

Features of the chemical potential of a quasi-two-dimensional electron gas at low-temperatures

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An analysis is made of the low-temperature behavior of the chemical potential μ of a quasi-two-dimensional electron gas near the resonance point (at the bottom of the miniband) and far from it. Low-temperature analytical formulas for $\mu(T)$ are obtained under the conditions of the existence of an arbitrary number of minibands. It is shown that with the increasing temperature near the resonance point, the chemical potential decreases linearly and exponentially slowly in the middle of the resonance points. Analytical formulas are compared to the numerical solutions.

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1. Introduction

The study of the properties of electron gas in quantum wells of semiconductor heterostructures is of both fundamental and applied interest. Dimensional quantization of carrier energies leads to the manifestation of a number of interesting low-dimensional effects.¹⁻¹⁴ In deep quantum wells, several minibands can exist.¹⁵⁻¹⁷

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The main reason for the manifestation of size-quantum effects in a gas is a stepwise change in the density of states at the resonance points, where the chemical potential μ is equal to the energy levels E_n of spatial quantization.¹ A change in the chemical potential relative to the energy levels of spatial quantization can be observed depending on the concentration n_s or the width of the quantum well L .

At present, it is well-known that in the approximation of a single miniband and at low-temperatures (near absolute zero), the chemical potential of a quasi-two-dimensional electron gas changes exponentially in a slow manner.^{8,9} The dependence $\mu(T)$ in the presence of several minibands was studied in Ref. 14; however, the results were obtained only by a numerical method. Since almost all thermodynamic quantities and kinetic coefficients are directly related to the chemical potential of the gas, it is clear that determining the function $\mu(T)$ is an urgent task.

In this paper, we study the temperature dependence of the chemical potential of a quasi-two-dimensional ideal gas at various two-dimensional (2D) concentrations of n_s (i.e., at different values of the Fermi energy). For dependence $\mu(T)$ near absolute zero, temperature analytical formulas are obtained under the conditions of the existence of an arbitrary number of minibands. The results showed that with increasing temperature near the resonance point, the chemical potential decreases linearly and exponentially slowly in the middle of the resonance points. Analytical results are compared with numerical calculations $\mu(T)$.

2. The Main Relationships

For the sake of simplification, we consider an ideal electron gas with a simple parabolic spectrum in a single quantum well of a heterostructure. In this case, the thermal transition of electrons from the quantum well to local levels and to the conduction bands of wide-gap material is not taken into account. In addition, the influence of the valence band is also neglected. Energy is measured from the bottom of the bulk semiconductor gap.

In a quantum well, the energy of the transverse motion is quantized, and the electron gas becomes quasi-two-dimensional. The dispersion of an electron can be represented as¹

$$E = \frac{\hbar^2 k^2}{2m} + E_n, \quad (1)$$

where $k^2 = k_x^2 + k_y^2$, m is the effective mass of the electron, E_n is the energy levels of the transverse motion. Finding the E_n levels is a quantum-mechanical part of the problem and we consider them known. The total 2D concentration is

$$n_s = g_0 \sum_{n=1}^M \int_{E_n}^{\infty} f(E) dE = g_0 T \sum_{n=1}^M \ln(1 + e^{\frac{\mu - E_n}{T}}), \quad (2)$$

where $g_0 = m/\pi\hbar^2$, M is the number of minibands in a given quantum well, T is the value $k_B T$, the k_B is Boltzmann constant, $f(E)$ is the Fermi-Dirac distribution

function

$$f(E) = \frac{1}{\exp\left(\frac{E-\mu}{T}\right) + 1}. \quad (3)$$

Solving Eq. (2), we can determine the chemical potential μ as a function of temperature T and 2D concentration n_s .

At absolute zero temperature, the chemical potential is equal to the Fermi energy, i.e., $T = 0, \mu = E_F$ and the distribution function $f(E)$ becomes stepwise

$$f(E) = \begin{cases} 1, & E < E_F, \\ 0, & E > E_F. \end{cases} \quad (4)$$

Then, for $T = 0$, Eq. (2) takes the form

$$n_s = g_0 \sum_{n=1}^M \int_{E_n}^{E_F} dE = g_0 \sum_{n=1}^M (E_F - E_n) \Theta(E_F - E_n), \quad (5)$$

where $\Theta(x)$ is the Heaviside step function. In Eq. (5), the terms under the sum sign must be positive. Negative terms are excluded by the function $\Theta(x)$.

From (2) and (5) also follows the equation

$$\sum_{n=1}^M (E_F - E_n) \Theta(E_F - E_n) = T \sum_{n=1}^M \ln(1 + e^{\frac{\mu - E_n}{T}}). \quad (6)$$

This equation defines the chemical potential of μ as a function of temperature T and the Fermi energy E_F . Since according to (5), E_F is uniquely related to the 2D concentration n_s , only the solution of Eq. (6) will be studied in what follows.

3. Precisely Solvable Models

In the simplest case of a single-band model $M = 1$, the solution of Eq. (6) has the form^{1,8,9}

$$\mu = E_1 + T \ln\left(e^{\frac{E_F - E_1}{T}} - 1\right) = E_F + T \ln\left(1 - e^{\frac{E_1 - E_F}{T}}\right), \quad E_F > E_1. \quad (7)$$

In the limit of sufficiently low-temperatures (after, near absolute zero), when $E_F - E_1 \gg T$, formula (7) has a simpler form

$$\mu \approx E_F - T e^{\frac{E_1 - E_F}{T}} \quad (8)$$

When there is only one miniband in a quantum well, model (7) is applicable only if $V - E_F \gg T$, (V is the depth of the quantum well). When the number of minibands is more than one $M > 1$, the single-zone model is applicable if $E_2 - E_F \gg T$. Otherwise, model (7) is unfair because it does not take into account the processes of thermal emission of electrons to overlying zones.

In the case of the two-band model $M = 2$, Eq. (6) reduces to a quadratic equation and its solution has the form

$$\mu = E_1 + T \ln \left(\sqrt{\left(1 - e^{\frac{E_2 - E_1}{T}}\right)^2 + 4e^{\frac{E_2 - E_1 + S}{T}}} - \left(1 + e^{\frac{E_2 - E_1}{T}}\right) \right) - T \ln(2), \quad (9)$$

where

$$s = \sum_{n=1}^2 (E_F - E_n)\Theta(E_F - E_n). \quad (10)$$

It should also be noted here that when the number of minibands is more than two $M > 2$, model (9) is valid if $E_3 - E_F \gg T$.

4. Asymptotic Formulas for Low-Temperatures and an Arbitrary Number of Minibands

1. Suppose that the chemical potential lies approximately in the middle of two successive levels of $E_N < \mu < E_{N+1}$ and the temperature is quite low $T \ll \mu - E_N, E_{N+1} - \mu$. Then, the right side of Eq. (6) can be reduced to

$$\sum_{n=1}^M T \ln(1 + e^{\frac{\mu - E_n}{T}}) \approx \sum_{n=1}^N (\mu - E_n) + T \ln(1 + e^{\frac{E_N - \mu}{T}}) + T \ln(1 + e^{\frac{\mu - E_{N+1}}{T}}). \quad (11)$$

In this representation, the second and third terms have the same degree of smallness. In the approximation under consideration, the left side of Eq. (6) is equal to

$$\sum_{n=1}^M (E_F - E_n)\Theta(E_F - E_n) = NE_F - \sum_{n=1}^N E_n. \quad (12)$$

Substituting (11) and (12) into (6), we have

$$\mu \approx E_F - \frac{T}{N} \left[\ln(1 + e^{\frac{E_N - \mu}{T}}) + \ln(1 + e^{\frac{\mu - E_{N+1}}{T}}) \right]. \quad (13)$$

If we take into account condition $T \ll \mu - E_N, E_{N+1} - \mu$, then this equation can be simplified further. For small x , we can use the expansion of $\ln(1 + x) \approx x$ and from (13) we obtain

$$\mu \approx E_F - \frac{T}{N} (e^{\frac{E_N - \mu}{T}} + e^{\frac{\mu - E_{N+1}}{T}}). \quad (14)$$

In a first approximation, on the right-hand side of (14), we can replace μ with E_F . Then we have

$$\mu \approx E_F - \frac{T}{N} (e^{\frac{E_N - E_F}{T}} + e^{\frac{E_F - E_{N+1}}{T}}). \quad (15)$$

It can be seen from (15) that near absolute zero temperatures the decrease in the chemical potential of a 2D gas is exponentially small. This correction is inversely proportional to the number of the subzone N . The admitted condition $T \ll \mu - E_N, E_{N+1} - \mu$ does not allow applying formulas (15) in cases where the Fermi energy is close to the E_N, E_{N+1} levels.

In the case $N = 1$, it follows from (15)

$$\mu \approx E_F - T(e^{\frac{E_1 - E_F}{T}} + e^{\frac{E_F - E_2}{T}}). \quad (16)$$

If the upper level is sufficiently far from the Fermi energy, then the second term inside the bracket can be neglected. Then result (8) follows from (16).

2. Let the Fermi energy lie near the N th-subband and the temperature be sufficiently low $T \sim T_N > 0$, $|\mu - E_N| \ll T \ll \mu - E_{N-1}, E_{N+1} - \mu$. Here, T_N is the temperature at which the chemical potential crosses the energy level of $\mu \sim E_N$. Then, the right-hand side of (6) can be simplified as follows:

$$\sum_{n=1}^M \ln(1 + e^{\frac{\mu - E_n}{T}}) \approx \frac{1}{T}(N - 1)\mu - \frac{1}{T} \sum_{n=1}^{N-1} E_n + \ln(1 + e^{\frac{\mu - E_N}{T}}). \quad (17)$$

Since $|\mu - E_N| \ll T$, then we can use the following decompositions:

$$e^{\frac{\mu - E_N}{T}} \approx 1 + \frac{\mu - E_N}{T}, \quad \ln\left(1 + \frac{\mu - E_N}{2T}\right) \approx \frac{\mu - E_N}{2T}.$$

Then, after some simplifications from (17), we have

$$\sum_{n=1}^M \ln(1 + e^{\frac{\mu - E_n}{T}}) \approx \frac{\mu}{T} \left(N - \frac{1}{2}\right) - \frac{E_N}{2T} - \frac{1}{T} \sum_{n=1}^{N-1} E_n + \ln 2. \quad (18)$$

In the approximation under consideration, the left side of Eq. (6) is equal to

$$\begin{aligned} \sum_{n=1}^M (E_F - E_n)\Theta(E_F - E_n) &= (N - 1)E_F - \sum_{n=1}^{N-1} E_n \\ &\quad + (E_F - E_N)\Theta(E_F - E_N). \end{aligned} \quad (19)$$

Substituting (18) and (19) in (6), we have

$$\mu = \frac{(N - 1)E_F + (E_F - E_N)\Theta(E_F - E_N) + \frac{E_N}{2} - T \ln 2}{N - \frac{1}{2}}. \quad (20)$$

In the case $E_F > E_N$ (20), it is simplified

$$\mu = \frac{NE_F - \frac{E_N}{2} - T \ln 2}{N - \frac{1}{2}}. \quad (21)$$

In the case $E_F < E_N$ (20), it is simplified

$$\mu = \frac{(N - 1)E_F + \frac{E_N}{2} - T \ln 2}{N - \frac{1}{2}}. \quad (22)$$

This shows that with increasing temperature, near the N th-level (bottom of the N th-subzone), the chemical potential decreases linearly. With the exact resonance $\mu = E_N, T = T_N, E_F > E_N$, from (20) we obtain

$$T_N = N \frac{E_F - E_N}{\ln 2}. \quad (23)$$

Thus, if the Fermi level is close enough to the N th-level, then the assumptions $T \sim T_N > 0, |\mu - E_N| \ll T \ll \mu - E_{N-1}, E_{N+1} - \mu$ are well satisfied. In deriving

Table 1. Calculation results of $\ln x$ and $\ln(2)/(N - 1/2)$.

N	$\ln(x)$	$\ln(2)/(N - 1/2)$
2	0.481	0.462
3	0.281	0.277
4	0.199	0.198
5	0.155	0.154
6	0.126	0.126

formulas (20)–(23), the upper levels of $n > N$ were neglected and the terms with numbers $n < N$ were summed approximately according to condition $T \ll \mu - E_{N-1}, E_{N+1} - \mu$. Otherwise, the dependence $\mu(T)$ and the temperature T_N at which the resonance $\mu = E_N$ is realized must be determined numerically from (6).

3. Consider the case when the Fermi energy is exactly equal to the N th energy level: $E_F = E_N$. With increasing temperature, the chemical potential mixes down from this level. If we proceed from (20)–(22), then setting $E_F = E_N$ we can obtain the following formula:

$$\mu \approx E_N - \frac{T \ln 2}{N - \frac{1}{2}}. \tag{24}$$

If we proceed from (6), then when condition $T \ll \mu - E_{N-1}, E_{N+1} - \mu$ is satisfied, putting $E_F = E_N$, we arrive at the following equation:

$$(N - 1)\mu + T \ln(1 + e^{\frac{\mu - E_N}{T}}) = (N - 1)E_N, \quad N > 1. \tag{25}$$

Introducing the notation $x = \exp[(E_N - \mu)/T]$, (25) we can reduce to

$$x + 1 = x^N, \quad N > 1. \tag{26}$$

Then, the chemical potential changes in temperature according to the following law:

$$\mu = E_N - T \ln x. \tag{27}$$

In the derivation of (24), expansions and the logarithm in a series were used, while in the derivation of formula (27) they refused this decomposition. For comparison, Table 1 shows the calculations of $\ln x$ and $\ln(2)/(N - 1/2)$.

It can be seen from the table that, for $N = 2$, their difference is about unity percent, and with the growth of N it rapidly decreases.

5. Comparisons with Numerical Results and Discussion of Results

For specific quantum wells of the heterostructure, the energy levels E_n are determined quantum mechanically. To numerically solve Eq. (6), we used a simple spectrum of $E_n = E_1 n^2, n = 1, 2, 3 \dots$ with a given E_1 (we considered the infinite potential well).

- (1) The effect of the number of minibands on the dependence of $\mu(T)$.

Suppose that in a quantum well there are several energy levels of spatial quantization. For example, at $E_1 = 0.005$ eV, the following quantum levels correspond: $E_n = 0.005, 0.02, 0.045, 0.08, 0.125, 0.18 \dots$ eV. Let the 2D electron concentration in the quantum well be such that the Fermi energy is between the levels $E_2 = 0.02$ eV and $E_3 = 0.045$ eV. In the numerical solution of Eq. (6), we limited ourselves to a finite number of minibands $M = 2, 3, 5$. The obtained dependences $\mu(T)$ for different values of the Fermi energy are presented in Fig. 1.

The line with $M = 2$ obtained by the numerical method exactly coincides with the analytical formula of the two-band model (9). With increasing temperature, the role of the thermal emission of electrons to the overlying minibands with $M = 3, 5$ grows, which can be seen from all the graphs in Figs. 1(a)–1(c). The two-band model works better at low-temperatures and when the Fermi energy is close to the E_2 level, Figs. 1(a) and 1(b). When the Fermi energy lies approximately in the middle of the levels E_2 and E_3 and at low-temperatures the chemical potential decreases exponentially slowly, this is clearly seen from Fig. 1(b). As the Fermi energy approaches the level E_2 or E_3 and at low-temperatures, the chemical potential decreases faster, as shown in Figs. 1(a) and 1(c). This sign indicates that the thermal transitions of electrons of overlying energy states are more intense where the density of energy states increases sharply.

- (2) Comparison of formula (15) with a numerical solution. Figure 2 presents a comparison of the dependences $\mu(T)$ obtained by the analytical formula (15) with the results of the numerical solution of Eq. (6) for different values of the Fermi energy. In the calculations, the following spectrum parameters were used: $E_1 = 0.005$ eV, $E_n = 0.005, 0.02, 0.045, 0.08, 0.125, 0.18 \dots$ eV, and the case where the Fermi energy is between the levels $E_3 = 0.045$ eV and $E_4 = 0.08$ eV ($N = 3$). In the numerical solution of Eq. (6), we limited ourselves to the maximum number of minibands $M = 5$.

From these graphical dependencies, we can conclude that if the Fermi energy E_F is located far from the size quantization level (in this case, from E_3 and E_4), then an exponentially slow decrease in the chemical potential is clearly observed in a wide temperature range $0 < T < 0.01$ eV, Fig. 2(b) This range decreases as the Fermi energy E_F approaches the bottom edges of the minibands E_3 and E_4 , Figs. 2(a) and 2(c), respectively.

- (3) Comparison of formula (20) with a numerical solution. Figure 3 shows the comparisons of the dependences $\mu(T)$ obtained by the analytical formula (20) with the results of the numerical solution of Eq. (6) for different values of the Fermi energy. The following spectral parameters were used in the calculations: $E_1 = 0.005$ eV, $E_n = 0.005, 0.02, 0.045, 0.08, 0.125, 0.18 \dots$ eV, and the case where the Fermi energy is between the levels $E_3 = 0.045$ eV and $E_4 = 0.08$ eV

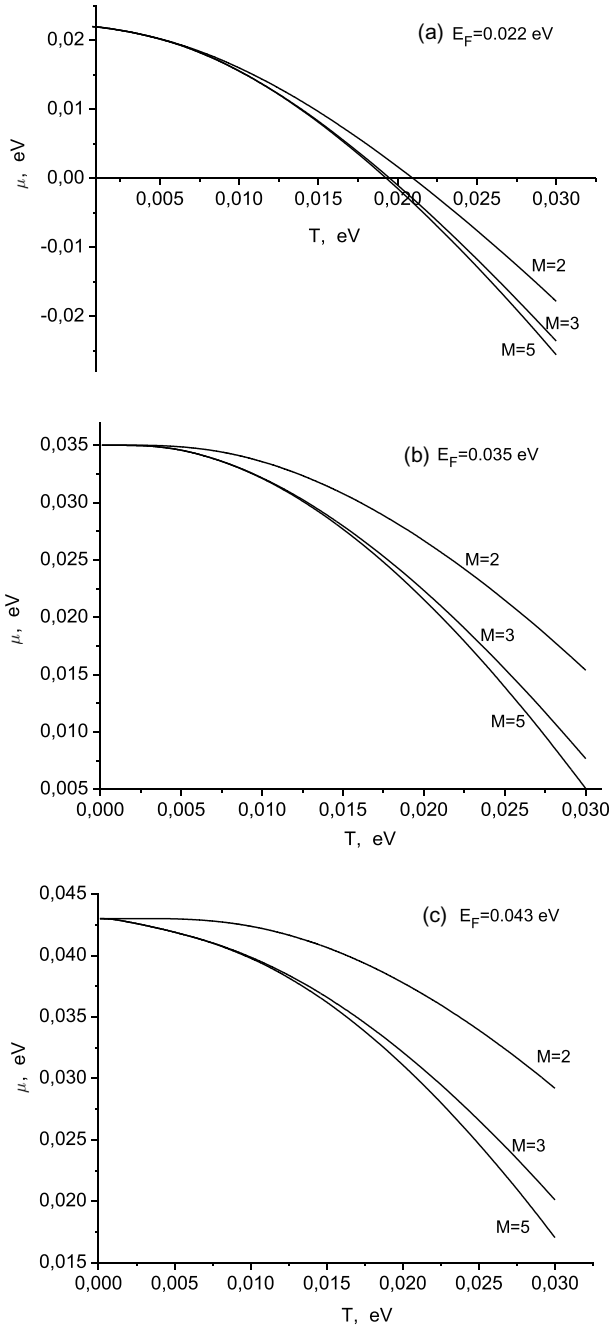


Fig. 1. Dependence of the chemical potential on the temperature of a quasi-two-dimensional electron gas. In numerical modeling, the contributions of different numbers of minibands $M = 2, 3, 5$ are considered. The Fermi energy is (a) $E_F = 0.022$ eV, (b) $E_F = 0.035$ eV and (c) $E_F = 0.043$ eV.

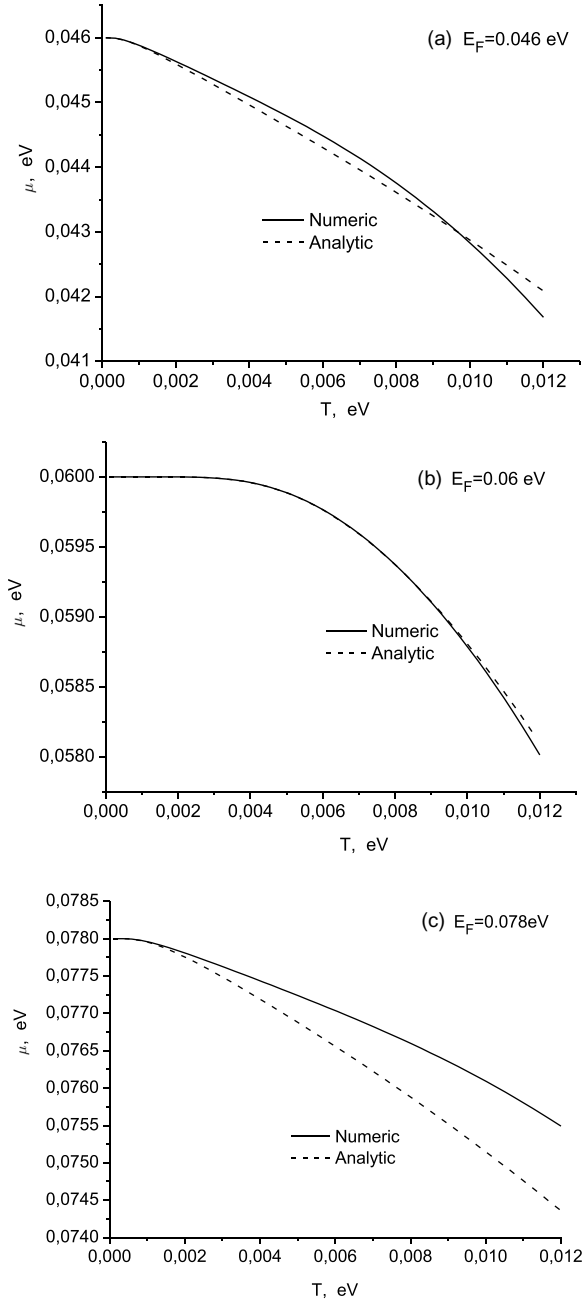


Fig. 2. Comparison of the dependence $\mu(T)$ obtained by analytical formula (15) with the results of numerical solutions of Eq. (6). The following parameters were used in the calculations: $E_1 = 0.005$ eV, $E_n = 0.005, 0.02, 0.045, 0.08, 0.125, 0.18 \dots$ eV. The Fermi energy is located between the levels $E_3 = 0.045$ eV and $E_4 = 0.08$ eV ($N = 3$): (a) $E_F = 0.046$ eV and (b) $E_F = 0.06$ eV and (c) $E_F = 0.078$ eV. In the numerical solution of Eq. (6), $M = 5$ is adopted.

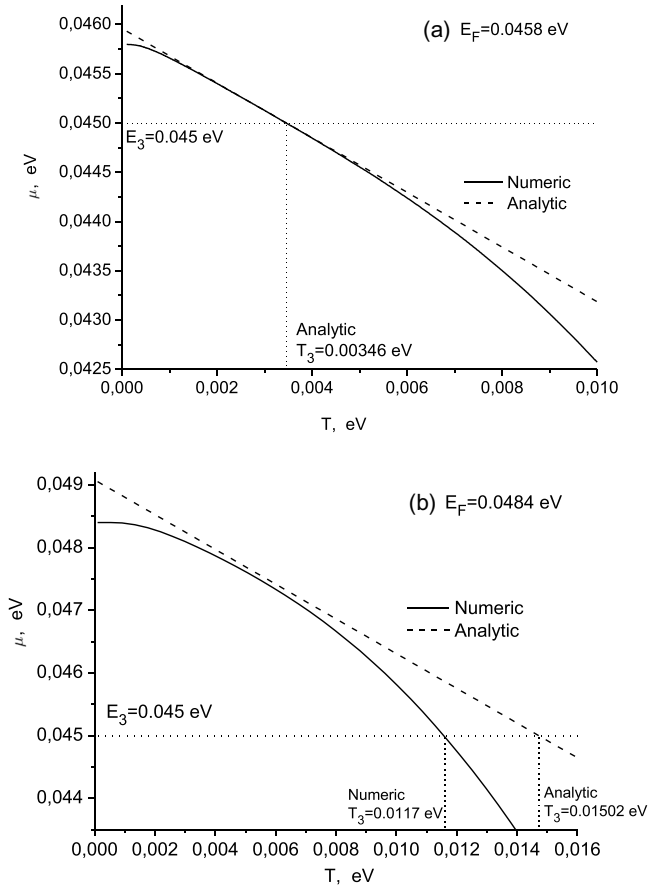


Fig. 3. Comparison of the dependence $\mu(T)$ obtained by analytical formula (20) with the results of numerical solutions of Eq. (6). The following parameters were used in the calculations: $E_1 = 0.005$ eV, $E_n = 0.005, 0.02, 0.045, 0.08, 0.125, 0.18 \dots$ eV. The Fermi energy is located between the levels $E_3 = 0.045$ eV and $E_4 = 0.08$ eV ($N = 3$): (a) $E_F = 0.0458$ eV and (b) $E_F = 0.0484$ eV. In the numerical solution of Eq. (6), $M = 5$ is adopted.

($N = 3$), but close to the level of E_3 . In the numerical solution, Eq. (6) was limited to the maximum number of minibands $M = 5$.

When the Fermi energy is close enough to the third level: $E_F = 0.0458$ eV and $E_3 = 0.045$ eV, then as can be seen from Fig. 3(a), the analytical formulas (20, 23) and the numerical model have a common intersection point $T_3 = 0.00346$ eV. When the Fermi energy is removed from the E_3 level: $E_F = 0.0484$ eV and $E_3 = 0.045$ eV [Fig. 3(b)], the intersection point obtained by analytical formula (23) is $T_3 = 0.01502$ eV, while the exact numerical result is $T_3 = 0.0117$ eV.

From these graphical dependencies, we can conclude that the closer the Fermi energy E_F to the level E_3 , the better the linear dependence (20) is satisfied and the more accurate the estimate (23). Such a regularity is also clearly visible in Fig. 4,

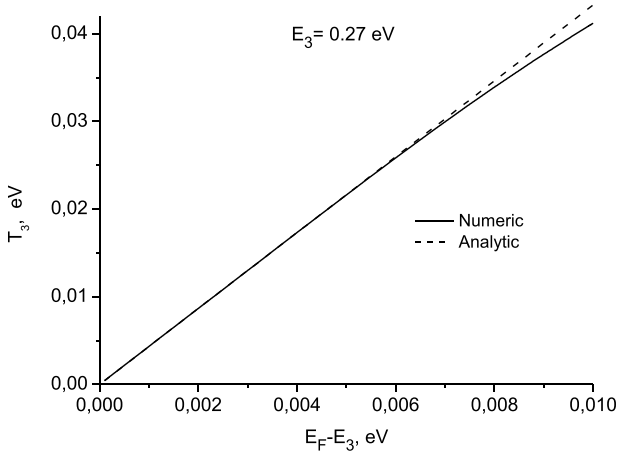


Fig. 4. Comparison of the dependence T_3 obtained by the analytical formula (23) with the results of numerical solutions of Eq. (6). The following parameters were used in the calculations: $E_1 = 0.03$ eV, $E_n = 0.03, 0.12, 0.27, 0.48, 0.75 \dots$ eV, $E_3 = 0.27$ eV ($N = 3$), $M = 5$.

where the dependences $T_3(E_F - E_3)$ are shown by the analytical formula (23) and the numerical solution (6).

6. Conclusions

Determining the law of variation of the chemical potential with respect to temperature is an important task for studying the thermodynamic properties of any gas, since almost all the observed thermodynamic parameters and kinetic coefficients are determined by this dependence. Analytical formulas for the temperature dependence of the chemical potential of a quasi-two-dimensional electron (or hole) gas are obtained in the low-temperature approximation. Cases are considered when the Fermi energy is located between the levels of dimensional quantization and is close to these levels. The case of exact resonance is also analyzed. The results show that with increasing Fermi energy, the dependence of the chemical potential on temperature alternates from a linear (at the resonance points) law to an exponentially small law of change (far from the resonance point).

- (i) The linear dependence of the chemical potential on temperature at the resonance points can be interpreted as follows. Only electrons near the Fermi level participate in the thermal excitation of the system. The number of such electrons is approximately equal to the product of the 'active layer' $\sim T$ and the density of states $N_T = Tg$. Each electron has energy of the order of T and the thermal energy gain is approximately equal to $E_T \sim N_T T$. We represent the temperature change in the chemical potential as $\mu \approx \varepsilon_F - \delta\mu$, where its increment due to the change in the total number of particles is $\delta\mu = (\delta E_T / \delta N)_T$. When any electrons are added to the systems, the Fermi

energy changes. Since, at the resonance point, the density of state changes abruptly, then $\delta\mu \approx \delta E_T/\delta N \neq 0$. Hence, it follows that $\delta\mu \approx \text{const} \cdot T$.

- (ii) In the middle of the resonance points, the density of the state does not change, hence $\delta\mu \approx \delta E_T/\delta N \sim T\delta g/\delta N = 0$ and thus $\mu \approx \varepsilon_F$. The exponential term (see for example (8)) is not obtained in this model. It cannot be expanded in powers of T . Thermal transitions of electrons to the Fermi level from distant $(E_F - E_1)$ points have a low probability, which is due to the Boltzman factor $\exp((E_1 - E_F)/T)$.

The numerical results coincided with the analytical ones in the areas of accepted assumptions. From the linear dependence (20), the quantization law of the one-particle entropy $s(N)$ also follows.^{12,18} Indeed, according to (20)

$$-(d\mu/dT)_{E_F} = \ln(2)/(N - 1/2) = s. \quad (28)$$

In this work, we used the ideal gas model with a simple parabolic spectrum in a single quantum well. Thus, a number of factors were not taken into account: collision processes, the thermal transition of electrons from a quantum well to local levels and into the conduction band of wide-gap material, and the effect of the valence band was also neglected. These tasks require a separate consideration.

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