Electrons in quantum dots: A comparison of interaction energies

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Recent studies of the effects of electron-electron interactions in quantum dots have utilized differing forms for the particle pair-interaction energy: the Coulomb energy and an energy that varies quadratically with particle separation (harmonic interaction). These two models have fundamentally different ground states for quantum dots in high magnetic fields. The ground state for the Coulomb case can have large total angular momentum, while the harmonic ground state is always at the minimum angular momentum. We bridge these two models, and show that the harmonic interaction is valid, i.e., is a good approximation to the Coulomb interaction, in systems where the electrons are strongly confined in the dot. We also demonstrate that while the Laughlin wave function is an exact eigenstate of the harmonic interaction, the harmonic interaction does not exhibit the fractional quantum Hall ground state because the relative angular momentum of the particles is not constrained to be the same for all particle pairs as for the Laughlin picture. This fact limits the validity of the harmonic interaction to systems with strong confinement, where the fractional quantum Hall effect is quenched.

I. INTRODUCTION

The discovery of the fractional quantum Hall effect by Tsui, Stormer, and Gossard,[1] and the subsequent explanation proposed by Laughlin[2] involving collective electron behavior, have demonstrated the important role of electron-electron interactions in the physics of low-dimensional systems. Of particular current interest are many-body effects in quantum dots in high magnetic fields. Quantum dots may be defined as two-dimensional electron gases (2DEG) that are laterally confined to effectively zero dimensions by an external potential. Two theoretical approaches to this problem have been (1) exact numerical diagonalization of a two-dimensional Hamiltonian for a small number of electrons interacting via the Coulomb potential, and (2) exact analytical solutions for arbitrary numbers of electrons interacting via a harmonic potential. The first discussion of these two approaches for an unconstrained 2DEG was given by Girvin and Jach.[3] Subsequently, the work has been extended to quantum dots with parabolic (harmonic) confinement potentials[4,5] as well as to one-dimensional channels.[6,7] In addition, the interactions have been treated in the Hartree approximation, ignoring exchange and correlation effects but modeling the full 3D quantum-dot geometry realistically, with results similar to those obtained with a harmonic interaction.[8]

Comparisons of the nature of the quantum-dot many-particle ground state predicted by the Coulomb[4] and harmonic[5] interactions exhibit dramatic qualitative differences. For the Coulomb case, the ground state of a confined system at high magnetic field can have a large total angular momentum. This fact was first pointed out by Laughlin,[10] who demonstrated that the ground-state angular momentum is inversely proportional to the confinement strength—the angular momentum for small clusters of particles goes up in integer multiples of the particle number.[3,10] This point is the key to understanding the results of Ref. 4 for the isolated quantum dot. On the other hand, in the region of confining potentials where it is physical, the harmonic interaction predicts a ground state with the lowest total angular momentum allowed by the Pauli principle to arbitrarily high magnetic fields. The purpose of this work is to provide a bridge between these two extremes, and to quantify the usefulness of the harmonic interaction approximation. In addition, we will discuss the role of the Laughlin wave function in the context of the quantum-dot problem, since it is well known that the Laughlin wave function, which is an approximate eigenstate of the Coulomb problem, is an exact eigenstate of the harmonic problem.[3] We will examine the results for small numbers of electrons in both models, since this is the only tractable way to approach the Coulomb problem without restrictive approximations. In addition, we will work in the range of magnetic field such that only the lowest Landau level is occupied—this is reasonable for the ground-state calculations that we are concerned about, since contributions from the other Landau levels have no effect on the results for the lowest Landau level[9] for these cases. The states in the higher Landau levels and the mixed states are combinations of the states in the lowest Landau level and their derivatives, and hence the lowest Landau-level representation may always be projected out.

II. THEORY

We begin by solving the single-particle problem, i.e., noninteracting electrons confined by a harmonic potential. It will be helpful to compare the results for the interacting system with those of the noninteracting one. The Hamiltonian for the one-particle problem is

$$H=\frac{(\mathbf{p}-e\,\mathbf{A})^2}{2m^*}+\tfrac{1}{2}m^*\omega_0^2|\mathbf{r}|^2\ , \tag{1}$$

where m^* is the effective mass, ω_0 is the confinement parameter, and $\mathbf{A}$ is the vector potential. In the symmetric gauge with the applied magnetic field along $+z$ and the

electron gas in the x-y plane ($\mathbf{A}=[-By/2, Bx/2, 0]$), the solutions to (1) in the lowest Landau level can be written for $l \geq 0$, as[11]

$$\psi_l(z)=\frac{(-1)^l}{\sqrt{\pi 2^l l!}} z^l e^{-|z|^2/4} . \tag{2}$$

Here $z=(x-iy)$, $-l$ is the orbital angular momentum quantum number (positive angular momentum states are not in the lowest Landau level), and the lengths in the problem are in units of the modified magnetic length given by

$$l_B^2=\frac{\hbar}{m^*\omega_0(B)} \tag{3}$$

and

$$\omega_0(B)=(\omega_0^2+\tfrac{1}{4}\omega_c^2)^{1/2} , \tag{4}$$

where $\omega_c=eB/m^*$ is the cyclotron frequency. The corresponding energy eigenvalues are given by

$$E=\hbar[\omega_0(B)\{l+1\}-l\omega_c/2] . \tag{5a}$$

For easy comparison to the results that follow, we write the noninteracting N-particle energy as

$$E=N\hbar\omega_0(B)+J\hbar[\omega_0(B)-\omega_c/2] . \tag{5b}$$

Here J is the total angular momentum.

For both the Coulomb problem and the harmonic problem, we will be interested in a harmonically confined, three-particle system. The three-particle problem provides ease of calculation and also provides a good example of general results for small systems. The Hamiltonian for the (interacting) problem may be written

$$H=\sum_i \frac{(\mathbf{p}_i-e\,\mathbf{A}_i)^2}{2m^*}+\tfrac{1}{2}m^*\omega_0^2\sum_i|\mathbf{r}_i|^2+\sum_{i,j}V(|\mathbf{r}_i-\mathbf{r}_i|) . \tag{6}$$

The Hamiltonian (6) will be the starting point for the calculations which follow.

III. RESULTS AND DISCUSSION

In this section we will solve Eq. (6) including two different forms of the interaction energy. We begin by examining the Coulomb problem, characterized by the interaction

$$V(|\mathbf{r}_i-\mathbf{r}_j|)=\frac{e^2}{4\pi\varepsilon\varepsilon_0}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|} , \tag{7}$$

where ε is the background dielectric constant. Following Ref. 3, we numerically diagonalize the Hamiltonian in the basis of eigenstates (2) for the lowest Landau level. If we restrict ourselves to the high-field regime, the complete basis for three particles is quite tractable,[3] and the two-particle interaction matrix elements may be easily evaluated.[3,12,13] In Fig. 1, we show the results of our calculations for the Coulomb problem for a variety of confining potentials, assuming a constant magnetic field of 10 T. Pictured are the single-particle energies [Eq. (5b) above, with the constant energy $\hbar\omega_0(B)$ per particle removed], the interaction energies, and the sum of these contributions as a function of total angular momentum J. The confinement energies are given by $\hbar\omega_0=2.5$ meV (a), $\hbar\omega_0=4$ meV (b),[14] and $\hbar\omega_0=6$ meV (c). To aid in understanding the figure, we first note that without any confinement the energy simply drops off with increasing angular momentum, such that $E\to 0$ as $J\to\infty$. The particles want to be further apart; without confinement there is no kinetic energy cost for this, and so all particles will simply leave the system (in real systems, there is always some confinement, which prevents the system from assuming the state $J=\infty$, i.e., all particles leaving the system). The interaction contribution to the energy therefore behaves (qualitatively) like the Coulomb energy itself—a sharp dropoff for small J (small separation), with much more shallow decline at large J (large separation). This is the reason that the minima at larger J show up in the total energy for low and intermediate confinement: since the kinetic-energy cost of the confinement goes up linearly with J, it overwhelms the in-

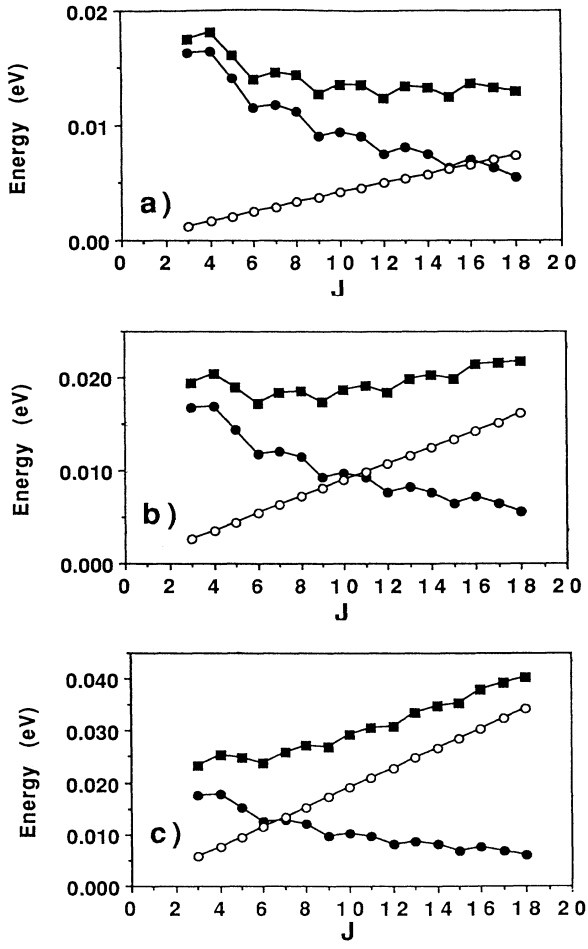

FIG. 1. The single electron (open dots) and interaction (closed dots) energies, together with their sum (squares), as a function of total angular momentum (in units of $\hbar$) for a quantum dot in a magnetic field of 10 T. The confinement energies are (a) 2.5 meV, (b) 4 meV, and (c) 6 meV, respectively.

teraction energy for large relative separation—the electrons are indeed confined, and the ground state is in the regime of large angular momentum. As we will see, this is the fractional quantum Hall regime (see below). Note also that the minima always occur at values of J which are integral multiples of the particle number.[10] On the other hand, large confinement energies simply prevent the electrons from getting too far apart [Fig. 1(c)]; the kinetic energy cost of the high J states is too great.

Turning to the harmonic problem, we adopt the interaction studied in Ref. 5, i.e.,

$$V(|\mathbf{r}_i-\mathbf{r}_j|)=2V_0-\tfrac{1}{2}m^*\Omega_0^2|\mathbf{r}_i-\mathbf{r}_j|^2 , \tag{8}$$

where V_0 and Ω_0 are parameters. This problem is quite interesting in that one may solve for the eigenstates and eigenvalues of (6) exactly by employing the center-of-mass and relative-mode ladder operators defined in Ref. 5; in particular, since we are interested only in states in the lowest Landau level (and dropping center-of-mass motion), we need only the relative mode raising operator to write the eigenstates of (6):

$$a_{ij}^{\dagger}=\left[\frac{1}{4m^*\hbar\Lambda}\right]^{1/2}\{m^*\Lambda(x_{ij}-iy_{ij})-i(p_{ij,x}-ip_{ij,y})\} , \tag{9}$$

where $\Lambda^2=\omega_0^2(B)-N\Omega_0^2$, x_{ij} and y_{ij} are the x and y components of the relative position operator for the particle pair i,j, and $p_{ij,x}$ and $p_{ij,y}$ are the x and y components of the relative momentum operator for the pair, respectively. The eigenstates in the lowest Landau level are then given by

$$|\Psi\rangle=\prod_{i<j}(a_{ij}^{\dagger})^{\alpha_{ij}}|0\rangle , \tag{10}$$

where the state $|0\rangle$ is the usual Gaussian in the relative and center-of-mass coordinates.[5] The α_{ij} are positive odd integers for *each* pair i,j to maintain antisymmetry of the wave function under particle exchange (assuming spin-polarized particles). The corresponding eigenvalues are

$$E=\hbar\{\omega_0(B)+(N-1)\Lambda\}+N(N-1)V_0 + \sum_{i<j}\alpha_{ij}\hbar(\Lambda-\omega_c/2) . \tag{11}$$

If we turn off the interactions, i.e., $V_0\to 0$ and $\Lambda\to\omega_0(B)$, we immediately recover Eq. (5b) above, provided that $\sum\alpha_{ij}=J$. We note that the energy of the interacting system is linear in J with a slope given by $(\Lambda-\omega_c/2)$. The slope must remain positive for the electrons to be confined—if the slope is negative, the system assumes the state $J=\infty$, as above (the positive slope condition here translates into the confinement condition $\omega_0>N^{1/2}\Omega_0$ noted in Ref. 5). Therefore, we see that the high-field ground state for this system, when the picture is physically reasonable, is always the state with the lowest J value, i.e., $\alpha_{ij}=1$ for all i,j. In Fig. 2(a) we show that the energy eigenvalues for the harmonic approximation can be adjusted to have reasonably good overlap with the full Coulomb problem (for three particles) in the regime of large confinement energies. Here $\hbar\omega_0=9$ meV, and the other parameters are fit to the $J=3$ energy: $\hbar\Omega_0=2.5$ meV and $V_0=3.6$ meV. Note that only odd J values are shown for the harmonic interaction. The even values of J would come from center-of-mass contributions and have been omitted [the reason for this omission is clarity: the eigenstates (10) above will next be compared to the Laughlin wave functions, which do not contain center-of-mass motion]. In Fig. 2(b) we show that for the parameters we have chosen, the interaction energies are in good agreement over a large range of relative particle separation.

An interesting comparison to make at this point is that of the Laughlin trial wave function and the states (10) above. The ground state of the 2DEG proposed by Laughlin[2] is

$$|m\rangle=\prod_{i<j}(z_i-z_j)^m\exp\left[-\tfrac{1}{4}\sum_i|z_i|^2\right] , \tag{12}$$

where m is an odd integer and z_i are the complex particle coordinates. We point out that dependence on relative

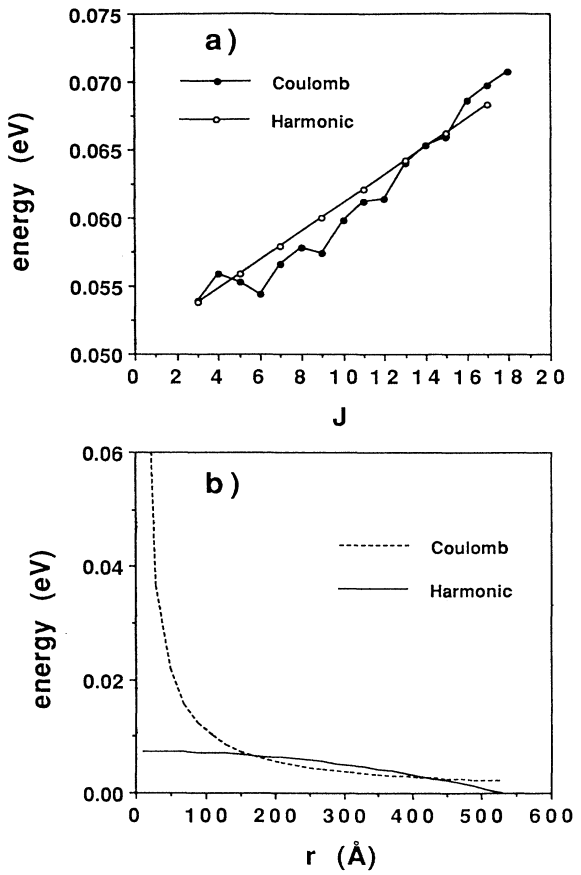

FIG. 2. (a) Comparisons of the total energy vs angular momentum for the Coulomb (closed dots) and the harmonic (open dots) interactions. (b) Comparisons of the two interaction energies as a function of particle separation for the parameters which give the fit in (a) (see text). Note the agreement over a large range of separations.

particle position for the states (12) and the states (10) are the same provided that the α_{ij} in Eq. (10) are the *same* for each particle pair—in other words, as long as the relative angular momentum is the same for each pair. This statement is important if we are to recover the results for total angular momentum and filling factor ν. If all α_{ij} are the same, then the sum becomes $J=\sum\alpha_{ij}=[N(N-1)/2]m$, where m is an odd integer. This is the usual result for large systems. We note that it is the restriction on relative angular momentum that makes the Laughlin functions work for the fractional quantum Hall effect; when the confinement is lowered, the system is not allowed to lower its energy by rearranging the relative angular momenta. The system remains in the $m=1$ state until the transition from $m=1$ to $m=3$, where it remains until the transition to $m=5$, etc. The Coulomb interaction has this feature "built in," i.e., the cusps in the ground-state energy at higher angular momentum in Fig. 1 are a reflection of this effect. Without an artificially imposed constraint, the exact solutions for harmonic interactions have only the $\alpha_{ij}=1$ ground state or else the confinement is released to the point where all the particles leave the dot.

Regarding the filling factor, it can be shown for the states (12) that the filling factor is given by $\nu=1/m$; therefore, the ground state of the quantum dot for large confinement (recall that for the ground state, $\alpha_{ij}=1$ for all pairs, which corresponds to the $m=1$ Laughlin state) occurs at $\nu=1$, and the fractional quantum Hall effect will not occur. On the other hand, the results for the Coulomb interaction indicate a ground-state crossover from high angular momentum states at lower confinement (larger quantum dots) to the minimum J at high confinement (smaller quantum dots). For the large J ground states, the arguments just presented give $\nu<1$, and the fractional quantum Hall effect should occur.[15,16]

In summary, we have examined the effect of confinement potentials on the ground state of a gas of interacting 2D electrons in a high magnetic field, utilizing two different forms of pair interactions. We find that the Coulomb interaction has ground states at angular momenta that are larger than the minimum value satisfying the Pauli exclusion principle, a feature not seen for harmonic interactions. The harmonic and Coulomb interactions are in good agreement for strongly confined systems. Comparing the quantum-dot eigenstates with the fractional quantum Hall ground state indicates that if the ground-state angular momentum is a minimum, then the filling fraction is $\nu=1$, and if $J>J_{\min}$ then $\nu<1$. Therefore, at a fixed magnetic field, the fractional quantum Hall effect will be quenched by confinement, and it is in this regime that the harmonic interaction is a reasonable approximation.

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