan zonali yarimo'tkazgichlar.

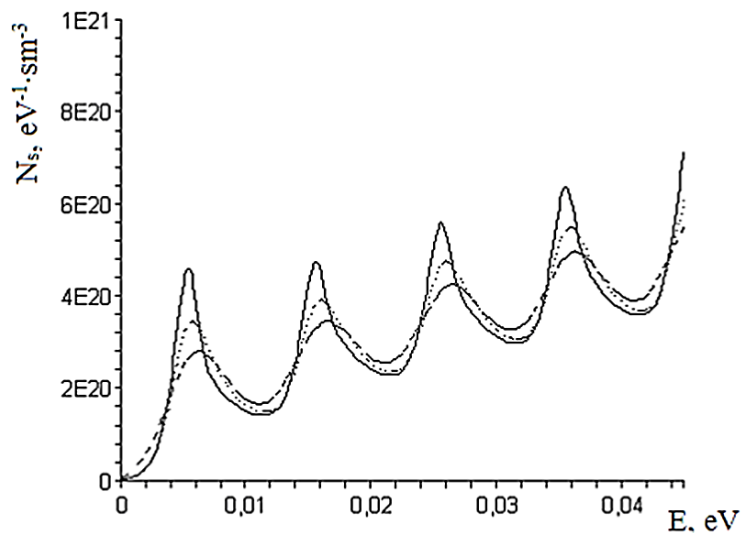
РАСЧЕТЫ ПЛОТНОСТИ ЭНЕРГЕТИЧЕСКИХ СОСТОЯНИЙ В КВАНТУЮЩЕМ МАГНИТНОМ ПОЛЕ С НЕПАРАБОЛИЧЕСКИМ ЗАКОНОМ ДИСПЕРСИИ

Аннотация: Исследуется температурная зависимость плотности состояний носителей заряда в квантующем магнитном поле для полупроводников с непараболическим (Кейновским) законом дисперсии, характерным для узкозонных соединений $A_{III}B_V$ и $A_{II}B_{VI}$, таких как InSb. Из кубического уравнения дисперсии получено аналитическое выражение для термодинамической плотности состояний при абсолютном нуле температуры, которое при соответствующем предельном переходе сводится к параболическому результату. Тепловое уширение уровней Ландау учитывается с помощью

производной по энергии от функции распределения Ферми–Дирака, что позволяет получить плотность состояний, зависящую от температуры. Численные расчёты для InSb показывают, что резкие пики уровней Ландау постепенно уширяются и сливаются в сплошной спектр при kT , превышающем $\hbar\omega_c$, что свидетельствует о том, что пренебрежение непараболическостью зоны приводит к некорректному описанию положения уровней Ландау и их теплового сглаживания.

Ключевые слова: плотность состояний, квантующее магнитное поле, уровни Ландау, непараболический закон дисперсии, модель Кейна, узкозонные полупроводники.

Introduction. The temperature dependence of the density of states in quantizing magnetic fields has been considered as a result of the thermal broadening of Landau levels [1-2]. These works showed that the continuous density-of-states spectrum, measured at liquid-nitrogen temperature, transforms into discrete Landau levels at low temperatures. However, these studies considered only the parabolic dispersion law

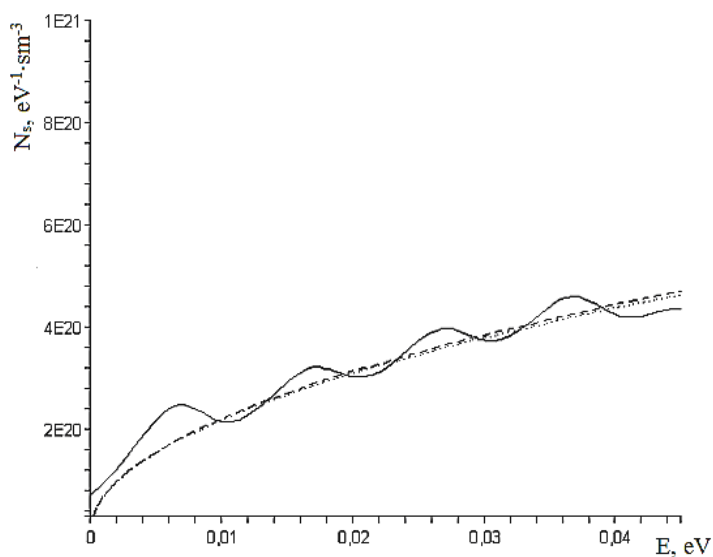


— function GN, the derivative of the level depletion degree with respect to energy

..... the derivative of the Fermi–Dirac function with respect to energy

- - the Gaussian function.

Fig.1. Temperature dependence of the density of energy states in a strong magnetic field ($H = 10$ kOe) at a temperature of $T = 10$ K.



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..... the derivative of the Fermi–Dirac function with respect to energy

- - the Gaussian function.

Fig.2. Temperature dependence of the density of energy states in a strong magnetic field ($H = 10$ kOe) at a temperature of $T = 35$ K.

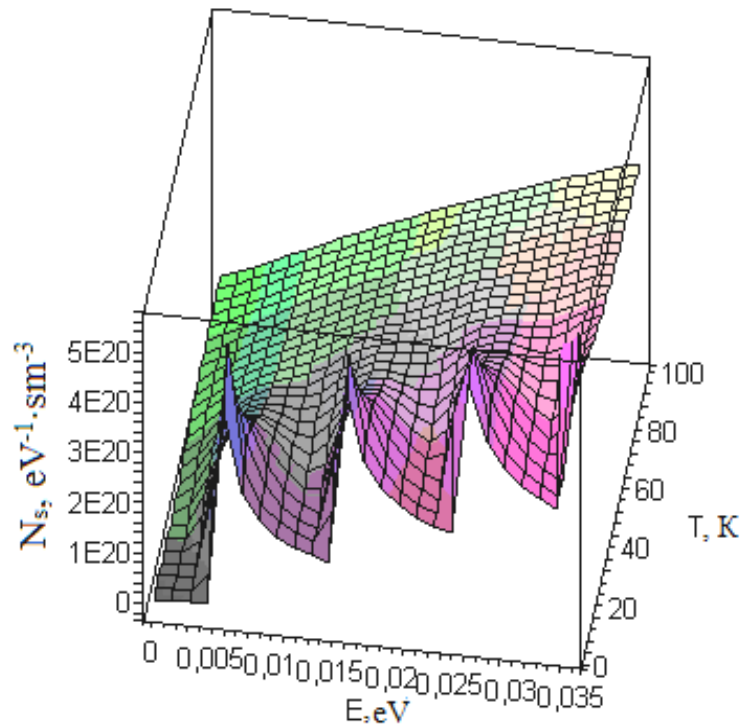


Fig.3. Density of states in the three-dimensional space N_s , E , T at $H = 10$ kOe.

If, however, the dispersion law is nonparabolic, as is the case, for instance, for electrons in $A_{III}B_V$ and $A_{II}B_{VI}$ compounds, the effective mass becomes energy-dependent.

Literature review. The temperature dependence of the density of states in quantizing magnetic fields has been studied as a consequence of the thermal broadening of Landau levels [1-2]. These works showed that the continuous density-of-states spectrum, measured at liquid-nitrogen temperature, transforms into discrete Landau levels as the temperature is lowered. However, this analysis was carried out only within the parabolic approximation for the energy dispersion, which does not account for the energy dependence of the effective mass observed in narrow-gap semiconductors.

In works [3-4], the density of energy states in a strong magnetic field at liquid-nitrogen temperature was determined for semiconductors with a nonparabolic dispersion law. In these works, the experimental results were compared with the Kane model in narrow-gap semiconductors such as InSb, and good agreement between theory and experiment was reported at a fixed, low temperature. However, the effect of temperature on the density of energy states in a quantizing magnetic field was not discussed, so the thermal evolution of the Landau-level structure in the presence of band nonparabolicity remained unexamined.

The theoretical basis for describing this nonparabolicity was laid out in work[5], where the energy levels of the conduction band in a magnetic field were obtained from a cubic dispersion equation arising from the interaction between the conduction band and the three valence bands (the Kane three-band model). Separately, in work [6] established that the thermodynamic density of states in a strong magnetic field, even without invoking nonparabolicity, has the form of a set of delta-function peaks separated by $\hbar\omega_c$, which provides the natural starting point for introducing thermal broadening.

Taken together, these studies leave a clear gap in the literature: the thermal-broadening formalism developed in works[1-2] has been applied only to carriers with a parabolic dispersion law, while the Kane-model density-of-states calculations in works[3-4] were restricted to a single, fixed temperature. A unified treatment that combines the nonparabolic (Kane) dispersion law with an explicit temperature dependence of the density of states — needed to describe narrow-gap semiconductors such as InSb over a wide temperature range — has not been presented, and this is the problem addressed in the present work.

Research methodology. In a magnetic field, the energy of free electrons with a parabolic dispersion law, taking into account the spin splitting of energy levels, takes the following form [3]:

$$E_n = \hbar\omega_c \left(n_c + \frac{1}{2} \right) + s\mu_B B + \frac{\hbar^2 k_z^2}{2m_e} \quad (1)$$

Here, μ_B is the Bohr magneton.

However, if the dependence of energy on the wave vector is not described by a quadratic function, as is the case, for example, for electrons in InSb, the energy levels of charge carriers in a magnetic field are not equidistant, since the cyclotron mass is determined by the expression

$$m_c = \frac{\hbar^2}{2\pi} \frac{\partial S}{\partial E} \quad (2)$$

The nonparabolicity of the conduction band in $A_{III}B_V$ and $A_{II}B_{VI}$ compounds arises as a result of the interaction between the conduction band and the three valence bands. In a magnetic field, the energy levels for the three energy bands are given by the cubic equation [5]:

$$E_{N\pm} (E_{N\pm} + E_g) (E_{N\pm} + E_g + \Delta) - P^2 \left[k_z^2 + (2N+1) \frac{1}{L^2} \right] \times \left(E_{N\pm} + E_g + \frac{2}{3} \Delta \right) \pm \frac{P^2 \Delta}{3L^2} = 0 \quad (3)$$

Here, E_N are the energies of electrons in the conduction band in a magnetic field, Δ is the spin-orbit splitting energy, and P is the matrix element.

Under this condition, the cubic equation (3) reduces to a quadratic one, whose solution for the conduction-band electrons has the form

$$E_{N\pm} = -\frac{E_g}{2} + \frac{1}{2} \sqrt{E_g^2 + 4E_g \left[\left(N + \frac{1}{2} \right) \hbar \omega_c + \frac{\hbar^2 k_z^2}{2m_n} \pm \frac{g_0 \mu_B H}{2} \right]} \quad (4)$$

Using expression (2) for the cyclotron mass, we find the difference in cross-sectional areas of two isoenergetic surfaces

$$\text{whose energies differ by: } \Delta E = \hbar \omega_c \quad \Delta S = \frac{2\pi m_c}{\hbar^2} \Delta E = \frac{2\pi m_c}{\hbar^2} \hbar \omega_c$$

The number of states per unit area in the $k_x k_y$ plane, arising from the quantization imposed by the cyclicity conditions, is equal to $L_x L_y / (2\pi)^2$.

From equation (4), we determine k_z without taking spin into account:

$$k_z = \frac{(2m)^{\frac{1}{2}}}{\hbar} \left(\frac{E^2 + E_g (E - (N + \frac{1}{2}) \hbar \omega_c)}{E_g} \right)^{\frac{1}{2}} \quad (5)$$

The electron motion along the z -axis is free, that is: $k_z = 2\pi n_z / L_z$. According to expressions (4) and (5), the number of states is:

$$n_z = \frac{(2m)^{\frac{1}{2}}}{\pi \hbar} \cdot \left(\frac{E^2 + E_g (E - (N + \frac{1}{2}) \hbar \omega_c)}{E_g} \right)^{\frac{1}{2}} \quad (6)$$

The total number of quantum states with energies less than E is equal to

$$N(E) = \frac{L_x L_y L_z m^{\frac{3}{2}}}{\pi^2 \hbar^3} \hbar \omega_c \cdot \sum_{N=0}^{N_{\max}} \left(\frac{E^2 + E_g (E - (N + \frac{1}{2}) \hbar \omega_c)}{E_g} \right)^{\frac{1}{2}} \quad (7)$$

As a result, we obtain the density of energy states per unit volume, without taking spin into account, for the Kane dispersion law in a magnetic field:

$$N_s^n(E, H) = \frac{dN(E)}{dE} = \frac{(m)^{\frac{3}{2}}}{(2)^{\frac{1}{2}} \pi^2 \hbar^3} \frac{\hbar \omega_c}{2} \sum_{N=0}^{N_{\max}} \frac{\frac{2E}{E_g} + 1}{\sqrt{\frac{E^2}{E_g} + E - (N + \frac{1}{2}) \hbar \omega_c}} \quad (8)$$

Here, is the thermodynamic density of energy states in a quantizing magnetic field with a nonparabolic dispersion law.

At, expression (8) reduces to the parabolic dispersion law (1). $N_s^n(E, H) E_g \rightarrow \infty$

Analysis and results. In work [6], the determination of the thermodynamic density of states in a strong magnetic field was discussed. The thermodynamic density of states of such a system represents a set of delta-function peaks separated from one another by $\hbar \omega_c$.

Thermal broadening will be taken into account using the energy derivative of the Fermi–Dirac distribution function. This yields a temperature-dependent density of energy states [1]. Thermal broadening of the levels in a magnetic field leads to

a smoothing of the discrete levels $\frac{df_0(E, \mu, T)}{dE}$

$$N_s^n(E, H, T) = \sum_{i=1}^n N_H^n(E_i, H) \frac{df_0(E_i, \mu, T)}{dE} \quad (9)$$

Here, is the density of states in a quantizing magnetic field at absolute zero temperature. This expression, as $T \rightarrow 0$, reduces to (8). As the temperature increases, the sharp peaks begin to smooth out (Fig.4), and at sufficiently high temperatures, $kT > \hbar\omega_c$, it transforms into a continuous density of states, and the magnetic field is no longer felt. This makes it possible to obtain a density of states that depends on temperature. Figure 4 shows the density of states in a magnetic field for InSb at the following parameter values: $N_s^n(E_i, H)$

$$, m_n^* = \frac{1}{70} m_0, E_g(0) = 0,234 \text{ eV}, B = 2 \text{ T}, \hbar\omega_c \approx 1,5 \cdot 10^{-3} \text{ eV}$$

At such low temperatures, the effect of thermal broadening is weak, and the density of states does not show noticeable deviation of N_s from its ideal form, which does not take temperature effects into account. Figure 5 shows $N_s(E, H)$ for temperatures of 1, 20, and 50 K. As can be seen from these figures, with increasing temperature, the sharp Landau-level peaks, caused by the quantization of electron energy levels in the plane perpendicular to the magnetic field, are gradually smoothed out.

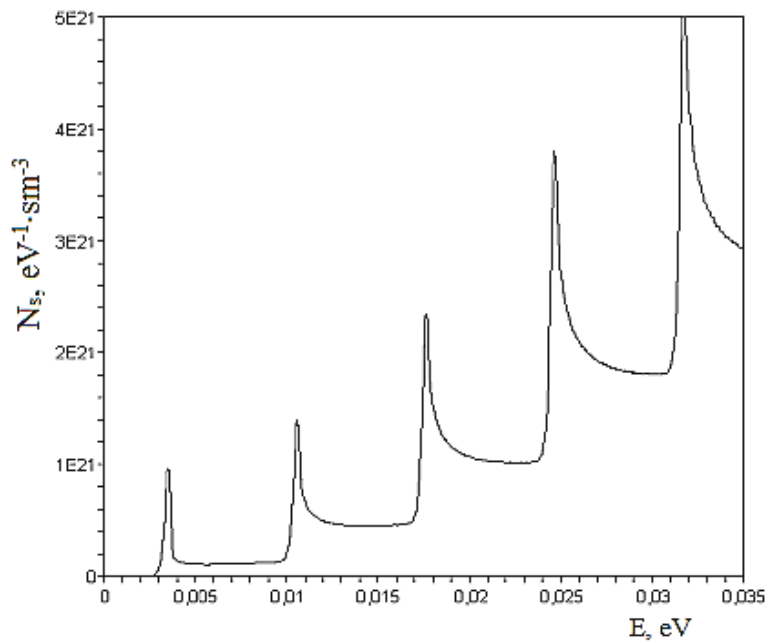


Fig.4. Density of energy states in a strong magnetic field $H = 20 \text{ kOe}$ at a temperature of $T = 1 \text{ K}$ with a nonparabolic dispersion law, calculated using formula (9).

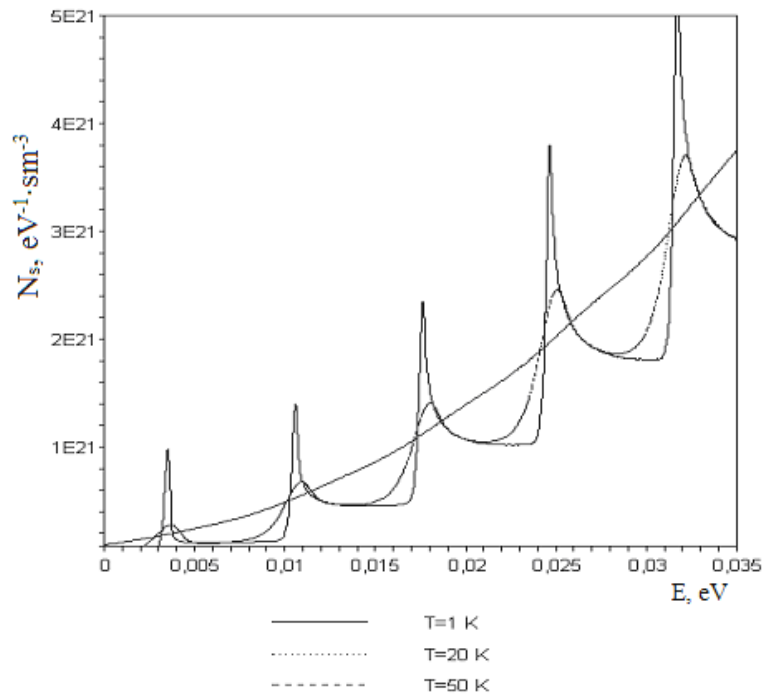


Fig.5. Temperature dependence of the density of energy states in a quantizing magnetic field with a nonparabolic dispersion law, calculated using formula (9).

Conclusion. An analytical method has been developed for determining the Landau levels and the corresponding density of energy states of electrons obeying the nonparabolic Kane dispersion law in a quantizing magnetic field. Starting from the cubic dispersion equation that accounts for the interaction between the conduction band and the three valence bands, the thermodynamic density of states at absolute zero was derived, correctly reducing to the known parabolic result in the appropriate limit. Incorporating thermal broadening through the energy derivative of the Fermi-Dirac distribution function yielded a temperature-dependent density of states applicable to narrow-gap semiconductors such as InSb.

Numerical calculations show that at low temperatures the density of states retains sharp, well-resolved Landau peaks, while with increasing temperature these peaks progressively broaden and merge into a continuous spectrum once kT exceeds $\hbar\omega_c$. These results demonstrate that neglecting band nonparabolicity leads to an incorrect description of Landau-level positions and their thermal smoothing in narrow-gap semiconductors, providing a quantitative basis for interpreting magneto-optical and magneto-transport experiments over a wide temperature range.

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