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Influence of Hole-Phonon Coupling on Magneto–Transport and Magnetocaloric Properties of the Dilute Ferromagnetic Semiconductor $Ga_{1-x}Mn_xAs$ in Confined Systems †

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Abstract: In this work the thermodynamic and magnetic properties of a two-holes parabolic quantum dot are studied in the presence of hole-hole and hole-phonon interactions in the range of temperature from 0 K to 50 K and in magnetic fields varying from −5 to 5 T. Calculations of energy levels of two-holes states have been performed with a resolution of the Schrödinger's equation and all thermodynamic functions are derived by using the canonical ensemble. Our formalism's numerical calculation is essentially applied to dilute ferromagnetic semiconductors $Ga_{1-x}Mn_xAs$ containing 3% Mn. The founded results show that the magnetic an thermodynamic properties are influenced by the magnetic field, hole-phonon and hole-hole interactions, and the confinement. The analysis of magnetization and susceptibility justifies that The $Ga_{1-x}Mn_xAs$ quantum dots with 3% Mn content are ferromagnetically even in the absence of a magnetic field, and show the antiferromagnetic behaviour under certain conditions. This results are similar with the majority of the previous works.

Keywords: Hole−Phonon Interaction; Diluted Magnetic Semiconductors; Magnetic Susceptibility

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2. Introduction

With the development of experimental techniques along with the theoretical understanding of the subject of spintronics and other related areas, the manipulation of quantum dots with the external magnetic, electric, and electromagnetic fields have gained a lot of prominence in recent times. The surge of the articles coming in literature is an Indicator of the importance of such studies [1–5]. It is also interesting to note that as far as Quantum heterostructures such as quantum wells, wires, and dots are concerned, applications based on electron states have been dominating the studies. Strange enough that applicationbased hole states of such quantum systems have received less attention. One possible reason for it may be slow mobility of holes compared to the electrons in confinement. Due to slow mobility, devices based on higher power consumption may lead lesser commercial demands. Also, higher input powers or fields may shorten lives of such devices. Despite these possible reasons, study of two (multiple) hole quantum devices is very interesting. As in the case of two electron systems, the Coulombic interaction between electrons under confinement remains dominant and plays an important part, while determining the energy states, matrix elements, and the modification of wave functions. More or less, hole-hole interaction plays the same role. The hole states in quantum wells, wires and dots are now slowly gaining interest in the recent times. As holes have strong spin-orbit coupling

(SOC) and this strong SOC helps in controlling the spin of hole states and that makes the possibility of hole states as qubits [6]. The large SOC of holes in QDs helps in overcoming recoherence [7,8]. The importance of hole states in QDs is documented in the literature, both in theory and experimentally [9]. However, two hole quantum dots or for that purpose many hole quantum dots, with hole-hole interaction being taken as Coulombic have not attracted due attention. In addition, studies based on multihole systems with all possible interactions such as Coulombic interaction between holes, hole- phonon interaction are scarce. Although such studies, on electronic counterpart, are there in the literature [10–12]. Recently two dimensional hole gases in presence of SOCs in quantum wells have been studied by Xiang et. al. [13]. They have shown that hole-hole coupling term responsible for SOC is very important as far as spin states of hole gases is concerned. In a recent experimental study Tai et. al. [14] have shown that 2-D hole gases can be manipulated through gating, that results in a high mobility of hole gases. Implying that the short comings of hole states based devices compared to electronic devices, may be managed or rectified, so that devices based on hole states become commercially viable [15]. Owing to the possible future importance of hole-based quantum structures, the studies on single/ multiple hole quantum dots have picked momentum in recent years e.g. Delaforce et. al. [16] have recently explored experimentally probe the low temperature transport in single hole quantum dots. van-Riggelen et. al. [17] have studied 2-D quantum dots array with each quantum dot having a single hole as charge career as possible means for quantum computation. This point is validated as the single hole state in a semiconductor QD is better suited for quantum information [18]. The beauty of working with the hole states is multifold. The hole states in self-assembled quantum dots have significant anisotropy compared to the electron states. So, prior to the studies related to applications of hole engineered devices, knowledge of hole states i.e., energies and wavefunctions is of immense fundamental and practical interest. In this work, we calculated energy eigenvalues and eigenfunctions of two-hole parabolic quantum dot, subjected to external magnetic field. Also, for the near to exact calculations, we have included the Coulombic hole-hole interaction and hole-phonon interactions into account.

The electron-phonon interactions are although quite weak compared to repulsive Coulombic hole-hole interactions. They are similar to spin-orbit interactions. But, their effect on the spectrum of the QDs is very interesting and this leads to modification of the response of QDs to external magnetic field. We have used Frohlich formation to take hole-phonon interaction into account. Here, we study the thermal and magnetic properties of two-hole QD in external magnetic field. The properties studied are the magnetization, magnetic susceptibility, specific heat, and entropy. Section II deals with the theoretical model used while in section III, the results are discussed in detail.

3. Background Theory

We start by describing our theoretical approach to determining the energy levels of two interacting holes confined in a quantum dot and subjected to a perpendicular magnetic field $\overrightarrow{B} = (0, 0, B)$ which is defined in the Lorentz gauge by the vector potential $\overrightarrow{A} = \frac{\overrightarrow{B} \times \overrightarrow{r}}{2}$. By taking into account the interaction with the LO-phonons, the system's energy can be calculated by solving the schrödinger equation $\mathcal{H}_{hh}|i\rangle = E_i^{hh}|i\rangle$, where $\mathcal{H}_{hh}$ is the Hamiltonian, which is defined as follows:

$$\begin{aligned}\mathcal{H}_{hh} = \frac{1}{2m_{hh}^*}\sum_{j=1}^{2}\left(\overrightarrow{P}_j - \frac{e\overrightarrow{A}_j}{c}\right)^2 + \frac{1}{2}m_{hh}^*\omega_0^2\sum_{j=1}^{2} r_j^2 + \frac{e^2}{\varepsilon_\infty|\overrightarrow{r}_1 - \overrightarrow{r}_2|} + \frac{1}{2}g^*B\mu_B\sum_{j=1}^{2}\hat{\sigma}_{z,j} \\ + \sum_{\vec{q}}\hbar\omega_{LO}\hat{a}_{\vec{q}}^{+}\hat{a}_{\vec{q}} + \sum_{\vec{q}}\sum_{j=1}^{2}\left[\hat{a}_{\overrightarrow{q}}V_{\overrightarrow{q}}(\exp(i\overrightarrow{q}\,\overrightarrow{r_j}) + H.c\right]\end{aligned} \quad (1)$$

The above symbols have the following meaning: m_{hh}^* represents the heavy-hole effective mass, $\hbar\omega_0$ is the energy scale of the parabolic confinement, c represents the light speed in a vacuum, g^* is the electron's Lande's factor, $\mu_B = \frac{e\hbar}{2m_0c}$ is the magneton of Bohr and $\hat{\sigma}_z$

is the Pauli matrice. The two last terms of eq 1 define the kinetic operator of a phonon and the Hamiltonian representing the hole−phonon coupling in the Fr$\ddot{o}$hlich formalism [19], resppectively, where $\hat{a}^{+}_{\vec{q}}\,(\hat{a}_{\vec{q}})$ is the phonon's creation (annihilation) operator with a $3D$ wave vector $\vec{q} = (\vec{q}_{\parallel}, \vec{q}_z)$, ω_{LO} is the LO-phonons frequency and $V_{\vec{q}}$ is the coefficient of hole−phonon coupling which defined by [20]:

$$V_{\vec{q}} = \left[\frac{2\pi e^2}{V}\frac{\hbar\omega_{LO}}{q^2}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)\right]^{1/2} \tag{2}$$

where V is the volume of the crystal in the optical branch and ε_0 and ε_∞ are the static and high dielectric constants, respectively.

In order to solve the schr$\ddot{o}$dinger equation of the system $\mathcal{H}_{hh}|i\rangle = E_i^{hh}|i\rangle$, we first introduce the relative and the center of mass (CM) parameters: ($\vec{r} = \vec{r_1} - \vec{r_2}$ and $\vec{R} = \frac{\vec{r_1}+\vec{r_2}}{2}$). Using the Lee Low Pines (LLP) method [21] the polaronic contribution can be further simplified, and the total Hamiltonian expression given by (eq 1) is a combination of two individual parts, $\mathcal{H}_{hh} = \mathcal{H}_{rel} + \mathcal{H}_{cm}$ and as a result, the system's energy spectrum is $E_{hh} = E_{cm} + E_{rel}$. Therefore we can write:

$$\mathcal{H}_{rel} = \frac{P_r^2}{2\mu} + \frac{1}{2}\mu\Omega^2 r^2 - \frac{1}{2}\omega_c L_z + \frac{e^2}{\varepsilon_\infty r} - \frac{2\alpha_{LO}\hbar\omega_{LO}}{u_{LO} r}(1 - \exp(-u_{LO} r)) - \alpha_{LO}\hbar\omega_{LO}\exp(-u_{LO} r) \tag{3}$$

and

$$\mathcal{H}_{cm} = \frac{P_R^2}{2M_0} + \frac{1}{2}M_0\Omega^2 R^2 - \frac{1}{2}\omega_c L_Z + \frac{M_0\hbar\omega_c g^* S}{4m_0} \tag{4}$$

here $\mu = m^*_{hh}/2$ and $M_0 = 2m^*_{hh}$, $\Omega = \sqrt{\omega_0^2 + \frac{\omega_c^2}{4}}$, $\omega_c = \frac{eB}{m^*_{hh}c}$, $L_{rel} = m\hbar$ and $L_{cm} = M\hbar$ are the angular momentum associated with relative motions and CM, respectively, where m and M are the angular momentum quantum numbers of relative and CM part, respectively. m and M can both take the values $0, \pm1, \pm2....$ The size $\dfrac{1}{u_{LO}}$ of the two interacting holes and the hole-phonon coupling constant α_{LO} are defined, respectively, as [22]:

$$u_{LO} = \sqrt{\frac{2M_0\omega_{LO}}{\hbar}}, \alpha_{LO} = \frac{e^2}{2\hbar\omega_{LO}}\left(\frac{2M_0\omega_{LO}}{\hbar}\right)^{1/2}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right). \tag{5}$$

Under this approach that the system's wave function $\Psi_{n,m}(\rho,\varphi)$ corresponding to relative and CM motion takes the following form:

$$\Psi_{n,m}(\rho,\varphi) = \frac{1}{\sqrt{2\pi}}\exp(im\varphi) f_{n,m}(\rho) \tag{6}$$

where $f_{n,m}(\rho)$ is the normalized radial wave function defined as. In the framework of the relative donor units $a^* = \frac{\varepsilon_\infty\hbar^2}{\mu e^2}$ for lenght and $R^* = \frac{\hbar^2}{2\mu a^{*2}}$ for energy [23]. The energies without Coulomb potential and polaronic terms, can be written as [12]:

$$E^{cm}_{NM} = 2\gamma_1(2N + |M| + 1) - M\gamma_2 + \frac{\gamma_2 g^* S M_0}{2m_0} \tag{7}$$

where $\gamma_1 = \frac{\hbar\Omega}{2R^*}$ and $\gamma_2 = \frac{\hbar\omega_c}{2R^*}$. By considering the hole−phonon coupling, the energy of the relative part can be calculated by computing the complete energy expression:

$$E^{rel}_{nm} = 2\gamma_1(2n + |m| + 1) - m\gamma_2 + \int_0^\infty r f^*_{n,m}(r) V^{int}_{h-ph}(r) f_{n',m'}(r)\delta_{nn'}\delta_{mm'} dr \tag{8}$$

where

$$V_{h-ph}^{int}(r) = \frac{e^2}{\varepsilon_\infty r} - \frac{2\alpha_{LO}\hbar\omega_{LO}}{u_{LO}r}(1-\exp(-u_{LO}r)) - \alpha_{LO}\hbar\omega_{LO}\exp(-u_{LO}r) \tag{9}$$

Once the wave functions and the energy eigenvalues are determined, one can calculate the associated thermodynamic and magnetic properties of $Ga_{1-x}Mn_xAs$ in in quantum dot systems. The thermodynamic and magnetic functions will be evaluated within the Boltzmann−Gibbs statistical framework utilizing the canonical partition function:

$$Z_c = \sum_i exp\left(-\beta E_i^{hh}\right) \tag{10}$$

where $\beta = 1/k_B T$ and k_B is the Boltzmann constant. T is the temperature expressed in Kelvin. In this approach, the main thermodynamic properties of the system can be deduced using Z_c: The heat capacity:

$$C_v = -k_B\beta^2\left(\frac{\partial\langle E\rangle}{\partial\beta}\right). \tag{11}$$

where E is the mean energy of the system. The entropy:

$$S = k_B\beta(\langle E\rangle - F_H). \tag{12}$$

where $F_H = F = -k_B T \ln Z_c$ is the Helmholtz free energy.

Magnetization and Magnetic susceptibility:

$$M = \frac{-1}{Z_c}\sum_i \frac{\partial E_i^{hh}}{\partial B} exp\left(-\beta E_i^{hh}\right); \chi = \frac{\partial M}{\partial B}. \tag{13}$$

4. Results and Numerical Analysis

The numerical calculation of our formalism is applied essentially for the dilute ferromagnetic semiconductor $Ga_{1-x}Mn_xAs$. Mn act as single acceptors in a GaAs host, it also adds a local magnetic moment. To characterize the relative strengths in the interplay of confinement we have introduced the length $l_0 = \sqrt{\frac{\hbar}{m_{hh}^*\omega_0}}$ of the harmonic potential, defined in terms of the heavy-hole mass. In this work we focalise our self on two limit values of confinement strength: $l_0 = 25$ Å($\hbar\omega_0 = 23.9$ meV) and $l_0 = 50$ Å($\hbar\omega_0 = 6$ meV). The first case corresponds to a strong confinement case with $l_0 \preceq a^*$ (a^* is the bohr radius given in table I) while the second case corresponds to a weak confinement with $l_0 \succ a^*$.

Table 1. $Ga_{1-x}Mn_xAs$ containing 3% Mn material parameters used in the calculations extracted from [24–29] for (Ga,Mn)As.

Material	$\frac{m_e^*}{m_0}$	$\frac{m_h^*}{m_0}$	$E_g(eV)$	ϵ_0	ϵ_∞	a^*(Å)	$R^*(meV)$	$\hbar\omega_{LO}(meV)$	$\hbar\omega_{TO}(meV)$	g^*	S
$Ga_{1-x}Mn_xAs$	0.067	0.5	1.50	13.99	11.8	25	24.4	33.29	36.25	2	$\frac{5}{2}$

The variation of mean energy as a function of temperature is presented in Figure 1. It is observed that as temperature rises, the system's mean energy increases as well. This is due to the fact that the system's kinetic energy becomes more important as temperature rises. It can be posited that the hole-phonons interaction decreases the mean energy of the system. By reinforcing the confinement strength, the mean energy increases.

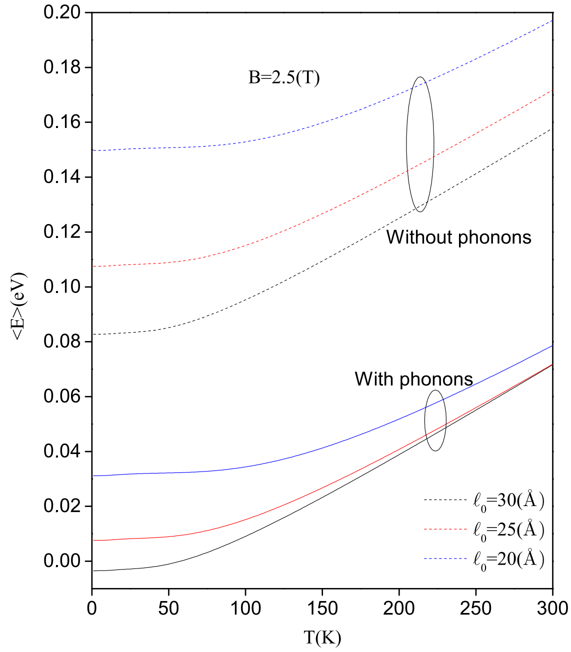
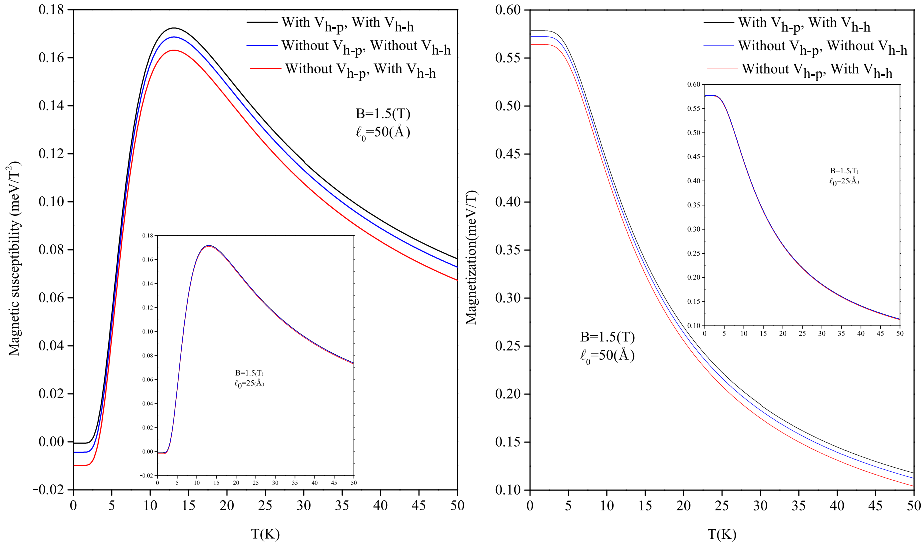


Figure 1. The evolution of the mean energy of two holes in quantum dot structures subjected to an applied magnetic field as a function of temperature taking into account the hole-phonon interactions and the size effect.

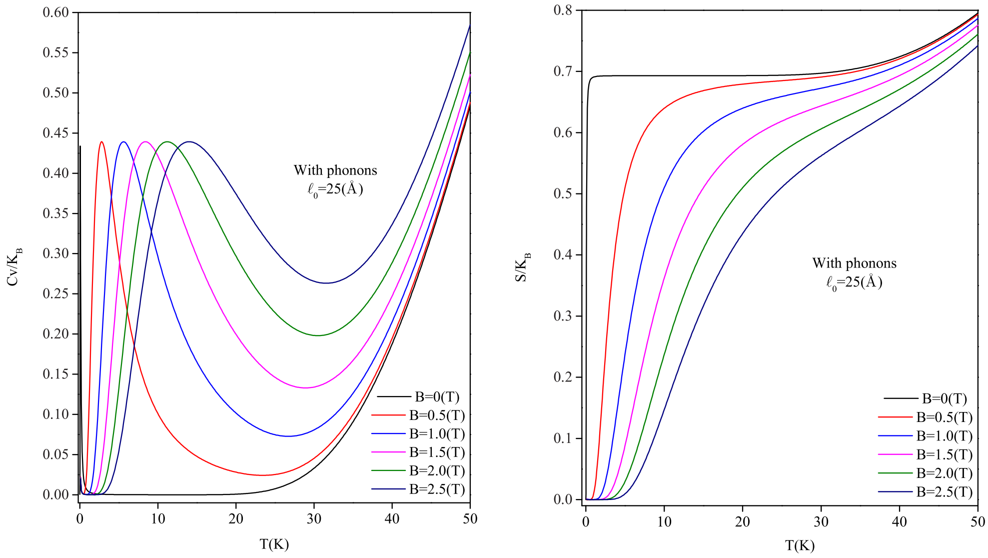
It is well known that the magnetization parameter M given by Equation (13) is the ability of the sample to retain induced magnetism in the presence of the magnetic field. The structural phase change is associated with a magnetic phase change which can be observed by studying the magnetization of the system as a function of temperature. In Figure 2, we present magnetic susceptibility (a) and magnetization (b) in $Ga_{1-x}Mn_xAs$ as function of temperature for two fixed parabolic confinement potential $l_0 = 50$ Åand $l_0 = 25$ Åcorresponding to weak and strong confinement, respectively, at $T = 5K$ with and without hole−phonon interaction (V_{h-p}) taking into account the hole−hole interaction (V_{h-h}). It is observed from the figure that for a given B the presence of hole−hole interactions($V_{h-h} \neq 0$) reduces the susceptibility (blue and red lines). However, with the introduction hole−phonon interactions(black line), we can see that the V_{h-p} reinforces the susceptibility of the system. It is interesting also to note that the polaron effect (hole−phonon coupling) in small confinement strength ($l_0 = 50$ Å) is larger compared with strong confinement strength ($l_0 = 25$ Å). The same behavior is observed for the magnetization curves(Figure 2b).

The heat capacity C_V of a given material is an important parameter which is the derivative of its thermal energy. Its calculation permits to obtain an integrated information of all the magnetic system's energy levels. Figure 3a, displays the variation of this quantity as function of temperature for various magnetic fields values $B = 0, 0.5, 1, 1.5, 2$ and 2.5T at $l_0 = 25$ Å. The first remark we can make here is that there is a peak observed in the heat capacity curves correspond to Schottky anomaly. In zero field the Schottky anomaly is observed at 0.11 K after this temperature value, the heat capacity starts to decrease. However a magnetic field applied between 0.5T and 2.5T causes a Zeeman splitting towards a spin system, therefore, it is possible to shift the specific heat anomaly to a certain temperature. The peak heat capacity, which is used in the randomization of the magnetic moments around T_c, is result of the heat absorption during the phase transition. Once a magnetic field is imposed, the randomization process of the magnetic moments takes place over a large range of temperature, which broadens the maximum peak [31].



(**a**) (**b**)

Figure 2. Variation of the magnetic susceptibility (**a**) and magnetization (**b**) of the two holes as function of temperature in the case of strong confinement ($l_0 = 25$ Å), and for weak confinement ($l_0 = 50$ Å) at $B = 1.5$T. The red and black lines correspond to the cases without and with phonons, respectively, taking into account the coulomb potential between two holes, the blue line is associated the case without coulomb potential and phonons.



(**a**) (**b**)

Figure 3. Heat capacity and entropy as a function of temperature in the presence of phonons, (**a**) in the range of magnetic field from $B = 0.5$ to $B = 2.5$T at $l_0 = 25$ Å, (**b**) for both strong ($l_0 = 25$ Å) and weak ($l_0 = 50$ Å) confinement cases.

The heat capacity is also directly dependent on the system's magnetic entropy $S(T, H)$ by $S = \int \frac{Cv}{T} dT$. Currently, this quantity is the object of increasing attention in the search for potential spintronics applications. The entropy also defines the disorder and the random character of the system. fig3b, illustrates the entropy variation (S(T,H) in (Ga,Mn)As with temperature for various magnetic fields values ($B = 0, 0.5, 1, 1.5, 2$ and 2.5T) at $l_0 = 25$ Å. It is worth noting that, at zero temperature, the entropy of the system is nul, while the temperature increases, S(T,H) also increases, because it increases the random character of the system by elevating the energy. We can observe also that as the magnetic field strength increases (from 0 to 2.5T), the entropy decreases.

5. Conclusions

In summary, thermodynamic and magnetic properties of the diluted ferromagnetic semiconductor $Ga_{1-x}Mn_xAs$ contained 3% Mn in Confined Systems have been studied in detail. The founded results show that the thermodynamic and magnetic properties properties are influenced by the magnetic field, hole−phonon and hole−hole interactions, and the confinement which is in a good agreement with previous works.

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