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RESEARCH ARTICLE

Mean energy and entropy of the electron gas in a semiconductor nanoplatelet: the role of the number of monolayers and geometric sizes

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ABSTRACT: This paper investigates the thermodynamic properties of an electron gas confined in a semiconductor nanoplatelet. Electrons are treated as non-interacting fermions, and the partition function of the system is calculated using the Boltzmann approximation. Using the resulting expressions for the partition function, the mean energy and entropy of the system are numerically calculated. The dependences of these thermodynamic parameters on temperature, the geometric parameters of the nanoplatelet, the number of monolayers, and the number of particles in the gas are examined. It is shown that size effects significantly influence the thermodynamic characteristics of the system, particularly at low temperatures and with small characteristic sizes of the nanoplatelet. The results obtained are of interest for describing the thermodynamic properties of electron systems in semiconductor nanostructures.

Keywords: Nanoplatelet; Electron Gas; Partition Function; Mean Energy; Entropy.

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1. INTRODUCTION

Semiconductor nanoplatelets are quasi - two - dimensional nanostructures with a thickness of several monolayers and controlled at the atomic level, while their lateral dimensions are one to two orders of magnitude larger than the thickness. In nanoplatelets, quantum confinement is realized only in one direction — along the thickness axis — which allows them to be considered an analogue of quantum wells. This fundamentally distinguishes them from quantum dots, in which the motion of charge carriers is confined in all three dimensions, whereas in nanoplatelets, carriers remain free in the plane of the plate [1–5]. Due to strong quantum confinement in one direction and large lateral dimensions, nanoplatelets have high exciton binding energy, high optical gain, and narrow photoluminescence lines [6–8]. The energy of nanoplatelets can be tuned with an accuracy of one monolayer, making them exceptionally attractive for optoelectronic applications. An important feature of semiconductor nanoplatelets is the formation of an electron gas in them — a system of delocalized charge carriers, the movement of which is significantly limited in the transverse direction. As a result of quantum confinement, the electron energy spectrum is split into discrete subbands corresponding to quantized states along the thickness of the plate, while the spectrum remains quasi-continuous in the plane of the structure. The number of filled subbands, and consequently the behavior of the electron gas, is determined by the size of the nanoplate and the number of nanolayers comprising it, opening the possibility of targeted control of the system's electronic properties.

The study of the quasi-two-dimensional electron gas is fundamentally important for understanding the physical phenomena in semiconductor materials, including charge transport, high-mobility phenomena,

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and the quantum properties of nanostructures that underlie modern electronic and nanotechnological devices [9, 10]. Among the thermodynamic characteristics of the system, the average energy and entropy occupy a special place. The average energy of the electron gas determines the thermal capacity of the system and is directly related to the nature of the filling of the energy levels, reflecting the influence of both size quantization and temperature effects. Entropy, in turn, serves as a measure of the statistical uncertainty of the system and is sensitive to changes in the number of accessible quantum states with variations in temperature, the geometric parameters of the nanoplatelet, and the number of particles in the system. Determining these thermodynamic quantities makes a fundamental contribution to the understanding necessary for the practical use of nanostructured materials in various technological applications.

Thus, a systematic theoretical study of the thermodynamic parameters of the electron gas in semiconductor nanoplatelets as a function of temperature, geometric characteristics of the structure, and the number of particles appears to be a relevant and significant task from both fundamental and applied perspectives. The aim of this work is to theoretically study the average energy and entropy of the noninteracting electron gas in a semiconductor nanoplatelet within the Boltzmann approximation, as well as to analyze the dependences of these thermodynamic parameters on temperature, nanoplatelet size, the number of nanolayers, and the number of particles in the system.

2. THEORETICAL MODEL

2.1. Electron states in NPL

Let us consider a non-interacting electron gas in a CdSe nanoplatelet (NPL). The CdSe NPL is modeled as a rectangular parallelepiped with lateral dimensions L_x and L_y, and a significantly smaller thickness L_z. Due to the disparity in spatial dimensions, quantum confinement is most pronounced along the z-axis. This strong anisotropy gives rise to a subband structure in which the in-plane motion is associated with discrete energy levels resulting from axial quantization. In the lateral directions (x and y), the carrier is confined within an ideal two-dimensional infinite potential well. In contrast, the axial potential consists of a finite confinement well together with a polarization-induced self-energy term. The electron self-potential along the z-axis is described within the framework proposed by Kumagai and Takagahara [11]. The resulting potential along the z-axis combines confinement and self-contributions:

$$V_{\text{tot}}(z) = V_{\text{conf}}(z) + V_{\text{self}}(z), \tag{1}$$

where $V_{\text{conf}}(z)$ is the finite confinement potential of the NPL and $V_{\text{self}}(z)$ is the polarization-induced self-potential described within the Takagahara framework [12–14]. For the lateral confinement potential, $V_{\text{conf}}(x, y)$, a two-dimensional infinite potential well with impenetrable boundaries is employed [15].

The eigensystems corresponding to the axial and planar directions were calculated numerically using the finite element method (FEM), as illustrated in Figure 1.

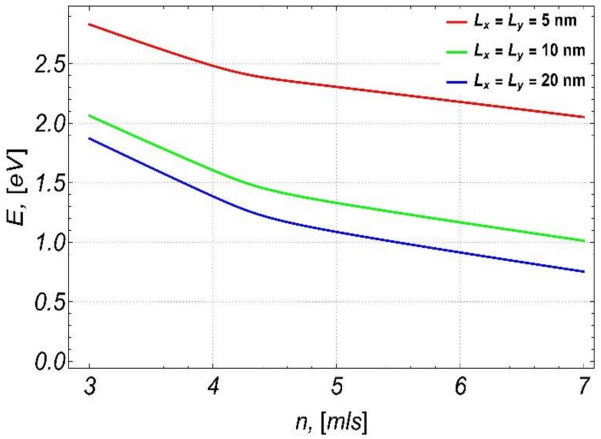


Fig. 1. Total energy dependency from monolayer numbers n for different NPL sizes L_x ; L_y.

2.2. Partition function

Now, let us assume that the NPL contains a weakly interacting electron gas with a discrete single-particle energy spectrum ε_i, where $i = 0, 1, \ldots, M-1$, containing a fixed number of particles N and available states M. Since electrons are fermions, the Pauli exclusion principle applies. The thermodynamic properties of such a system can be described within the Boltzmann approximation (Figure 2), for which the partition function is given by

$$Z(N) = \frac{1}{N!} \sum_{\nu} e^{-\beta \varepsilon_\nu}, \tag{2}$$

where $\beta = \frac{1}{k_{\text{B}} T}$ is the inverse temperature, k_{B} is the Boltzmann constant, T is the absolute temperature, and ν denotes the set of quantum states.

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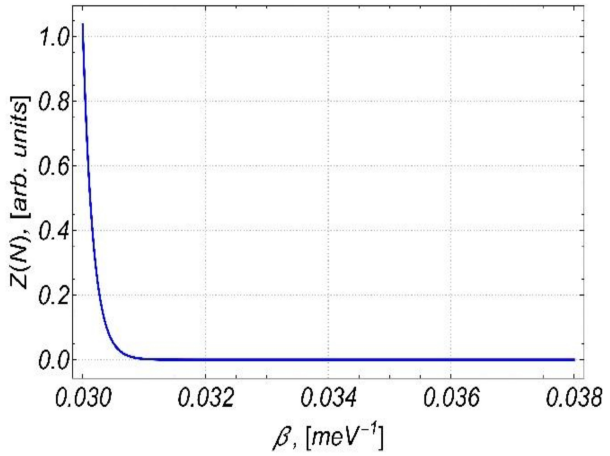


Fig. 2. Partition function dependency on inverse temperature β.

2.3. Mean energy

Having obtained the partition function $Z(N)$, we can proceed to calculate the thermodynamic and magnetic properties of the electron gas. The mean energy is given by

$$E = -\frac{1}{Z(N)}\frac{\partial Z(N)}{\partial \beta} \tag{3}$$

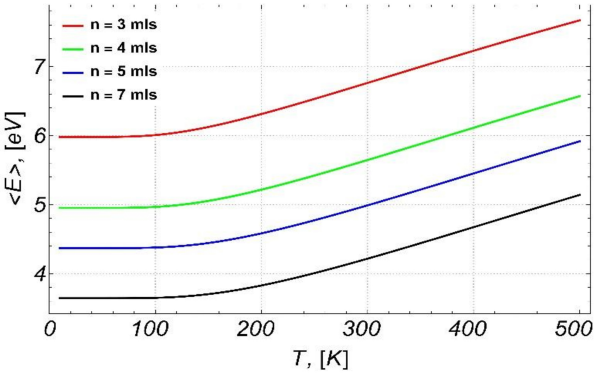


Fig. 3. Mean energy dependency from temperature T for different monolayer numbers n.

The dependence of the mean energy on temperature is shown in Figure 3. As can be seen from the graphs, a very weak increase is observed at relatively low temperatures, while the increase is more significant at relatively high temperatures. It should also be noted that an increase in the number of monolayers leads to a decrease in the mean gas energy due to a decrease in the size quantization effect in the axial direction. Figure 4 shows the dependence of the mean energy on the number of particles in the gas for different nanoplatelet base lengths. An increase in the number of particles leads to a linear increase in the mean energy. As in the previous case, increasing the nanoplatelet size results in a decrease in the mean energy due to the reduced effect of planar size quantization.

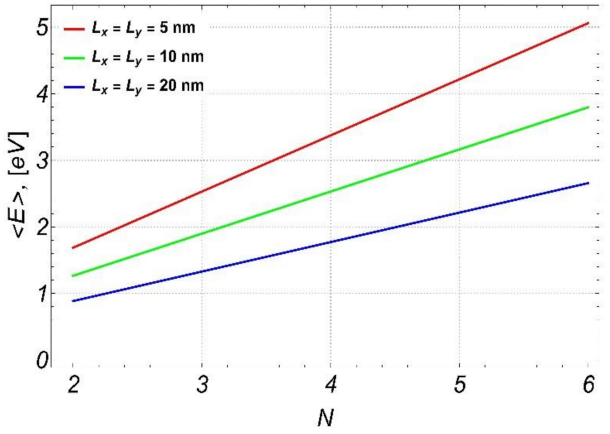


Fig. 4. Mean energy dependency from particle numbers for different NPL sizes L_x ; L_y.

2.3. Entropy

The entropy is given by

$$S = \frac{\partial}{\partial T}\left(\frac{1}{\beta}\ln Z(N)\right) \tag{4}$$

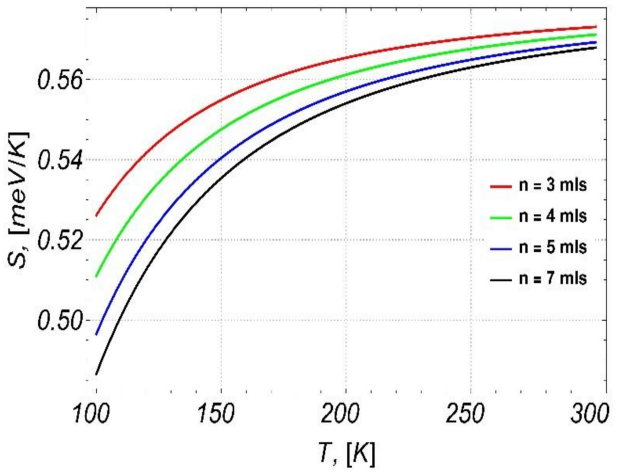


Fig. 5. Entropy dependency from temperature T for different monolayer numbers n .

Figure 5 shows the dependence of gas entropy on temperature for different values of the number of monolayers. An increase in temperature leads to an increase in entropy due to increased temporal motion of particles. However, as temperatures approach room temperature, saturation of the dependence is observed. An increase in the number of monolayers leads to a decrease in gas entropy

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due to increased particle localization. However, an increase in temperature leads to a decrease in this effect.

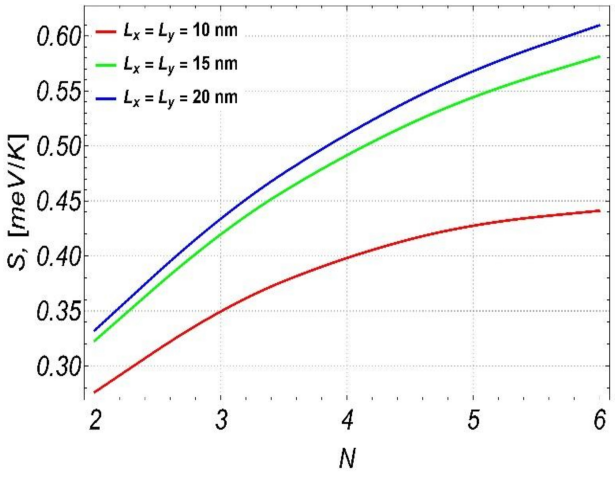


Fig. 6. Entropy dependency from particle numbers for different NPL sizes L_x ; L_y.

Figure 6 shows the dependence of gas entropy on the number of particles in the gas for different base lengths. An increase in the number of particles for a fixed nanoplatelet size leads to an increase in gas entropy. This can be explained by the fact that the freedom of particle movement decreases, thereby increasing chaos in the system.

4. CONCLUSION

In this work, we carried out a theoretical investigation of the thermodynamic characteristics of an electron gas confined in CdSe semiconductor nanoplatelet. Using the Boltzmann approximation to compute the partition function, we derived expressions for the mean energy and entropy of the system and performed numerical calculations. The analysis demonstrated that the geometric parameters of the nanoplatelet, its thickness, number of monolayers, and lateral dimensions, strongly affect the thermodynamic behavior of the electron gas, particularly at low temperatures and for small structural sizes. It was established that reducing the number of monolayers leads to significant changes in the energy spectrum and, consequently, to variations in both mean energy and entropy. Moreover, the number of particles in the system plays an important role in determining the filling of quantum states and the degree of statistical uncertainty. The obtained results confirm the key role of size effects in shaping the thermodynamic properties of nanostructured materials and show the possibility of deliberately controlling these properties by tuning the geometry of nanoplatelets. This opens up prospects for practical applications of electron gases in nanoplatelets in the design of new optoelectronic and nanophotonic devices, where control over energy and entropy characteristics may be critically important. Thus, the present study contributes to the fundamental understanding of quasi two-dimensional systems and provides a basis for further applied developments in nanophysics and nanotechnology.

DECLARATIONS

Ethical Approval

We affirm that this manuscript is an original work, has not been previously published, and is not currently under consideration for publication in any other journal or conference proceedings. All authors have reviewed and approved the manuscript, and the order of authorship has been mutually agreed upon.

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Availability of data and material

The datasets used and/or analyzed during the current study are available from the corresponding author on reasonable request.

Conflicts of Interest

The authors declare that they have no financial or personal interests that could have influenced the research and findings presented in this paper. The authors alone are responsible for the content and writing of this article.

Authors' contributions

M.K. Manvelyan: Writing – original draft, Visualization, Software, Investigation; **M.A. Mkrtchyan**: Writing – original draft, Software, Investigation, Methodology, Supervision.

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