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Interacting electrons in quantum dots

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Abstract

The ground states of N-electron parabolic quantum dots in the presence of a perpendicular magnetic field are investigated. Rigorous lower bounds to the ground-state energies are obtained. It is shown that our lower bounds agree well with the results of exact diagonalization. Analytic results for the lower bounds to the ground-state energies of the quantum dots in a strong magnetic field (known as electron molecule) agree very well with numerically calculated lower bounds.

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1. Introduction

In recent years, there has been intense study of nanostructures such as quantum dots (QD) [1–5], where quasi-two-dimensional islands of electrons are laterally confined by an externally imposed potential that, in a good approximation, is parabolic. In Ref. [6], the electronic states of interacting electrons in three-electron QD are calculated without making assumptions about the shape of the confining potential and dimensionality of the problem.

Theoretical investigations of the ground states of QD have been reported in many papers. As for the standard Hartree and Hartree–Fock (HF) approximations, there are doubts about their accuracy, since the exchange and correlation energies can be significant in QD [7,8].

A simple way to incorporate the interaction between electrons is to use the Post model [9], where inter-electron repulsion is replaced by the harmonic interaction [10]. For a critical analysis of this approximation, see Ref. [11]. The Post model [9] was used for a problem in nuclear physics in Ref. [12].

Numerical calculations using exact-diagonalization techniques were carried out in Refs. [13–19]. These calculations are computationally extensive and limited to a few ($\leqslant 6$) electrons.

The ground states of an N-electron QD in magnetic fields have been measured up to $N \leqslant 50$ [20].

The purpose of this work is to provide a rigorous lower bounds to the ground-state energy of N-electron QD in magnetic fields for any N. We show that our lower bounds for ground states agree well with the exact results of the diagonalization method.

This Letter is organized as follows. In Section 2, we generalize a lower-bound method developed by Hall and Post [21] for the case of N-electron QD in a magnetic field B. In Section 3, lower bounds are found analytically in the large B limit. In Section 4, we

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describe our calculations. A summary and conclusions are given in Section 5.

2. Lower bounds

The Hamiltonian for N interacting electrons confined in a parabolic QD, in the presence of a magnetic field B perpendicular to the dot, can be written as

$$H = \frac{1}{2m^*}\sum_{i=1}^{N}\vec{p}_i^{\,2} + \frac{1}{2}m^*\Omega^2\sum_{i=1}^{N}\vec{r}_i^{\,2} - \frac{\omega_c}{2}L_z + \sum_{i<j}\frac{e^2}{\epsilon|\vec{r}_i-\vec{r}_j|} + g^*\mu_b B S_z, \tag{1}$$

where m^* is the electron effective mass, $\Omega^2 = \omega_0^2 + \omega_c^2/4$, ω_0 is the parabolic confinement frequency, ω_c is the cyclotron frequency, L_z is the z component of the total orbital momentum, ϵ is the dielectric constant, g^* is the effective g-factor, μ_b is the Bohr magneton, and S_z is the z component of the total spin.

In our numerical calculations we use the effective mass $m^* = 0.067m_e$ (m_e is the free-electron mass) of GaAs QD.

Now we introduce the center-of-mass coordinates, $\vec{R} = (1/N)\sum_{i=1}^{N}\vec{r}_i$ and $\vec{P} = \sum_{i=1}^{N}\vec{p}_i$.

Using

$$\sum_{i=1}^{N}\vec{r}_i^{\,2} = N\vec{R}^2 + \frac{1}{N}\sum_{i<j}\big(\vec{r}_i-\vec{r}_j\big)^2, \tag{2}$$

$$\sum_{i=1}^{N}\vec{p}_i^{\,2} = \frac{\vec{P}^2}{N} + \frac{1}{N}\sum_{i<j}\big(\vec{p}_i-\vec{p}_j\big)^2, \tag{3}$$

and

$$\vec{L} = \sum_{i=1}^{N}\vec{r}_i\times\vec{p}_i = \vec{R}\times\vec{P} + \frac{1}{N}\sum_{i<j}\big(\vec{r}_i\times\vec{p}_i + \vec{r}_j\times\vec{p}_j - \vec{r}_i\times\vec{p}_j - \vec{r}_j\times\vec{p}_i\big), \tag{4}$$

we can rewrite Eq. (1) as

$$H = H_{\rm cm} + H_{\rm rel} + H_z, \tag{5}$$

where the first term is the center-of-mass energy, the second term is the relative energy and the last term is the Zeeman energy, with $H_z = g^*\mu_b B S_z$. $H_{\rm cm}$ and $H_{\rm rel}$ are given by

$$H_{\rm cm} = \frac{\vec{P}^2}{2m^*N} + \frac{m^*N\Omega^2\vec{R}^2}{2} - \frac{\omega_c}{2}\big(\vec{R}\times\vec{P}\big)_z \tag{6}$$

and

$$H_{\rm rel} = \sum_{i<j}H_{ij}, \tag{7}$$

where

$$H_{ij} = \frac{(\vec{p}_i-\vec{p}_j)^2}{2m^*N} + \frac{m^*\Omega^2(\vec{r}_i-\vec{r}_j)^2}{2N} + \frac{e^2}{\epsilon|\vec{r}_i-\vec{r}_j|} - \frac{\omega_c}{2N}\big(\vec{r}_i\times\vec{p}_i + \vec{r}_j\times\vec{p}_j - \vec{r}_i\times\vec{p}_j - \vec{r}_j\times\vec{p}_i\big)_z. \tag{8}$$

Hence we have for the ground state energy

$$E = \hbar\Omega + E_{\rm rel} + g^*\mu_b B S_z, \tag{9}$$

where

$$E_{\rm rel} = \langle\psi|H_{\rm rel}|\psi\rangle, \tag{10}$$

and $\psi(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)$ is the ground state wave function. Using the symmetric properties of ψ we can rewrite Eq. (10) as

$$E_{\rm rel} = \frac{N(N-1)}{2}\langle\psi|H_{12}|\psi\rangle. \tag{11}$$

Introducing the Jacobi coordinates $\vec{\zeta}_i$ as

$$\vec{\zeta}_i = \sum_{j=1}^{N}U_{ij}\vec{r}_j, \tag{12}$$

with

$$U_{ij} = \begin{cases}(i)^{-1} & \text{if } j < i+1,\\ -1 & \text{if } j = i+1,\\ 0 & \text{if } j > i+1,\end{cases} \tag{13}$$

we have

$$H_{12} = -\frac{2}{m^*N}\Delta_{\zeta_1} + \frac{m^*\Omega^2\zeta_1^2}{2N} + \frac{e^2}{\epsilon\zeta_1} - \frac{\omega_c}{N}\left(\vec{\zeta}_1\times\frac{\hbar}{i}\nabla_{\zeta_1}\right)_z, \tag{14}$$

where $\vec{\zeta}_1 = \vec{r}_1 - \vec{r}_2$.

Projecting $|\psi\rangle$ on the complete basis $|n\rangle$, generated by the effective two-body Hamiltonian H_{12}, $H_{12}|n\rangle =$

$E_n|n\rangle$, and using

$$\langle\psi|H_{12}|\psi\rangle = \sum_n E_n \big|\langle\psi|n\rangle\langle n|\psi\rangle\big| \geqslant E_g,$$

we get

$$E \geqslant \hbar\Omega + \frac{N(N-1)}{2}E_g + g^*\mu_b B S_z, \tag{15}$$

where E_g is the ground state energy of the effective two-body Hamiltonian H_{12} (for the completely spin polarized states, $S_z = N\hbar/2$ and E_g is the energy of the lowest antisymmetric state of the effective two-body Hamiltonian H_{12}). Eq. (15) is a generalization of the Hall–Post method (which is restricted to the case with only inter-particle forces present and no external potential) for obtaining lower bounds to the ground-state energy of N-electron QD in a magnetic field B.

3. Large B limit

We introduce dimensionless units by making the following transformation: $\vec{\rho} = (1/a)\vec{\zeta}_1$, where $a = \sqrt{\hbar/(m^*\omega_0)}$.

Using the above dimensionless notation and polar coordinates $\rho_x = \rho\sin\theta$ and $\rho_y = \rho\cos\theta$, we can write the effective two-body eigenvalue problem $H_{12}|\phi_g\rangle = E_g|\phi_g\rangle$ as

$$\begin{aligned}\tilde{H}_{12}u(\rho) &= \left[-\frac{2}{N}\frac{d^2}{d\rho^2} + \frac{2(\ell^2-1/4)}{N\rho^2}\right.\\ &\quad\left. + \frac{1}{2N}\left(1+\frac{\lambda^2}{4}\right)\rho^2 + 2\frac{\gamma_c}{\rho} - \frac{\ell\lambda}{N}\right]u(\rho)\\ &= \tilde{E}u(\rho),\end{aligned} \tag{16}$$

where $\lambda = \omega_c/\omega_0$, $\phi_g(\rho,\theta) = e^{i\ell\theta}u(\rho)/\sqrt{\rho}$, $\gamma_c = \alpha\sqrt{m^*c^2/(\hbar\omega_0)}/2$, and $\tilde{E} = E_g/(\hbar\omega_0)$.

The two-body equation, Eq. (16), can be solved numerically to find E_g for any arbitrary value of ℓ. The optimal ℓ value, restricted to odd integers for polarized states, minimizes the energy. The two-electron QD has been the subject of intensive study [3,4,8,22–26].

In the large magnetic field limit, ℓ becomes large and the term $1/4$ in $(\ell^2 - 1/4)$ can be neglected [17], and Eq. (16) can be rewritten as

$$\left[-\frac{2}{N}\frac{d^2}{d\rho^2} + V_{\text{eff}}(\rho)\right]u(\rho) = \tilde{E}u(\rho), \tag{17}$$

where

$$V_{\text{eff}}(\rho) = \frac{2\ell^2}{N\rho^2} + \frac{1}{2N}\left(1+\frac{\lambda^2}{4}\right)\rho^2 + 2\frac{\gamma_c}{\rho} - \ell N\lambda. \tag{18}$$

In the large-B limit the effective potential V_{eff}, Eq. (18), has a deep minimum, therefore a good approximation to $\tilde{E}$ can be obtained by making the Taylor expansion of V_{eff} about its minimum [17]. Thus the approximate E_g is

$$E_g \approx \frac{2}{N}\left[\frac{3}{4}(2\gamma_c N)^{2/3} + \frac{1}{2}\sqrt{\lambda^2+3}\right]\hbar\omega_0. \tag{19}$$

Substitution Eq. (19) into Eq. (15) gives

$$\begin{aligned}E &\geqslant E_{\text{low}} \approx \mathcal{E}\\ &= \hbar\Omega + (N-1)\left[\frac{3}{4}(2\gamma_c N)^{2/3} + \frac{1}{2}\sqrt{\lambda^2+3}\right]\hbar\omega_0\\ &\quad + g^*\mu_B B S_z.\end{aligned} \tag{20}$$

Note that the large N limit of E_{low} is independent of magnetic field in this approximation (see also Ref. [16]).

4. Numerical results

We begin with the single-electron basis functions $\chi_{n\ell}(\rho)$, associated with Hamiltonian

$$H_0 = -\frac{d^2}{d\rho^2} + \frac{\ell^2-1/4}{\rho^2} + \frac{1}{4}\left(1+\frac{\lambda^2}{4}\right)\rho^2 - \frac{\lambda\ell}{2}. \tag{21}$$

These functions were found more than seventy years ago [27],

$$\begin{aligned}\chi_{n\ell}(\rho) &= A_{n\ell}\rho^{\ell+1/2}e^{-(1/4)(1+\lambda^2/4)^{1/2}\rho^2}\\ &\quad\times L_n^\ell\left(\frac{1}{2}\left(1+\frac{\lambda^2}{4}\right)^{1/2}\rho^2\right),\end{aligned} \tag{22}$$

where L_n^ℓ are associated Laguerre polynomials and

$$A_{n\ell} = \left[\frac{1}{2}\left(1+\frac{\lambda^2}{4}\right)^{\ell+1}\frac{n!}{(n+\ell)!}\right]^{1/2}. \tag{23}$$

In order to solve Eq. (16) we introduce

$$\chi_{n\ell}^{\beta}(\rho) = \sqrt{\beta}\chi_{n\ell}(\beta\rho) \tag{24}$$

Table 1
Convergence of the method, Eqs. (25) and (26), for lower bounds, E_g, with increasing M for the three-electron QD with $\epsilon = 13.1$ and $\hbar\omega_0 = 0.01$ meV. $S_z = 3\hbar/2$ and $B = 0$ is assumed [18]

M	1	4	5	6	7	8
E_g (meV)	0.373368	0.336831	0.336681	0.336659	0.336659	0.336659

and expand $u(\rho)$, Eq. (16), in the basis $\chi^{\beta}_{n\ell}$, i.e., we seek solution of the form

$$u^M(\rho) = \sum_{n}^{M} c_N^{\beta} \chi^{\beta}_{n\ell}(\rho). \tag{25}$$

The conventional choice for the parameter β is $\beta = 1$ (see, for example, [4]). However, for finite M, the choice $\beta = 1$ is not the optimal choice. The most reliable β is obtained from

$$\frac{d}{d\beta}\langle u^M | \tilde{H} | u^M \rangle = 0. \tag{26}$$

We apply the method, Eqs. (25) and (26), to compute the lower bounds.

Consider a two-dimensional three-electron QD with $\epsilon = 13.1$ and $\hbar\omega_0 = 0.01$ meV without a magnetic field, $B = 0$ [18]. Let M be the number of functions in Eq. (25). Examples of the lower bound to the completely spin polarized three-electron state, $S_z = 3\hbar/2$, corresponding to the different M are given in Table 1. The fast convergence is evident. Comparison of the converging result of Table 1, $E_g = 0.336659$ meV with exact diagonalization calculations of Ref. [18], $E_g = 0.3393$ meV, shows that our lower bound is a very good approximation with relative error of about 0.7% for the ground state energy of the three-electron QD without a magnetic field.

Now consider the GaAs QD with $\epsilon = 12.4$ and $\hbar\omega_0 = 4$ meV in a strong magnetic field, $B = 20$ T [19]. Examples of the lower bounds to the completely spin polarized N-electron ground state, $E_{\rm low}$, for up to $N = 6$ electrons are given in Table 2. Numerical results $E_{\rm low}$ agree with large B approximation, $\tilde{E}$ (Eq. (20)) to better than 0.1%.

From Table 2, we can see that the calculated lower bounds agree well with exact-diagonalization results, $E_{\rm ed}$ [19]. The relative error, $\Delta = (E_{\rm ed} - E_{\rm low})/(2E_{\rm ed})$, is less than 2%.

We have also calculated the chemical potential of QD, $\mu_A(N) = E(N+1) - E(N)$. $\mu_A(N)$ is measured by the single-electron capacitance spectroscopy method [20,28] since the transfer of the $(N+1)$th electron from the electrode to the QD occurs when the chemical potential of the electrode, μ_E, is equal to the μ_A.

Table 2
Results for lower bounds $E_{\rm low}$, chemical potential μ_A, large B analytical approximation $\mathcal{E}$, Eq. (20), and $\Delta = (E_{\rm ed}\,[19] - E_{\rm low})/(2E_{\rm ed}\,[19])$ for N-electron GaAs QD with $\epsilon = 12.4$ and $\hbar\omega_0 = 4$ meV in a strong magnetic field, $B = 20$ T. $S_z = N\hbar/2$ is assumed

Number of electrons N	$E_{\rm low}$ (meV)	μ_A (meV)	$\mathcal{E}$ (meV)	Δ (%)
1	17.4810	24.2141	17.4810	
2	41.6951	28.5087	41.6910	
3	70.2038	32.0032	70.1483	0.2
4	102.207	35.1570	102.168	0.7
5	137.364	38.2630	137.366	1.4
6	175.627	40.6922	175.482	1.8

5. Summary and conclusion

In summary, we have generalized the Hall–Post lower-bound method [21] for the case of the N-electron parabolic QD in the presence of a perpendicular magnetic field.

It is shown that our rigorous lower bounds agree well with the results of exact diagonalization. For example, lower bounds to the completely spin polarized ground state energy of the three-electron QD agree with exact-diagonalization results to better than 1%. For the case of six-electron QD, the relative error is less than 2%.

Analytic results for the lower bounds to the ground-state energies of the QD in a strong magnetic field (the QD analogue of a Wigner crystal [29] known as

electron molecule [19]) agree with numerical lower bounds to better than 0.1%.

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