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Thermodynamic Properties of a Quantum Ring Perturbed with Quantum Wells and Impurities

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In this work, we study the thermodynamic properties of a quantum ring in the presence of an additional quantum well and impurity in its circumstance. Effects of the number of impurities, impurities strengths, quantum ring radiuses and potential well depth on the mean energy, specific heat and entropy of a quantum ring have been investigated. We have seen that, if the temperature or quantum ring radius increases the entropy of the system also increases. Adding few impurities just at low temperatures can change the specific heat. At low temperatures and for small radius quantum rings, adding a quantum well even with a very small height can create a sharp sensible peak in the specific heat diagram versus temperature.

Keywords: Quantum rings, Mean energy, Specific heat, Entropy and tight binding model.

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1. INTRODUCTION

Rapid progress in the nano-science and nanotechnology makes the study of low-dimensional semiconductor hetero-structures as nanostructures essentials. superlattices, quantum wires, quantum dots, quantum wells quantum rings are the more promising systems [1-2]. These structures can change the physical properties through confining the charge carriers in one, two, and three dimensions.

In the past few years, several investigations on the heat capacity and entropy of nanostructures [3-6] have been made. Entropy can show the missing information on a concrete state of the system. Entropy is an elementary information concept. Effects of a single magnetic ion [6], helium-like confinement [7], electron-electron interactions [8], on the thermodynamics properties have also been studied. But, there is not a comprehensive study on the thermodynamic properties of a quantum ring with a quantum well in its circumstance. During our last works, we have studied the Physical properties of GaN/AlN constant total effective radius multi-well quantum rings (CTER-MWQR) under well number variation effects [9], optical properties of two-electron [10] and impurity included [11] GaN/AlN constant total effective radius multi-shell quantum rings (CTER-MSQR) and dots (CTER-MSQD). Finally, we have studied the miniband formation scenario in GaN/AlN CTEL-MSQDs [12].

Thermodynamics of a system with large number of particles within the Statistical mechanics theory can be studied by using of the probability theory. In order to calculate the physical quantities, an appropriate way is to use from energy fluctuations in the canonical ensemble. Within this method, in the present work, we have studied effects of the number of impurities, impurities strengths, quantum ring radiuses and potential well depth on the mean energy, specific heat and entropy of a quantum ring in the presence of an additional quantum well and impurity in its circumstance.

2. FORMALISM

A quantum ring with N number of sites of similar atoms can be modeled by a tight binding Hamiltonian as:

$$\hat{H}=\sum_{n=1}^{N}\left[\left(2t+V_n\right)c_n^{\dagger}c_n-tc_{n+1}^{\dagger}c_n-tc_n^{\dagger}c_{n+1}\right] \qquad (1)$$

Where $t=\hbar^2/\left(2m_e a^2\right)$, me, N, a, $c_n^{\dagger}$, c_n are the hopping matrix element, electron mass, number of sites, lattice constant, creation and annihilation operators, respectively. The additional on-site potentials V_n form a rectangular potential well of depth VConf within the circumstance of the quantum ring.

By using of the diagonalization of the Hamiltonian (1) the eigen-energies of the system can be obtained. By using of the energy fluctuations in the canonical ensemble correspondence with the microcanonical ensemble we can obtain the specific heat and entropy of the system. For this purpose, at the first step we find the mean energy as,

$$U\equiv\langle E\rangle=\frac{\sum_r E_r\exp\left(-\beta E_r\right)}{\sum_r\exp\left(-\beta E_r\right)} \qquad (2)$$

Where $\beta=1/T$. By differentiating it with respect to the parameter beta and holding the energy values E_r constant, we obtain,

$$\frac{\partial U}{\partial\beta}=-\frac{\sum_r E_r^2\exp\left(-\beta E_r\right)}{\sum_r\exp\left(-\beta E_r\right)}+\left[\frac{\sum_r E_r\exp\left(-\beta E_r\right)}{\sum_r\exp\left(-\beta E_r\right)}\right]^2 =\langle E\rangle^2-\langle E^2\rangle \qquad (3)$$

Now the specific heat can be given by

$$C_V=-\frac{1}{T^2}\frac{\partial U}{\partial\beta}=\frac{\partial U}{\partial\beta}T =\frac{1}{T^2}\left(\langle E\rangle^2-\langle E^2\rangle\right) \qquad (4)$$

Finally the entropy of the system can be written as

$$S=\frac{1}{TZ}\sum_r E_r\exp\left(-\beta E_r\right)+Ln\left(Z\right) \qquad (5)$$

where $Z=\sum_r\exp\left(-\beta E_r\right)$ is the partition function.

3. RESULTS AND DISCUSSION

In our calculations, we have studied the quantum rings with a quantum well in its circumstance. Effects of quantum well confining potential depths $V_{\text{conf}} = 0.1t$, $0.2t$, $0.4t$, $0.7t$, $1t$, $1.7t$ and $2.5t$, quantum ring radiuses $R = 50$ Å, 100 Å and 200 Å, as well as 1, 2 and 7 number of impurities with different strengths $I_S = 0.1t$, $1t$, and $2.5t$ on the mean energy, specific heat and entropy of the system have been studied. For comparison purposes we have also studied the quantum ring in the absence of the quantum wells or impurities within its circumstance (clean ring).

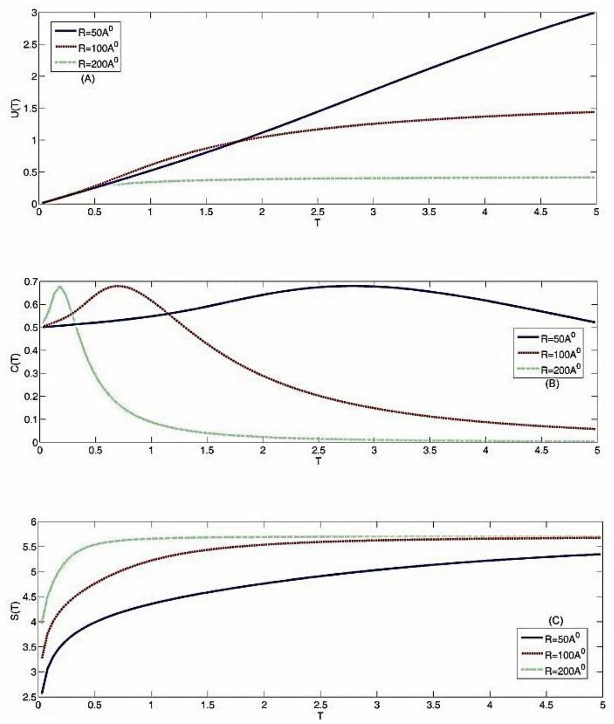

Fig. 1 – Panel (A): variation of the mean energy as a function of the temperature for a clean quantum ring (without additional quantum well or impurity) with radiuses $R = 50$ Å, 100 Å and 200 Å. Lines details have been specified on the panel. Panels (B) and (C) are same as the panel (A) but they show the specific heat and entropy of the system, respectively

By using of the diagonalization of the tight binding Hamiltonian (1), eigen-energies of the quantum ring system can be obtained. Then by using of the equations (2), (4) and (5) we are able to calculate the mean energy, specific heat and entropy of the system. At first, we assume a clean ring with no impurity of additional quantum well. In the figure 1: Panel (A): We have presented the variation of the mean energy as a function of the temperature for a clean quantum ring with radiuses $R = 50$ Å, 100 Å and 200 Å. Lines details have been specified on the panel. Panels (B) and (C) are same as the panel (A) but they show the specific heat and entropy of the system, respectively. The mean energy changes linearly with temperature for a 50 Å quantum ring. If we increase the ring radius to 100 Å and 200 Å, the non-monotonic behavior of the mean energy will be revealed. For this larger radius quantum rings, the mean energy saturates at a critical temperature. This critical temperature reduces when the quantum ring radius increases. The corresponding specific heats have been plotted in the panel (B). These specific heats have a peak when we plot then as a function of the temperature. The position of the peak decreases when we increase the quantum ring radiuses. At the same time the full width at half maximum (FWHM) of the peaks reduces as the quantum ring radiuses increases. However, roughly speaking we can say that at high temperatures the specific heat decreases when the quantum ring radiuses increases. In the Panel (C) of this figure we have presented the variation of the entropy as a function of the temperature. As the temperature increases the entropy of the system also increases and then saturates. Another fact is that by increasing of the quantum ring radius the entropy of the system also increases.

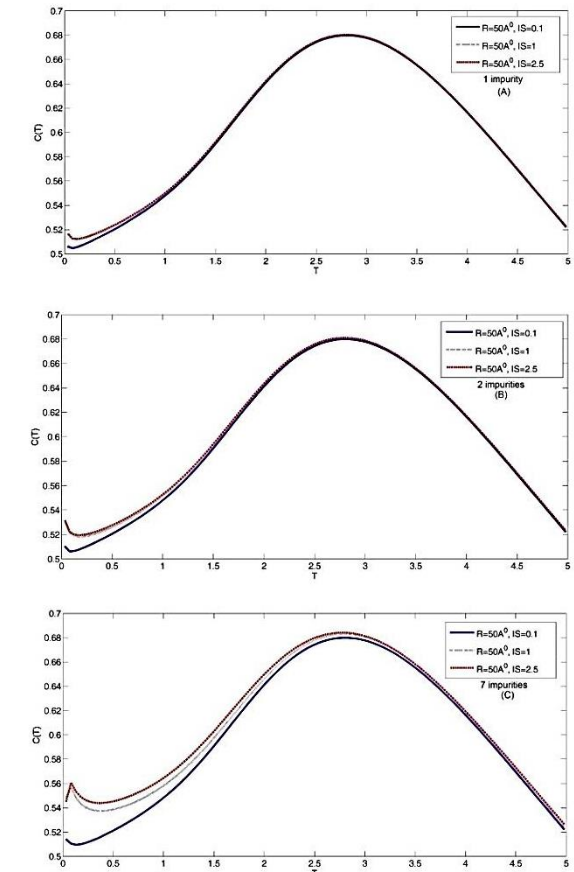

Fig. 2 – Panel (A): variation of the specific heat as a function of the temperature for a quantum ring with an impurity. We assume $R = 50$ Å and different impurity strengths $I_S = 0.1t$, $1t$ and $2.5t$. Lines details have been specified on the panel. Panels (B) and (C) are same as the panel (A) but they show the specific heat of the systems with 2 and 7 number of impurities, respectively

At this step we add some impurities with different strengths to the quantum ring and study the specific heat of the system. In the figure (2) we have shown the variation of the specific heat as a function of the temperature for a quantum ring with an impurity (Panel (A)). We have assumed $R = 50$ Å and changed the impurity strengths $I_S = 0.1t$, $1t$ and $2.5t$. Lines details have been specified on the panel. As it is clears from this panel, at high temperatures the specific heat does not change if we increase the impurity strength. But at low temperatures (near the origin), the specific heat increases if we increase the impurity strengths. If we increase the number of impurities to 2 and repeat the panel (A), we find the panel (B). Adding another impurity also change the specific heat at low temperatures. However, for this new system with 2 impurities, the specific heat increases more when we increase the impurity strength. Another fact is that by adding an impurity to the panel (A) we can affect the specific heat at higher temperatures. In the panel (B), different lines have been separated at higher temperatures. Now, we increase the number of impurities to 7 and plot the panel (C). All things are similar to that of we have described for the panel (B) but there is a difference.

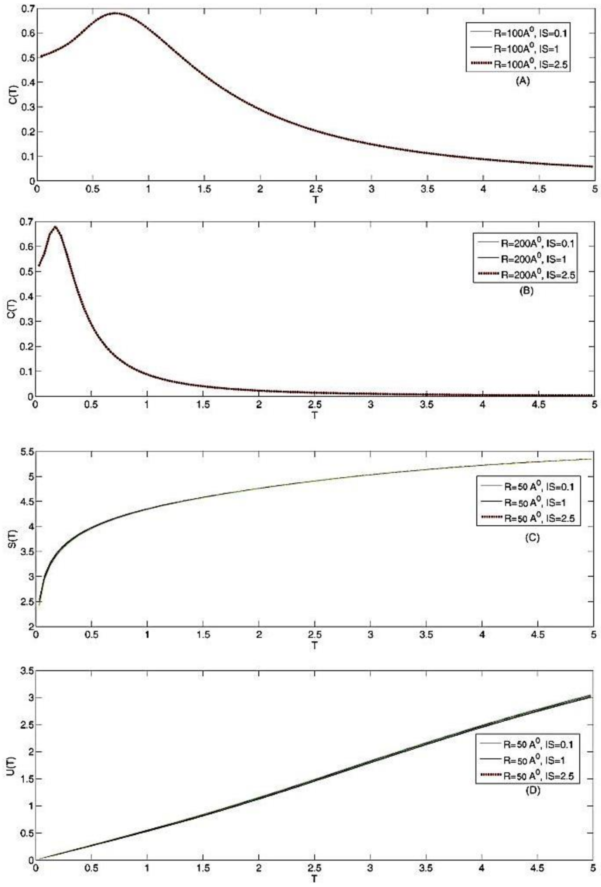

Fig. 3 – Panel (A): variation of the specific heat as a function of the temperature for a quantum ring with 7 impurities. We assume $R = 100$ Å and different impurity strengths $I_S = 0.1t$, $1t$ and $2.5t$. Panel (B) is same as the panel (A) but it depicted for $R = 200$ Å. Panels (C) and (D) are same as the panel (A) but they show the specific heat and entropy of the system, respectively. In the two last panels we assumed $R = 50$ Å

For the system with 7 number of impurities the specific heat increases as the impurity strengths increase (this occur for larger temperature interval), but as the impurity strength increases a new peak will be created in the specific heat diagram at low temperatures. The heights of this peak also increase when the impurity strength increases. To see the effect of the quantum ring radius when there is an impurity in it, we have plotted the variation of the specific heat as a function of the temperature for a quantum ring with 7 impurities in the Panel (A) of the Figure 3.

We assume $R = 100$ Å and changed the impurity strength $I_S = 0.1t$, $1t$ and $2.5t$. As we can see, by increasing of the impurity strength nothing changes. Panel (B) is same as the panel (A) but it depicted for $R = 200$ Å. Comparing the panel (A) and (B) reveals that: the specific heat peak position moves to lower temperatures when we increase the quantum ring radius. However, the specific heat of this system also do not change when we increases the impurity strength.

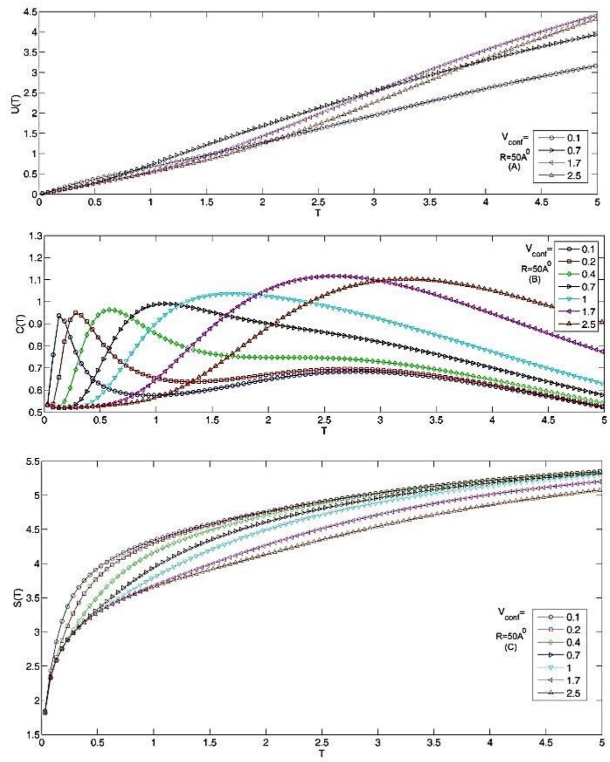

Fig. 4 – Panel (A): variation of the mean energy as a function of the temperature for a quantum ring with an additional quantum well in its circumstance. We assumed the quantum radius $R = 50$ Å as well as different confining potential depths $V_{\mathrm{conf}} = 0.1t$, $0.7t$, $1.7t$ and $2.5t$. Lines details have been specified on the panel. Panels (B) and (C) are same as the panel (A) but they show the specific heat and entropy of the system, respectively. In the two last panels we have studied more confining potential depths $V_{\mathrm{conf}} = 0.1t$, $0.2t$, $0.4t$, $0.7t$, $1t$, $1.7t$ and $2.5t$

At this point we study the effect of a quantum well in the circumstance of a quantum ring. Panel (A) of the Figure (4) presents the variation of the mean energy as a function of the temperature. Here, we assumed the quantum radius $R = 50$ Å as well as different confining potential depths $V_{\mathrm{conf}} = 0.1t$, $0.7t$, $1.7t$ and $2.5t$. Lines details have been specified on the panel.

As it is clear, the mean energy increases when the temperature increases. However, this behavior is linear for systems with small confining potentials. But if we increase the confining potential depth, the mean energy of the system grows more rapidly and in a non monotonic behavior. In the next panel (B), we have plotted the corresponding specific heat of the system.

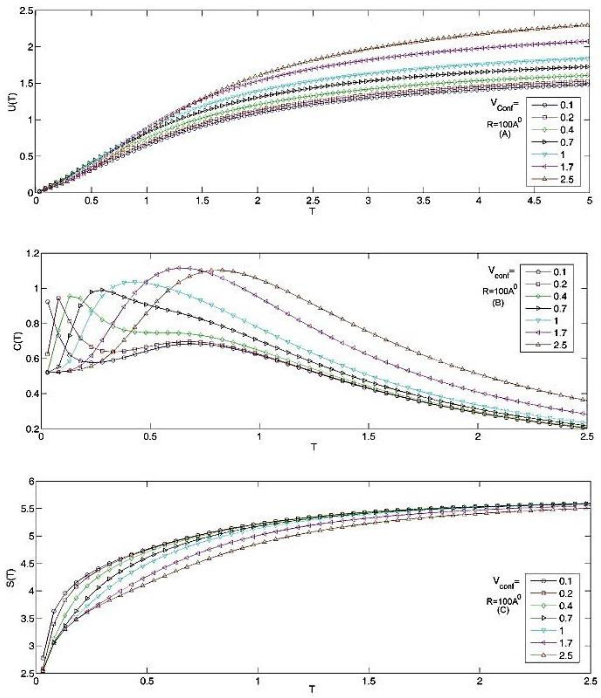

Fig. 5 – this figure is same as the Figure (4) but here we have assumed quantum radius $R = 100$ Å and in all panels we have used confining potential depths $V_{conf} = 0.1t$, $0.2t$, $0.4t$, $0.7t$, $1t$, $1.7t$ and $2.5t$

In this panel and the panel (C), we have studied more confining potential depths $V_{conf} = 0.1t$, $0.2t$, $0.4t$, $0.7t$, $1t$, $1.7t$ and $2.5t$. If we compare the blue solid line of the panel (B) of the Figure 1 with this diagram we see that adding a quantum well even with a very small height $V_{conf} = 0.1t$, can create a sharp sensible peak in the specific heat diagram as a function of the temperature. However, a quantum well can be regarded as a bunch of impurities brought together. For quantum rings with a quantum well in its circumstance this phenomenon is more considerable. For a quantum ring with a quantum well in its circumstance ($V_{conf} = 0.1t$), there are two peaks in the diagram of the specific heat as a function of the temperature. One of these peaks is sharp and the other has been broadened. By increasing of the confining potential V_{conf} these two peaks merge. The peak of the systems with larger V_{conf} is larger and has been more broadened. Panel (C) also is same as the panel (A) but it shows the entropy of the system. As we can see in this panel, as the confining potential V_{conf} increases the entropy of the system decreases.

We see that for all confining potential depths, the mean energy increases and then saturates as the temperature increases (Fig. 5). For $V_{conf} = 0.1t$ there is not the peak which appeared in the panel (B) of the Figure 4 for quantum ring radius $R = 50$ Å, but if we increase the confining potential to $V_{conf} = 0.2t$, that peak again will be created. We received that, at high temperatures all systems with different confining potential have same entropy. But they are more distinct at low temperatures.

4. CONCLUSIONS

In the this study, we investigated the effects of the number of impurities, impurities strengths, quantum ring radiuses and potential well depth on the mean energy, specific heat and entropy of a quantum ring. We showed that, for clean rings, the mean energy changes linearly with temperature for small radius quantum rings while for large radius quantum rings the mean energy saturated at a critical temperature and this critical temperature decreased as the quantum ring radius increased. Specific heat peak position and FWHM of the peak occurred in lower temperatures when the quantum ring radiuses increased. When the temperature or quantum ring radius increased the entropy of the system also increased. Adding few impurities just at low temperatures could change the specific heat. At these temperatures the specific heat increased when we increased the impurity strengths. However, by adding more impurities we could affect the specific heat at higher temperatures. As the impurity strength increased a new peak created in the specific heat diagram at low temperatures. In the presence of the quantum well in the circumstance of the quantum ring, as the confining potential depth increased the mean energy of the system changed in a non-monotonic manner. Adding a quantum well even with a very small height could create a sharp sensible peak in the specific heat diagram as a function of the temperature. This phenomenon occurred at low temperatures and for quantum rings with small radiuses. Finally, as the confining potential height increased, entropy of the system decreased.

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