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Research Article

On the Heat Capacity of a Quasi-Two-Dimensional Electron Gas

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Numerical and analytical results of the investigation of the thermodynamic properties of a quasi-2D electron gas are presented. The density of states, the temperature derivative of the chemical potential, and the heat capacity of the gas at the resonance points and away from it are analyzed. It is shown that, in the dependence of the heat capacity on the chemical potential, there are additional steps at the resonance points. The width of the additional steps increases with temperature. With the increase in temperature, when the main steps are practically blurred, there are still visible marks from the additional steps.

1. Introduction

A quasi-two-dimensional electron gas in heterostructural quantum wells causes both fundamental and applied interest, since the spatial quantization of the carrier energy leads to the manifestation of interesting low-dimensional effects [1–8]. Of particular interest is the behavior of a two-dimensional electron gas in a magnetic field [9–15], since the latter can significantly change the properties of the system.

Under certain conditions, the effects of size quantization appear in the observed thermodynamic quantities even in the absence of a magnetic field [16–23].

It is known that the main reason for the manifestation of size-quantum effects in a gas is a stepwise change in the density of states at critical points, i.e., at the points of resonance, where the chemical potential μ is compared with the energy levels E_n of spatial quantization [1]. Such a change in the density of states manifests itself in one form or another in all the observed thermodynamic quantities. The change in the chemical potential relative to the energy levels of spatial quantization can be observed depending on the concentration n_s or width of the quantum well L.

In [18], the entropy, which is incident on a single particle $s = (\partial S/\partial n_s)_T = -(\partial \mu/\partial T)_{n_s}$ in a quasi-two-dimensional electron gas, is studied as a function of the chemical potential μ. It turned out that at low temperatures it has narrow peaks at the resonance points $\mu = E_n$ ($n = 1, 2, 3...$), and the height and width of these peaks depend on the temperature and the scattering event (degree of disorder).

In this paper, the heat capacity of a quasi-two-dimensional ideal gas is studied as a function of the chemical potential at different temperatures. Based on known thermodynamic relationships, the density of states, the temperature derivative of the chemical potential, and the heat capacity of a two-dimensional electron gas are analyzed. For these quantities, low-temperature asymptotic formulas are obtained.

Numerical simulations show that, in the dependence of the heat capacity on the chemical potential, at the resonance points $\mu = E_n$ ($n = 1, 2, 3...$) there are additional steps. The width of the additional steps is proportional to the temperature and they are connected by sharp changes in the value $d\mu/dT$ at the resonance point. In conclusion, the results of the work are briefly summarized.

2. Basic Relationships

Let us consider an ideal electron gas with a simple parabolic spectrum. Energy is measured from the bottom of the zone of a massive semiconductor. In a heterostructural quantum well, the energy of the transverse motion is quantized, and the electron gas becomes quasi-two-dimensional. One-particle spectrum can be represented in the form [1]

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

where $k^2 = k_x^2 + k_y^2$-wave vector, E_n are the energy levels of the transverse motion, and is the effective mass of the electron. The total two-dimensional concentration is

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

where $g_0 = m/\pi\hbar^2$ and $f(E)$ is the Fermi-Dirac distribution function. The thermodynamic density of a state [9] is defined as

$$g_s = \frac{\partial n_s}{\partial \mu} = g_0 \sum_n \frac{1}{e^{(E_n - \mu)/T} + 1} \quad (3)$$

Expressions for the heat capacity of a gas can be obtained by differentiating the total energy

$$U_s = g_0 \sum_n \int_{E_n}^{\infty} E f(E)\, dE \quad (4)$$

by temperature, i.e., $C_s = \partial U_s / \partial T$. We represent it in the form

$$C_s = C_1 + \frac{d\mu}{dT} C_2 \quad (5)$$

where

$$C_1 = g_0 \sum_n \int_{(E_n - \mu)/2T}^{\infty} \frac{x(\mu + 2xT)}{\cosh(x)^2} dx \quad (6)$$

$$C_2 = \frac{g_0}{2} \sum_n \int_{(E_n - \mu)/2T}^{\infty} \frac{\mu + 2xT}{\cosh(x)^2} dx \quad (7)$$

here $x = (E - \mu)/2T$. A temperature derivative of the chemical potential $d\mu/dT = -B/A$ can be found from the conditions of constancy of the number of particles (2), where

$$B = \sum_n \left[\ln\left(1 + e^{(\mu - E_n)/T}\right) + \frac{E_n - \mu}{T\left(e^{(E_n - \mu)/T} + 1\right)} \right] \quad (8)$$

$$A = \sum_n \frac{1}{e^{(E_n - \mu)/T} + 1} \quad (9)$$

First, let us analyze the low-temperature asymptotics of these formulas.

(i) Let the chemical potential μ be near the level E_N, and the temperature is sufficiently low $\mu \sim E_N$, $T << E_N - E_{N-1}$. Then in the expressions (6) and (7) all the summands with $\mu \sim E_N < E_n$ exponentially small and N–1 the term with $\mu \sim E_N > E_n$ give a finite contribution. By retaining also the N - term (since $\mu \sim E_N$), from (6) and (7) we obtain ($N > 1$)

$$\begin{aligned} C_1 &= g_0 (N-1) \int_{-\infty}^{\infty} \frac{x(\mu + 2xT)}{\cosh(x)^2} dx \\ &\quad + g_0 \int_{(E_N - \mu)/2T}^{\infty} \frac{x(\mu + 2xT)}{\cosh(x)^2} dx \\ C_2 &= \frac{g_0}{2} (N-1) \int_{-\infty}^{\infty} \frac{\mu + 2xT}{\cosh(x)^2} dx \\ &\quad + \frac{g_0}{2} \int_{(E_N - \mu)/2T}^{\infty} \frac{\mu + 2xT}{\cosh(x)^2} dx \end{aligned} \quad (10)$$

The first integrals in these expressions are calculated analytically. Then

$$C_1 = g_0 \left[(N-1) T \frac{\pi^2}{3} + \int_{(E_N - \mu)/2T}^{\infty} \frac{x(\mu + 2xT)}{\cosh(x)^2} dx \right] \quad (11)$$

$$C_2 = g_0 \left[(N-1) \mu + \frac{1}{2} \int_{(E_N - \mu)/2T}^{\infty} \frac{\mu + 2xT}{\cosh(x)^2} dx \right] \quad (12)$$

The remaining integrals in (11) and (12) can also be calculated analytically, but the results are cumbersome. These integrals can be calculated numerically with good accuracy.

Similarly, near the resonance point $\mu \sim E_N$ under the condition $T << E_N - E_{N-1}$ of (8) and (9) we have

$$\begin{aligned} B &= \ln\left(1 + e^{(\mu - E_N)/T}\right) + \frac{E_N - \mu}{T\left(e^{(E_N - \mu)/T} + 1\right)} \\ A &= N - 1 + \frac{1}{e^{(E_N - \mu)/T} + 1} \end{aligned} \quad (13)$$

Thus, near the resonance point $\mu \sim E_N$ under the condition $T << E_N - E_{N-1}$ the quantity is equal $d\mu / dT$ to

$$\begin{aligned} &\frac{d\mu}{dT} \\ &= -\frac{\left(e^{(E_N - \mu)/T} + 1\right) \ln\left(1 + e^{(\mu - E_N)/T}\right) + (E_N - \mu)/T}{\left(e^{(E_N - \mu)/T} + 1\right)(N-1) + 1} \end{aligned} \quad (14)$$

In the approximation considered, for the density of states (3) we can obtain the following formula:

$$g_s = g_0 \left[N - 1 + \frac{1}{e^{(E_N - \mu)/T} + 1} \right] \quad (15)$$

The quantity $d\mu/dT$ also determines the entropy per electron $s = (\partial S/\partial n_s)_T = -(\partial \mu/\partial T)_{n_s}$, and the low-temperature dependence $s(\mu)$ is studied in detail in [18]. Using (11), (12), and (14), according to formula (5), we can find the specific heat value near the resonance point $\mu = E_N$, and also the line shape $C_s(\mu)$ near $\mu \sim E_N$.

(ii) Suppose that the chemical potential μ is between the levels E_{N-1} and E_N, i.e., $E_{N-1} < \mu < E_N$ and the temperature is low enough $T << E_N - E_{N-1}$. Then in the expressions (11) and (12) the values of the integrals are exponentially small. Neglecting them, we obtain

$$C_1 = g_0 (N-1) T \frac{\pi^2}{3} \quad (16)$$

$$C_2 = g_0 (N-1) \mu \quad (17)$$

Under the conditions considered, the quantity $d\mu/dT$ in formula (14) is exponentially small. Thus, according to (5), the specific heat in this limit has the form

$$C_s = C_1 = g_0 (N-1) T \frac{\pi^2}{3} \quad (18)$$

and the density of state (15) reduces to the form

$$g_s = g_0 (N-1) \quad (19)$$

It can be seen from the comparisons (18) and (19) that when the condition $E_{N-1} < \mu < E_N$, $T << E_N - E_{N-1}$ and $T << |E_N - \mu|$, both the density of the state and the

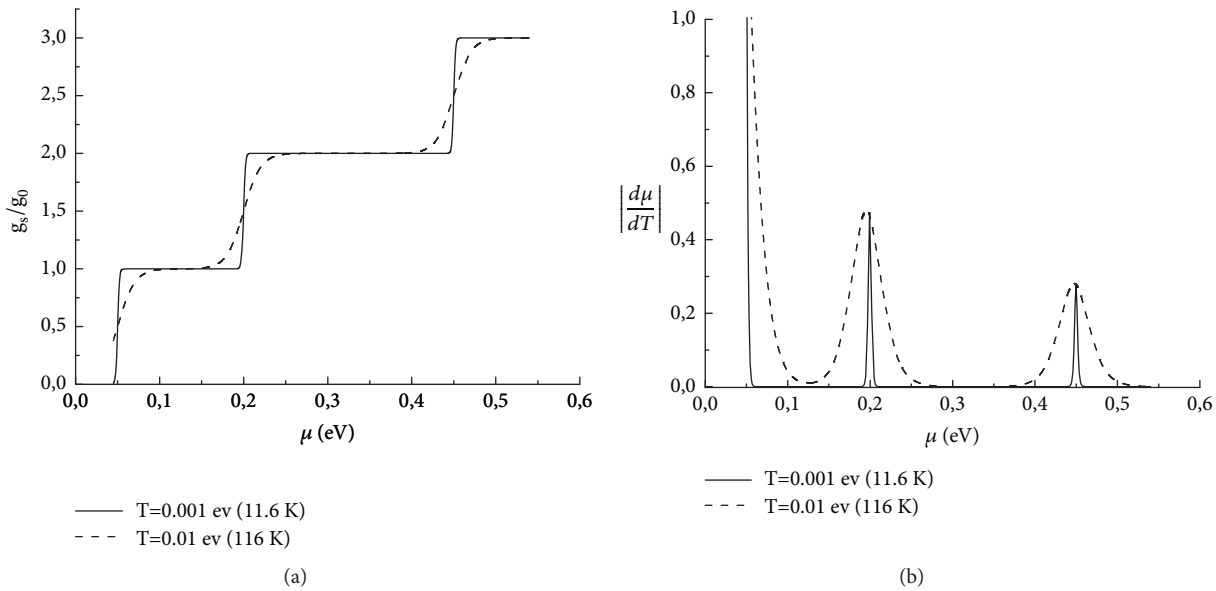

Figure 1: Dependences (a) of the density of states $g_s(\mu)/g_0$ and (b) a derivative of the chemical potential $|d\mu/dT|$ at $E_1 = 0.05$ eV different temperatures: T = 0.001 eV (11.6 K), solid lines, and T = 0.01 eV (116 K), dashed lines.

heat capacity of a quasi-two-dimensional ideal gas g_s, vary abruptly with increasing chemical potential μ

$$\frac{3C_s}{\pi^2 T} = g_s = N - 1 \tag{20}$$

(3) At low temperatures at the resonance points $T << E_N - E_{N-1}$ and $\mu = E_N$ from (11) and (12) we have

$$C_1 = g_0 \left[(N-1)\, T \frac{\pi^2}{3} + \int_0^\infty \frac{x\left(E_N + 2xT\right)}{\cosh(x)^2} dx \right] \tag{21}$$

$$C_2 = g_0 \left[(N-1)\, \mu + \frac{1}{2} \int_0^\infty \frac{E_N + 2xT}{\cosh(x)^2} dx \right] \tag{22}$$

The integrals in these expressions are calculated analytically. Then

$$C_1 = g_0 \left[T \frac{\pi^2}{3} \left(N - \frac{1}{2} \right) + E_N \ln(2) \right] \tag{23}$$

$$C_2 = g_0 \left[E_N \left(N - \frac{1}{2} \right) + T \ln(2) \right] \tag{24}$$

Similarly, it follows from (14) that

$$\frac{d\mu}{dT} = -\frac{\ln(2)}{N - 1/2} \tag{25}$$

Thus, at the resonance point the heat capacity (5) is

$$\begin{aligned} C_s &= C_1 + \frac{d\mu}{dT} C_2 \\ &= g_0 \left(N - \frac{1}{2} \right) T \frac{\pi^2}{3} \left\{ 1 - \frac{3 \ln(2)^2}{\pi^2 (N - 1/2)^2} \right\} \\ &\approx g_0 \left(N - \frac{1}{2} \right) T \frac{\pi^2}{3} \end{aligned} \tag{26}$$

For N=2, the second term in the curly bracket is approximately equal 0,065 but decreases rapidly with growth. It is approximately equal to half the sum of the successive steps of the heat capacity (18) obtained under the condition $E_{N-1} < \mu < E_N$. In a similar way, from (15) we can find an expression for the density of states at the resonance point

$$g_s = g_0 \left[N - \frac{1}{2} \right] \tag{27}$$

And in this limit the jumps in the specific heat (26) are due to a change in the density of states (27)

$$\frac{3C_s}{\pi^2 T} \approx g_s = N - \frac{1}{2} \tag{28}$$

3. Numerical Results and Discussion

At not too low temperatures, the dependence of the heat capacity on the chemical potential can be obtained only numerically, on the basis of relations (5) - (9). The explicit form of the electron spectrum in a heterostructural quantum well can be determined by solving the quantum-mechanical problem. In the future, in numerical calculations, we use its simple approximation $E_n = E_1 n^2$, $n = 1, 2, 3 \ldots$

First, consider the dependence of the density of states $g_s(\mu)$ and the derivative $d\mu/dT$ of the chemical potential μ. The results of numerical simulations of these quantities using formulas (3) and (8) and (9) are $E_1 = 0.05$ eV shown in Figure 1.

The nature of the dependence $g_s(\mu)$ is well known [2]. According to (3), the total density of the state is equal to the sum of the density of states of sequentially located overlapping minibands. Sharp jumps are observed at sufficiently low temperatures, when the chemical potential crosses the bottom of the miniband.

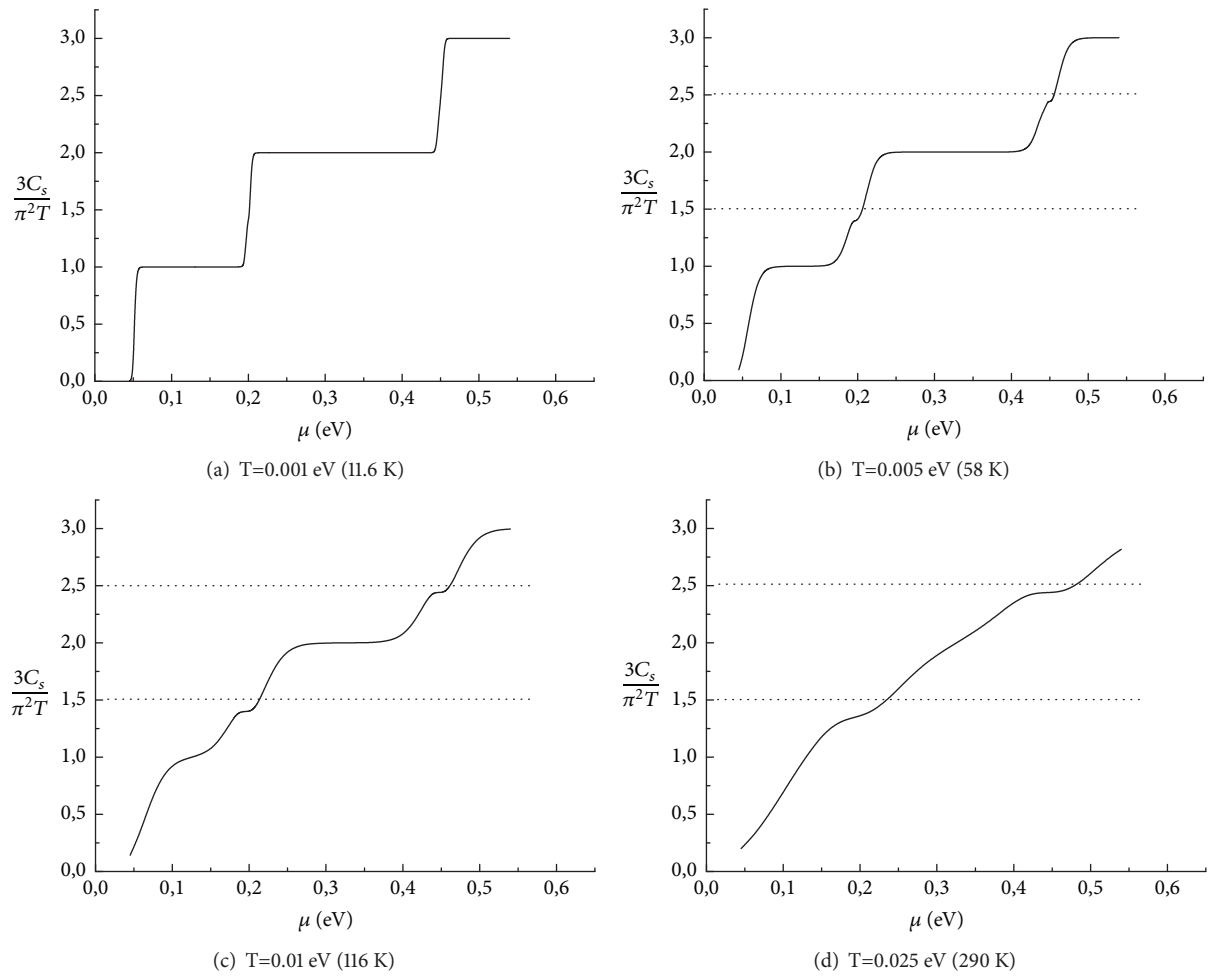

Figure 2: Dependences of the heat capacity of a quasi-two-dimensional electron gas on the chemical potential at $E_1 = 0.05$ eV and different temperatures: (a) T = 0.001 eV (11.6 K), (b) T = 0.005 eV (58 K), (c) T = 0.01 eV (116 K), and (d) T = 0.025 eV (290 K).

With increasing temperature, sharp step changes $g_s(\mu)$ turn into a smoother dependence (dashed line in Figure 1(a)). As can be seen from the relations (3), this is due to the smoothing of the Fermi-Dirac step near $E \sim \mu$ the temperature increase.

The nature of the dependence of $d\mu / dT$ on the chemical potential was studied in detail in [18]. As can be seen from the graph (solid line in Figure 1(b)), at sufficiently low temperatures at resonance point $\mu = E_n$ the value $d\mu / dT$ has sharp peaks. According to formula (25), the height of these peaks depends on the quantum level number N and is independent of temperature and effective mass. The height of the peaks decreases with increasing quantum number N. As the temperature increases, the widths of these peaks increase (the dashed line in Figure 1(b)). Inside the miniband $E_{N-1} < \mu < E_N$, where the density of state is constant (at $T \longrightarrow 0$) and the derivative of $d\mu / dT$ is exponentially small.

As can be seen from the figure, at low temperatures the steps of $g_s(\mu)$ and the peaks in $d\mu/dT$ are well described by the asymptotic formulas (19), (25), and (27). Near the resonance point, the shape of the lines can also be described with the help of relations (14) and (15).

Let us now consider the dependence of the specific heat on the chemical potential $C_s(\mu)$. The results of numerical calculations based on the relations (5)-(9), at $E_1 = 0.05$ eV are shown in Figure 2.

According to Figure 2(a), at sufficiently low temperatures, the specific heat varies abruptly, i.e., practically repeating the dependence of the density of states (see Figure 1(a)). This is also seen from the analytical result (20). The peak width of derivative $d\mu / dT$ at the resonance point is also small $\sim T$ and is not noticeable in the graph.

With increasing temperature, additional weak steps appear at resonance points $\mu = E_n$, Figure 2(b). With further temperature increase, the width of these steps increases, which is more noticeable in the graph of Figure 2(c). We note that as the temperature increases, the steps blur simultaneously. According to Figure 2(d), at temperature T=290 K, the main steps are practically blurred and the traces of additional steps are still noticeable.

As can be seen from the figure, at low temperatures, far from the resonance point $E_{N-1} < \mu < E_N$, the steps in dependence $C_s(\mu)$ are well described by formula (18) and at the resonance point by formula (28).

The low-temperature value of the heat capacity at the resonance point $3C_s(\mu = E_N)/(\pi^2 T) \approx N - 1/2$ in Figures 2(b)–2(d) is represented by a horizontal dot line, which are obtained for $N = 2, 3$. A small deviation from the numerical result is due to the approximation admitted in (26).

4. Conclusions

In this paper, based on a simple model, the results of an analysis of the heat capacity of a quasi-two-dimensional ideal gas are presented. The calculations do not take into account many factors, such as the scattering process, electron-electron interaction, and so on. which can significantly affect the results.

In spite of this, it was found that in a simple model of a quasi-two-dimensional ideal gas, depending on the specific heat from the chemical potential other than the basic ones-ladder-like steps that are connected by the peculiarities of the density-of-states variations, there are still additional steps-the values of $d\mu$ / dT due to negative peaks at the resonance points. The width of the additional steps increases with temperature. With an increase in temperature, when the main steps are practically blurred, there are still visible marks from the additional steps (see Figure 2(d)).

Asymptotic analyzes of the density of state $g_s(\mu)$, derivative $d\mu/dT$, and heat capacity $C_s(\mu)$ at low temperatures, both at resonance points and far from it, are carried out. Simple formulas are obtained for them. Such singularities of heat capacity, obtained on the basis of a simple model, serve as a test when considering more realistic models.

Data Availability

The results of this study are included in the article and can be made freely available. Also, the authors embedded original figure in the text manuscript.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

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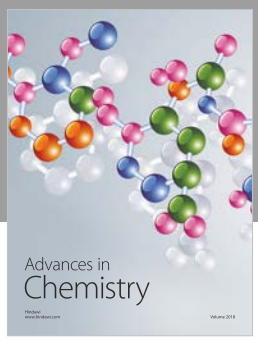

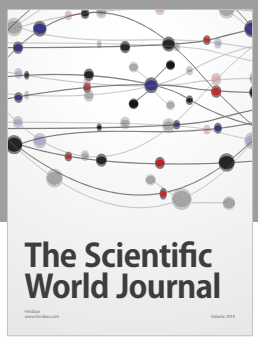

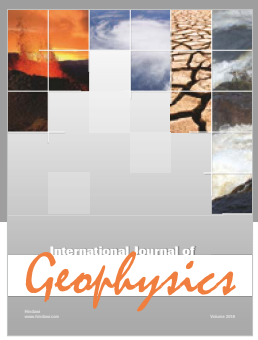

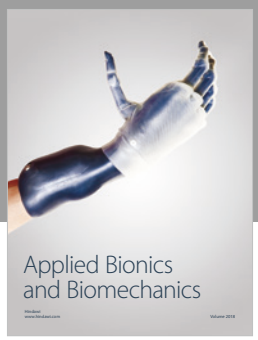

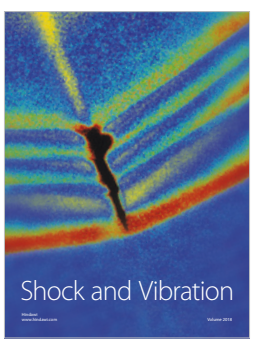

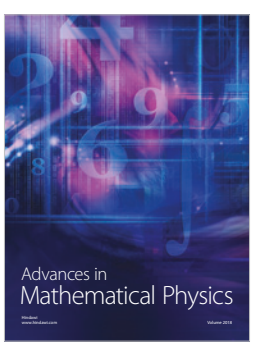

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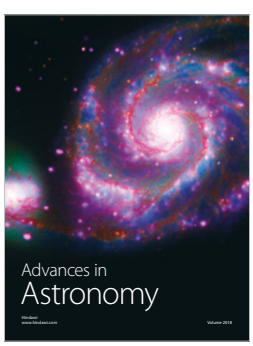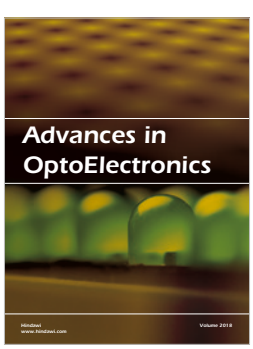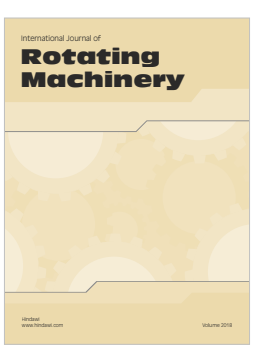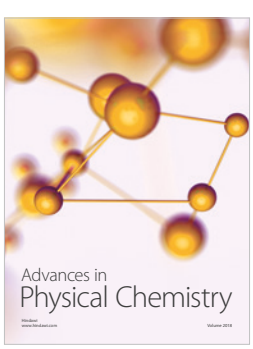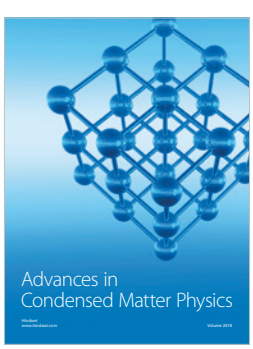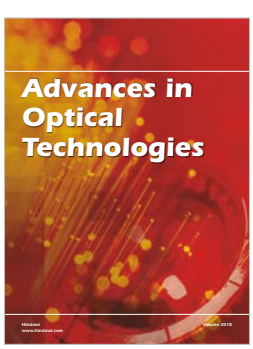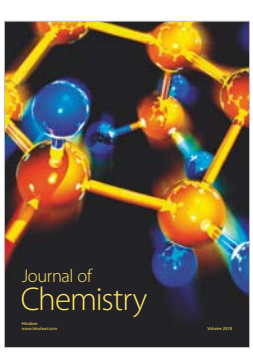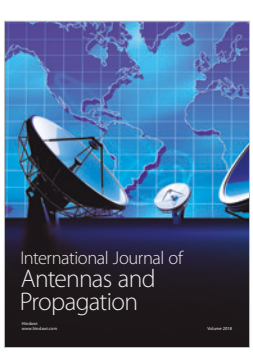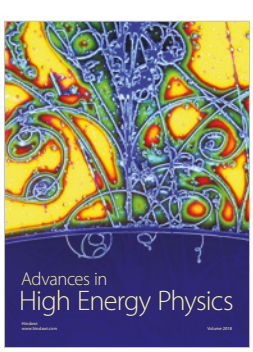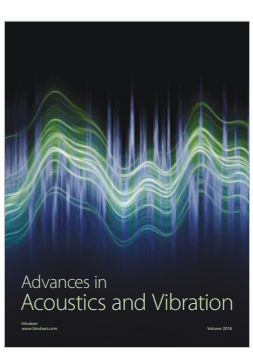
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