Exactly Solvable Model of Interacting Particles in a Quantum Dot

N. F. Johnson[1,2] and M. C. Payne[1]
[1]*Cavendish Laboratory, Cambridge University, Cambridge, United Kingdom*
[2]*Universidad de Los Andes, Bogota, Columbia*
(Received 1 April 1991)

A simple, yet physically reasonable, model is presented which describes an arbitrary number of interacting particles in a quantum dot. Exact analytic expressions are obtained for the energy spectrum as a function of particle number and magnetic field.

PACS numbers: 73.20.Dx, 73.20.Mf, 73.40.Kp

Recent progress in semiconductor technology now allows the fabrication of zero-dimensional structures, called quantum dots [1–8], where islands of two-dimensional electrons are laterally confined by an imposed potential. The number of electrons in a quantum dot can be varied over a considerable range, and recent far-infrared absorption [1–3], capacitance spectroscopy [5], and conductance [8] measurements have yielded data with rich structure. However, a full understanding of the experimental results requires knowledge of the many-electron energy spectrum for a quantum dot. The few existing theoretical treatments of the energy spectrum have been computationally intensive and have employed either the Hartree approximation [9], whose neglect of exchange and correlation effects may be significant in quantum dots [10], or direct numerical diagonalization [11,12], which is limited by convergence problems to treating just a few (<6) electrons. In this Letter we present a simple, yet physically reasonable, model which describes a quantum-dot system that contains an arbitrary number of interacting particles. The many-body problem is solved *exactly*, yielding analytic expressions for the energy spectrum as a function of external magnetic field and particle number. By obtaining exact solutions we automatically include all the effects of exchange and correlation.

The two features of the present model which permit an exact, analytic solution of the many-body problem are as follows. (1) The bare (i.e., unscreened), two-dimensional confining potential $V(\mathbf{r}_i)$ for the ith particle is taken to be parabolic. It has been shown theoretically that for electrons contained in a parabolic potential there is strong absorption of far-infrared light at the frequency corresponding to the bare parabola [13–17]. This theoretical prediction is consistent with recent experimental measurements on quantum dots [4]. Further evidence that the bare potential in many quantum-dot samples is close to parabolic is provided by simple electrostatic models [18]. (2) The interaction potential $V(\mathbf{r}_i,\mathbf{r}_j)$ between particles i and j moving in the two-dimensional confining potential in the x-y plane [19] is taken to saturate at small particle separation and decrease quadratically with increasing separation. The interaction between two electrons in free space would, of course, vary as $|\mathbf{r}_i-\mathbf{r}_j|^{-1}$. However, in quantum-dot structures, the form of $V(\mathbf{r}_i,\mathbf{r}_j)$ is modified in a nontrivial way by the presence of image charges in adjacent layers of gates. Furthermore, the wave functions of the electrons confined in the quantum dots have a small but finite extent perpendicular to the x-y plane [19]. This results in a slight smearing of the electron charges along the perpendicular (z) direction. Hence the interparticle repulsion will tend to saturate at small interparticle separations. We choose as our model for the interaction

$$V(\mathbf{r}_i,\mathbf{r}_j)=2V_0-\tfrac{1}{2}m^*\Omega^2|\mathbf{r}_i-\mathbf{r}_j|^2, \tag{1}$$

where m^* is the particle effective mass; V_0 and Ω are positive parameters within the model. Reasonable values for V_0 and Ω will be discussed later in the Letter.

We consider a parabolic quantum dot in the x-y plane [19] in the presence of a magnetic field B along the z axis. The dot contains N interacting particles (e.g., electrons) with charge $-e$ where e is positive, g-factor g^*, spatial coordinates $\{\mathbf{r}_i\}$, and spin components $\{s_{z,i}\}$ along the z axis. The total Hamiltonian H can be written as $H=H_{\text{space}}+H_{\text{spin}}$, where H_{space} and H_{spin} only depend on spatial and spin coordinates, respectively [20]. Explicitly,

$$H_{\text{space}}=\frac{1}{2m^*}\sum_i\left(\mathbf{p}_i+\frac{e\mathbf{A}_i}{c}\right)^2+\frac{1}{2}m^*\omega_0^2\sum_i|\mathbf{r}_i|^2+\sum_{i<j}V(\mathbf{r}_i,\mathbf{r}_j) \tag{2}$$

and

$$H_{\text{spin}}=-g^*\mu_B B\sum_i s_{i,z}, \tag{3}$$

where the momentum and vector potential associated with the ith particle are given by $\mathbf{p}_i=(p_{i,x},p_{i,y})$ and $\mathbf{A}_i=(A_{i,x},A_{i,y})$, respectively, and μ_B is the Bohr magneton. The eigenstates of H can be written as the product of spatial and spin eigenstates obtained from H_{space} and H_{spin}, respectively. The z component of the total spin S_Z is equal to $\sum_i s_{i,z}$ and represents a good quantum number for the system. Choosing a circular gauge $\mathbf{A}_i=B(-y_i/2, x_i/2,0)$, Eq. (2) becomes

$$H_{\text{space}}=\frac{1}{2m^*}\sum_i\mathbf{p}_i^2+\frac{1}{2}m^*\omega_0^2(B)\sum_i|\mathbf{r}_i|^2+\sum_{i<j}\left(2V_0-\frac{1}{2}m^*\Omega^2|\mathbf{r}_i-\mathbf{r}_j|^2\right)+\frac{\omega_c}{2}\sum_i L_{i,z}, \tag{4}$$

where $\omega_0^2(B)=\omega_0^2+\omega_c^2/4$, $\omega_c=eB/m^*c$, and the z component of angular momentum for particle i is given by $L_{i,z}=x_ip_{i,y}-y_ip_{i,x}$. We now make a transformation to center-of-mass and relative coordinates using the following transformation:

$$\mathbf{R}=(X,Y)=\frac{1}{N}\sum_i \mathbf{r}_i,\quad \mathbf{P}=(P_X,P_Y)=\sum_i \mathbf{p}_i;\quad \mathbf{r}_{ij}=(x_{ij},y_{ij})=\mathbf{r}_i-\mathbf{r}_j,\quad \mathbf{p}_{ij}=(p_{ij,x},p_{ij,y})=\mathbf{p}_i-\mathbf{p}_j\,. \tag{5}$$

This transformation replaces the $2N$ coordinates of the initial system by $2[1+(N/2)(N-1)]$ coordinates. Now H_{space} can be cast into a convenient form by defining the following center-of-mass mode raising (A^+,B^+) and lowering (A^-,B^-) operators:

$$\begin{aligned} A^{\pm}&=\left(\frac{1}{4Nm^*\hbar\omega_0(B)}\right)^{1/2}[Nm^*\omega_0(B)(X\mp iY)\mp i(P_X\mp P_Y)]\,,\\ B^{\pm}&=\left(\frac{1}{4Nm^*\hbar\omega_0(B)}\right)^{1/2}[Nm^*\omega_0(B)(X\pm iY)\mp i(P_X\pm P_Y)]\,, \end{aligned} \tag{6}$$

and relative mode raising (a_{ij}^+,b_{ij}^+) and lowering (a_{ij}^-,b_{ij}^-) operators $(i\neq j)$

$$\begin{aligned} a_{ij}^{\pm}&=\left(\frac{1}{4m^*\hbar\Omega_0}\right)^{1/2}[m^*\Omega_0(x_{ij}\mp iy_{ij})\mp i(p_{ij,x}\mp ip_{ij,y})]\,,\\ b_{ij}^{\pm}&=\left(\frac{1}{4m^*\hbar\Omega_0}\right)^{1/2}[m^*\Omega_0(x_{ij}\pm iy_{ij})\mp i(p_{ij,x}\pm ip_{ij,y})]\,, \end{aligned} \tag{7}$$

where $\Omega_0=[\omega_0^2(B)-N\Omega^2]^{1/2}$. We take $\omega_0>N^{1/2}\Omega$ so that all N electrons remain confined to the dot (i.e., $\Omega_0>0$) for all values of B (see later). These center-of-mass and relative mode ladder operators satisfy *most* of the usual commutation relations, e.g., $[A^-,A^+]=1$ and $[A^{\pm},a_{ij}^{\pm}]=0$. However, the difference lies in the relative mode ladder operators which do *not* fully commute among themselves. In particular,

$$[a_{ij}^-,a_{kl}^+]=[b_{ij}^-,b_{kl}^+]=c_{ijkl}\,, \tag{8}$$

where $c_{ijkl}=2$ if $i=k$ and $j=l$; $c_{ijkl}=-2$ if $i=l$ and $j=k$; $c_{ijkl}=1$ if $i=k$ but $j\neq l$; $c_{ijkl}=-1$ if $i=l$ but $j\neq k$; and $c_{ijkl}=0$ if $i\neq k,l$ and $j\neq l,k$. Equation (4) can now be written equivalently as

$$H_{\text{space}}=H_{\text{c.m.}}+H_{\text{rel}}\,, \tag{9}$$

where

$$H_{\text{c.m.}}=\left(\hbar\omega_0(B)-\frac{\hbar\omega_c}{2}\right)A^+A^-+\left(\hbar\omega_0(B)+\frac{\hbar\omega_c}{2}\right)B^+B^-+\hbar\omega_0(B)$$

and

$$H_{\text{rel}}=\left(\hbar\Omega_0-\frac{\hbar\omega_c}{2}\right)\frac{1}{N}\sum_{i<j}a_{ij}^+a_{ij}^-+\left(\hbar\Omega_0+\frac{\hbar\omega_c}{2}\right)\frac{1}{N}\sum_{i<j}b_{ij}^+b_{ij}^-+(N-1)\hbar\Omega_0+N(N-1)V_0\,.$$

Note that the total Hamiltonian H $(=H_{\text{space}}+H_{\text{spin}})$ and the commutation relations for the ladder operators can equally well describe N interacting fermions *or* bosons.

We now investigate the eigenvalues and eigenstates corresponding to H, ignoring for the moment any requirements on the symmetry of the eigenstates under exchange of two particles. Consider a particular eigenstate $|0,S_Z\rangle$ of H corresponding to a total spin S_Z and eigenvalue $E_0(S_Z)$, and with the additional property that $D|0,S_Z\rangle=0$, where D is a_{ij}^-, b_{ij}^-, A^-, or B^-. The (unnormalized) spatial part of $|0,S_Z\rangle$ is given by

$$\exp\left[-\frac{Nm^*\omega_0(B)}{2\hbar}(X^2+Y^2)\right]\exp\left[-\frac{m^*\Omega_0}{2N\hbar}\sum_{i<j}(x_{ij}^2+y_{ij}^2)\right] \tag{10}$$

and the eigenvalue is given by

$$E_0(S_Z)=\hbar\omega_0(B)+(N-1)\hbar\Omega_0+N(N-1)V_0-(g^*m^*/2m_0)\omega_cS_Z\,. \tag{11}$$

It can be shown that states of the form $(A^+)^{N_A}(B^+)^{N_B}|0,S_Z\rangle$ are eigenstates of H and correspond to a ladder of

center-of-mass modes with eigenvalue $E_0(S_Z)+N_A[\hbar\omega_0(B)-\hbar\omega_c/2]+N_B[\hbar\omega_0(B)+\hbar\omega_c/2]$. These eigenvalues depend only on the frequency of the bare parabola and the cyclotron frequency, and are independent of the number of electrons in the quantum dot. As a result of the curious commutation relations in Eq. (8) the energy spacing for the ladders of relative modes is not immediately obvious. Consider the excitation described by $a_{12}^{+}|0,S_Z\rangle$. Using Eq. (8) it follows that

$$Ha_{12}^{+}|0,S_Z\rangle=E_0(S_Z)a_{12}^{+}|0,S_Z\rangle+\frac{1}{N}\left(\hbar\Omega_0-\frac{\hbar\omega_c}{2}\right)\left(2a_{12}^{+}+\sum_{k>2}(a_{1k}^{+}-a_{2k}^{+})\right)|0,S_Z\rangle. \tag{12}$$

Since $a_{1k}^{+}-a_{2k}^{+}=a_{12}^{+}$, we have

$$\begin{aligned}Ha_{12}^{+}|0,S_Z\rangle&=E_0(S_Z)a_{12}^{+}|0,S_Z\rangle+\frac{1}{N}\left(\hbar\Omega_0-\frac{\hbar\omega_c}{2}\right)[2a_{12}^{+}+(N-2)a_{12}^{+}]|0,S_Z\rangle\\&=\left[E_0(S_Z)+\left(\hbar\Omega_0-\frac{\hbar\omega_c}{2}\right)\right]a_{12}^{+}|0,S_Z\rangle.\end{aligned} \tag{13}$$

The state $a_{12}^{+}|0,S_Z\rangle$ is therefore an eigenstate of H. It can similarly be shown that a ladder of relative modes for each pair of particles i and j can be generated by products of a_{ij}^{+} and b_{ij}^{+}. The eigenstates of the total Hamiltonian H are therefore given by

$$(A^{+})^{N_A}(B^{+})^{N_B}\prod_{i<j}(a_{ij}^{+})^{\alpha_{ij}}(b_{ij}^{+})^{\beta_{ij}}|0,S_Z\rangle, \tag{14}$$

where N_A, N_B, α_{ij}, and β_{ij} are positive integers. The corresponding eigenvalues are given by

$$E=E_0(S_Z)+N_A\hbar[\omega_0(B)-\omega_c/2]+N_B\hbar[\omega_0(B)+\omega_c/2]+\sum_{i<j}[\alpha_{ij}\hbar(\Omega_0-\omega_c/2)+\beta_{ij}\hbar(\Omega_0+\omega_c/2)]. \tag{15}$$

It is clear from Eq. (15) that the ordering of the energy levels will depend on the relative strengths of ω_c (i.e., magnetic field), ω_0 (i.e., the parabolic potential), Ω (i.e., the interaction potential), and N (the particle number), thereby yielding a rich crossing of levels as these parameters are varied [21]. The state $|0,S_Z\rangle$ corresponds to the lowest-energy state for a given total spin S_Z.

So far we have calculated the energy of the states without regard to the fermionic or bosonic character of the individual particles. The special symmetry of the wave function is an additional requirement which selects the physically meaningful eigenstates from among the much larger number of mathematically possible solutions in Eq. (14). The properly symmetrized states corresponding to particles of given statistics are easily identifiable by noting that (1) $a_{ij}^{+}=-a_{ji}^{+}$ and $b_{ij}^{\pm}=-b_{ji}^{\pm}$ under interchange of spatial coordinates for particles i and j, whereas $A^{\pm}$ and $B^{\pm}$ remain unchanged, and (2) $|0,S_Z\rangle$ is symmetric under interchange of spatial coordinates of any two particles. For N *fermions* of spin $\frac{1}{2}$, only states that are antisymmetric under interchange of two particles are allowed. In a large magnetic field, the lower-energy eigenstates will be completely spin polarized, yielding $S_Z=N\hbar/2$. Since the spin state is totally symmetric, the corresponding spatial states must be antisymmetric. Hence in Eq. (14), N_A and N_B can take any values while the sum $\alpha_{ij}+\beta_{ij}$ would be chosen to be an odd integer for each pair i and j. From Eq. (14), the state

$$\prod_{i<j}a_{ij}^{+}|0,S_Z\rangle$$

is the lowest-energy state for large magnetic field ($S_Z=N\hbar/2$) and has a corresponding energy given by Eq. (15),

$$E=\hbar\left[\omega_0(B)+\frac{1}{2}(N-1)(N+2)\Omega_0-\frac{1}{4}N\left(N-1+\frac{g^{*}m^{*}}{m_0}\right)\omega_c\right]+N(N-1)V_0. \tag{16}$$

It is interesting to note that the spatial part of the corresponding wave function is given by

$$\left(\prod_{i<j}(x_{ij}-iy_{ij})\right)\exp\left(-\frac{Nm^{*}\omega_0(B)}{2\hbar}(X^2+Y^2)\right)\exp\left(-\frac{m^{*}\Omega_0}{2N\hbar}\sum_{i<j}(x_{ij}^2+y_{ij}^2)\right), \tag{17}$$

which represents a simple generalization of the Laughlin trial wave function. A full discussion of this result will be presented elsewhere [21]. As the magnetic-field strength B is reduced, competition from other spatial states ($S_Z=N\hbar/2$) leads to a rich crossing of energy levels which depends on particle number N. For example, for three spin-polarized particles the state described by $a_{12}^{+}b_{23}^{+}$ (and its permutations) becomes lower in energy than $a_{12}^{+}a_{23}^{+}a_{13}^{+}$ when $\omega_c<[1/2(\omega_0^2-3\Omega^2)]^{1/2}$. States with $S_Z<N\hbar/2$ compete for ground-state status as B is further reduced [22], and at $B=0$ states with the same

spatial wave function but different S_Z can become degenerate. For three weakly interacting particles, the $B=0$ ground state is fourfold degenerate and corresponds to a linear combination of a_{ij}^{+}'s. For a system of N *bosons* with spin 1, only states that are symmetric under interchange of two particles are allowed, and $|0,S_Z\rangle$ with $S_Z=N\hbar$ is the lowest-energy eigenstate. The corresponding energy is given by Eq. (11) which yields $N\hbar\omega_0$ as the interaction and magnetic field are turned off, as expected for N independent oscillators.

Obviously the model electron-electron interaction $V(\mathbf{r}_i,\mathbf{r}_j)$ is not correct for all electron separations $r=|\mathbf{r}_i-\mathbf{r}_j|$, but the interaction parameters can be adjusted to give the best fit to the true interaction for the dominant range of r, which will increase with N. Equation (1) implies $V(\mathbf{r}_i,\mathbf{r}_j)>0$ (i.e., repulsion) only if $r<r_c$, where $r_c=2V_0^{1/2}/(m^*\Omega^2)^{1/2}$. In order for the model to be physically reasonable, r_c should be greater than the typical electron-electron separation $\bar{r}$ implied by the wave function in Eq. (17) [i.e., $\bar{r}=(N\hbar/2m^*\Omega_0)^{1/2}$]. Choosing $\hbar\Omega=5.6$ meV, $V_0=10$ meV, and $\hbar\omega_0=15$ meV (see Ref. [8]) for a GaAs quantum dot yields a reasonable fit to the true electron-electron interaction for $r<r_c$, where $r_c=350$ Å, and implies that up to seven electrons will remain confined to the dot at $B=0$ (i.e., $\Omega_0>0$). It is reassuring to see that even when the dot is full ($N=6$), $\bar{r}<r_c$ over the B fields of interest ($\bar{r}=108$ Å at 30 T and $\bar{r}=220$ Å at 0 T).

An interesting prediction of the present model is the weakening of the magnetic-field dependence of the N-electron energy levels due to the electron-electron interaction, which is in qualitative agreement with recent experimental data of Ref. [8]. In addition, the present model for $N=2$ electrons gives results within 30% of the full Coulomb calculation of Ref. [12] for the lower-lying energy levels [21].

Although the experimental dots of interest [1–8] are quasi two dimensional [19], dots with more three-dimensional character could be treated theoretically by introducing a parabolic confinement in the z direction, and making a suitable choice of V_0 and Ω for the dominant range of r [21]. In addition, experimental dots with nonparabolic confinement can be described using a perturbation theory based on the exact many-body solutions presented here. This leads to hybridization of the center-of-mass and relative modes [21].

We thank E. M. Restrepo, D. Khelmnitskii, M. Feingold, and B. Simons for valuable discussions. This work was supported by St. John's College, Cambridge (N.F.J.), and by the Royal Society (M.C.P.).

[1] T. Demel, D. Heitmann, P. Grambow, and K. Ploog, Phys. Rev. Lett. **64**, 788 (1990).
[2] A. Lorke, J. P. Kotthaus, and K. Ploog, Phys. Rev. Lett. **64**, 2559 (1990).
[3] C. T. Liu, K. Nakamura, D. C. Tsui, K. Ismail, D. A. Antoniadis, and H. I. Smith, Appl. Phys. Lett. **55**, 168 (1989).
[4] Ch. Sikorski and U. Merkt, Phys. Rev. Lett. **62**, 2164 (1989).
[5] W. Hansen, T. P. Smith, III, K. Y. Lee, J. A. Brum, C. M. Knoedler, J. M. Hong, and D. P. Kern, Phys. Rev. Lett. **62**, 2168 (1989).
[6] J. Alsmeier, E. Batke, and J. P. Kotthaus, Phys. Rev. B **41**, 1699 (1990).
[7] M. A. Reed, J. N. Randall, R. J. Aggarwal, R. J. Matyi, T. M. Moore, and A. E. Wetsel, Phys. Rev. Lett. **60**, 535 (1988).
[8] M. Tewordt, L. Martin-Moreno, V. J. Law, M. J. Kelly, D. Ritchie, J. Frost, M. Pepper, and G. A. C. Jones, in Proceedings of the International Symposium on Nanostructures and Mesoscopic Systems, Sante Fe, 1991 (to be published).
[9] A. Kumar, S. E. Laux, and F. Stern, Phys. Rev. B **42**, 5166 (1990).
[10] G. W. Bryant, Phys. Rev. Lett. **59**, 1140 (1987).
[11] P. A. Maksym and T. Chakraborty, Phys. Rev. Lett. **65**, 108 (1990).
[12] U. Merkt, J. Huser, and M. Wagner, Phys. Rev. B **43**, 7320 (1991).
[13] L. Brey, N. F. Johnson, and B. I. Halperin, Phys. Rev. B **40**, 10647 (1989).
[14] L. Brey, N. F. Johnson, Jed Dempsey, and B. I. Halperin, in Proceedings of the NATO Advanced Research Workshop on Light Scattering in Semiconductor Structures and Superlattices, Mont Tremblant, Quebec, 1990 (Plenum, New York, to be published).
[15] F. M. Peeters, Phys. Rev. B **42**, 1486 (1990).
[16] S. K. Yip, Phys. Rev. B **43**, 1707 (1991).
[17] Q. P. Li, K. Karrai, S. K. Yip, S. Das Sarma, and H. D. Drew (unpublished).
[18] Jed Dempsey, N. F. Johnson, L. Brey, and B. I. Halperin, Phys. Rev. B **42**, 11708 (1990); see Ref. [8] therein.
[19] The z-direction confinement in the experimental dots of interest is strong, hence the electrons essentially lie in the lowest z subband. The free motion is therefore constrained to the x-y plane.
[20] We ignore the effect of spin-orbit coupling which can be shown to be small.
[21] N. F. Johnson and M. C. Payne (to be published).
[22] States with $S_Z<N\hbar/2$ can be formed from a linear combination of all possible spin configurations corresponding to S_Z. See C. Cohen-Tannoudji, *Quantum Mechanics* (Wiley, New York, 1977), p. 1384. For a given S_Z, we can *always* construct a spin state that is symmetric.