Exchange interaction effects in the thermodynamic properties of quantum dots

L. G. G. V. Dias da Silva and Nelson Studart

1Department of Physics and Astronomy, Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, Ohio 45701-2979
2Departamento de Física, Universidade Federal de São Carlos, 13565-905 São Carlos SP, Brazil

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We study electron-electron interaction effects in the thermodynamic properties of quantum-dot systems. We obtain the direct and exchange contributions to the specific heat \( C_v \) in the self-consistent Hartree-Fock approximation at finite temperatures. An exchange-induced phase transition is observed and the transition temperature is shown to be inversely proportional to the size of the system. The exchange contribution to \( C_v \) dominates over the direct and kinetic contributions in the intermediate regime of interaction strength \( (r_s \sim 1) \). Furthermore, the electron-electron interaction modifies both the amplitude and the period of magnetic field induced oscillations in \( C_v \).

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I. INTRODUCTION

Research on semiconductor quantum dots (QD)s and nanostructures have drawn considerable effort in recent years. In particular, the study of electron-electron interaction effects on the ground-state and excited-state of QDs has been a very active subject. A variety of methods have been used in such studies, ranging from the exact diagonalization of few electron systems\(^{2,3,4,5,6,7}\) to sophisticated numerical schemes based on the density functional theory, quantum Monte Carlo simulations and mean-field approximations.\(^{8,9,10,11,12,13,14,15,16}\) Among the last ones, the self-consistent Hartree-Fock (SCHF) approximation has been successfully applied to QDs in a number of works\(^{9,10,11,12,13,14,15,16}\), which focused attention on calculations of the pair-correlation function\(^\star\) and addition spectra\(^{10,11}\) and on configurations of the Wigner-like molecule in the strong interacting regime.\(^{12,13}\)

A less pursued track is the use of SCHF to study magnetic and thermodynamic properties of semiconductor QDs.\(^{14,15,16}\) Electron-electron interaction was shown to give an important contribution to thermodynamic properties such as the magnetization\(^{7,4,5}\) and the magnetic susceptibility.\(^{5,16}\) Another quantity of experimental interest is the specific heat \( C_v \), which has been studied in a number of works in both non-interacting\(^{17,18}\) and interacting\(^{2,15}\) QD systems. In Ref.\(^{15}\), Dean and coworkers reported an interesting interaction-induced phase transition in parabolic QDs with \( N = 6 \) electrons. This phase transition manifests itself as sharp drops in the specific heat as the temperature reaches a critical value. Nevertheless, a systematic study on how such a transition depends on the interaction coupling parameter \( r_s \) of the dot, which measures the relative electron-electron interaction strength, remains to be performed.

In this paper, we address the role of the exchange interaction in the thermodynamic properties of non-parabolic QDs. Specifically, we study the kinetic, direct and exchange contribution to the specific heat in a finite-temperature Hartree-Fock approach.\(^{10,12}\) In a previous work using this method,\(^\star\) we have shown that the exchange interaction contribution is the dominant term in magnetic properties such as the zero-field susceptibility in the intermediate regime of interaction strength \( (r_s \sim 1) \).

II. THE MODEL

We consider the problem of \( N \) interacting electrons confined in a 2D square quantum dot of size \( L \) and subjected to an external magnetic field \( B \) perpendicular to the electron system. To account for screening effects, the electron-electron interaction is modeled by an Yukawa-type potential\(^\star\) and the model Hamiltonian reads as

\[
H = \sum_{n=1}^{N} h(r_n) + \sum_{n<n'} e^{-\kappa |r_n-r_{n'}|} \epsilon_{tr} \frac{|r_n-r_{n'}|}{|r_n-r_{n'}|},
\]

where \( r_n \) indicates the position of the \( n \)th electron. We consider low \( g \)-factor QDs, so that the Zeeman term can be safely disregarded. Above, \( \kappa \) gives the effective interaction range and \( \epsilon_{tr} \) is the background dielectric constant. For \( \kappa = 0 \), there are no screening effects and the “bare” Coulomb interaction is recovered.

The single-particle Hamiltonian \( h(r) \) is given by

\[
h(r) = \frac{1}{2m^*} \left[ \mathbf{p} + \frac{e}{c} \mathbf{A}(r) \right]^2 + u(r),
\]

where \( m^* \) is the effective mass, \( \mathbf{p} \) is the momentum operator, \( \mathbf{A}(r) \) is the vector potential and \( u(r) \) is the on-site potential.
where \( m^* \) is the electron effective mass and \( u(\mathbf{r}) \) is the hard-wall confining potential. The vector potential \( \mathbf{A} \) is chosen in the symmetric gauge, namely, \( \mathbf{A} = (-B y / 2, B x / 2, 0) \). Hereafter, the magnetic field is expressed in units of \( \Phi / \Phi_0 \), where \( \Phi = B A \) is the magnetic flux through the system area \( A \) and \( \Phi_0 = \hbar c / e \) is the quantum flux unit.

A key parameter in our analysis is \( L/a_B^2 \), the QD length \( L \) in units of the effective Bohr radius \( a_B^2 = \hbar^2 / m^* e^2 \) which gives the relative strength of the e-e interaction as compared to the kinetic energy of the system. For a square dot of side \( L \), the potential energy scales with \( L^{-1} \) while the kinetic energy scales with \( L^{-2} \). Therefore, as \( L \) is increased, the potential energy becomes increasingly more important.

The many-body ground-state energy is obtained in the finite-temperature SCHF approximation. The SCHF equations read as

\[
\begin{align*}
\hbar^2 \phi_i(\mathbf{r}) + \sum_j \left[ n_j \int d\mathbf{r}' \phi'_j(\mathbf{r}') v(\mathbf{r}, \mathbf{r}') \phi_j(\mathbf{r}') \right] & \phi_i(\mathbf{r}) \\
- \sum_j \left[ n_j \int d\mathbf{r}' \phi'_j(\mathbf{r}') v(\mathbf{r}, \mathbf{r}') \phi_j(\mathbf{r}) \phi_i(\mathbf{r}') \right] & = \varepsilon_{HF} \phi_i(\mathbf{r}),
\end{align*}
\]

where the sums run over all HF orbitals. Here \( n_i = \{ \exp[(\varepsilon_{HF} - \mu)/k_B T] + 1 \}^{-1} \) is the Fermi occupation number of the \( i \)th HF orbital with corresponding wave function \( \phi_i(\mathbf{r}) \) and energy \( \varepsilon_{HF} \). As in the standard procedure, the chemical potential \( \mu \) is determined by requiring that \( N = \sum_i n_i \). We truncate the number of orbitals and take only the \( M \geq 2N \) lowest energy states into account.

The SCHF ground-state energy is given by

\[
E_{HF}^g = T_{HF} + V_d^{HF} - V_x^{HF} = \sum_i n_i \langle \phi_i | h | \phi_i \rangle + \frac{1}{2} \sum_{i,j} n_i n_j \left( \langle \phi_i \phi_j | v | \phi_i \phi_j \rangle \right.
\]
\[
- \langle \phi_i \phi_j | v | \phi_i \phi_j \rangle \right),
\]

where \( \{ \phi_i \} \) are the HF orbitals, self-consistent solutions of Eq. 3 and \( T_{HF}, V_d^{HF} \) and \( V_x^{HF} \) are the kinetic, direct and exchange contributions to the ground-state energy respectively. We are interested in the intermediate interaction strength regime \( (r_s \sim 1) \). In this regime, the direct interaction term \( V_d^{HF} \) is the leading contribution to the \( E_{HF}^g \), followed by \( T_{HF} \) and \( V_x^{HF} \) respectively.

The details on the matrix elements calculations and the Hartree-Fock method can be found on Refs. 2 and 16 respectively.

We calculate the specific heat \( C_v \) of the system in this SCHF approximation, namely:

\[
C_v = \left( \frac{\partial U}{\partial T} \right)_V
\]

where \( U \) is the internal energy and \( T \) is the system temperature. The first-order exchange and Hartree contributions to \( C_v \) can be accounted for by approximating \( U \approx E_{HF}^g \) so that for \( E_{HF}^g \), given by Eq. 4 there are kinetic \( (C_v^{kin}) \), direct \( (C_v^d) \) and exchange \( (C_v^x) \) contributions to \( C_v \).

III. RESULTS AND CONCLUSIONS

We analyze the behavior of the specific heat \( C_v \) as a function of relevant parameters of the system, i.e. the temperature \( T \), the interaction strength \( L/a_B^2 \), the magnetic field \( \Phi / \Phi_0 \), the potential range \( \kappa^{-1} \) and the number of electrons \( N \). The results given in this section are for the Coulomb case \( (\kappa = 0) \) with \( N = 10 \) electrons in the dot. We should mention that QDs with up to \( N = 20 \) electrons and with the screened interaction \( (\kappa \neq 0) \) were also considered and the same overall qualitative features were observed. In the remaining of this section, energy and temperature are given in units of the typical scales for the system, namely \( E_L = \hbar^2 / (m^* L^2) \) and \( T_L = E_L / k_B \) respectively.

![FIG. 1](color online) (a): Ground-state energy \( E_{HF}^g \) as function of temperature for \( N = 10 \) electrons and \( r_s = 0.89 \). The kinetic \( (b) \), exchange \( (c) \) and direct \( (d) \) contributions to \( E_{HF} \) are also plotted.

The ground-state energy \( E_{HF}^g \) increases with temperature as shown in Fig. 1 for \( N = 10 \) and \( r_s = 0.89 \). Nevertheless, this increase is not smooth and a sudden change in slope is observed at a certain temperature \( T^* \). By analyzing the kinetic energy \( T_{HF} \), the direct term \( V_d^{HF} \) and the exchange contribution \( V_x^{HF} \) given by Eq.
observed in the temperature range $T < T/T_L$. As signatures of phase transitions, we
observe clearly that the change in slope is a feature due to the exchange interaction, since neither $T_{HF}$ or $V_d$ display cusps at $T = T^*$. The insets show the noninteracting case is referred to as "$L/a_B^* = 0" or "r_s = 0". The noninteracting curve does not display any sharp drops.

Discontinuities in the specific heat are usually regarded as signatures of phase transitions. In fact, such transitions are accompanied by a charge reordering in the ground state distribution, as shown in the insets of Fig. 2. A sharp drop develops for a wide range of values of the interaction strength parameter (for simplicity, the noninteracting case is referred to as "$L/a_B^* = 0" or "r_s = 0". The noninteracting curve does not display any sharp drops.

The abrupt change in slope in the energy causes a discontinuity in the specific heat $C_v(T)$ at $T = T^*$, as expected. Furthermore, we observe clearly that the change in slope is a feature due to the exchange interaction, since neither $T_{HF}$ or $V_d$ display cusps at $T = T^*$ (Figs. 1d).

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In Fig. 3, we see that both $V_d^{HF}$ and $V_x^{HF}$ decrease with $T$, as expected. Furthermore, we observe clearly that the change in slope is a feature due to the exchange interaction, since neither $T_{HF}$ or $V_d$ display cusps at $T = T^*$ (Figs. 1d).

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The susceptibility of QD systems depends on the magnetic field amplitude. The oscillation period is defined more clearly for even higher parameter, the higher harmonics are suppressed and an even higher value of the interaction strength parameter, the higher harmonics are suppressed and an oscillation period is defined more clearly. For even higher values of the interaction strength parameter, the higher harmonics are suppressed and an oscillation period is defined more clearly. For even higher values of the interaction strength parameter, the higher harmonics are suppressed and an oscillation period is defined more clearly. For even higher values of the interaction strength parameter, the higher harmonics are suppressed and an oscillation period is defined more clearly. For even higher values of the interaction strength parameter, the higher harmonics are suppressed and an oscillation period is defined more clearly. For even higher values of the interaction strength parameter, the higher harmonics are suppressed and an oscillation period is defined more clearly. For even higher values of the interaction strength parameter, the higher harmonics are suppressed and an oscillation period is defined more clearly. For even higher values of the interaction strength parameter, the higher harmonics are suppressed and an oscillation period is defined more clearly..

Experiments to verify our findings using single quantum-dots are likely too demanding. The specific heat has been measured in multi-layer 2D electron gases in the Landau regime with heat-pulse and steady-state ac-temperature calorimetry techniques, with resolutions in $C_v$ still much lower than the required to test our results. One possible way to overcome such difficulty is to perform experiments in ensembles of nearly identical dots in a multi-layer configuration so that the contribution from single dots is amplified. This is, nonetheless, an experimentally challenging task which would bring a new understanding to the many-body effects in the thermodynamics of such small-scale devices.

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