Symmetry of ‘molecular’ configurations of interacting electrons in a quantum dot in strong magnetic fields

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A molecular description for magic-number configurations of interacting electrons in a quantum dot in high magnetic fields developed by one of the authors has been elaborated for four, five, and six electron dots. For four electrons, the magic spin-singlet states are found to alternate between two different resonating valence bond (RVB)-like states. For the five-electron spin-polarized case, the molecular description is shown to work for the known phenomenon of magic-number sequences that correspond to both the N-fold symmetric ring configuration and a (N − 1)-fold symmetric one with a center electron. A six-electron dot is shown here to have an additional feature in which inclusion of quantum mechanical mixing between classical configurations, which are deformed and degenerate, restores the N-fold symmetry and reproduces the ground-state energy accurately.

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I. INTRODUCTION

Quantum dots are two-dimensional (2D) electron systems confined in a small (∼ few hundred nanometer) region and have attracted much attention as artificial atoms [1]. A remarkable feature of these ‘atoms’ is their controllability. A dramatic feature in fact arises when quantum dots are placed in high magnetic fields, where specific total-angular momentum (L) states are stabilized with downward cusps in the energy against L. The cusps, originally found from numerical calculations [2], are called ‘magic numbers’ in the angular momenta. When the magnitude of magnetic field is varied, the true ground state changes from one magic-number state to another. Some of the cusps occur at the same fractional filling factors as the fractional quantum Hall effect in bulk systems.

In a different light, quantum dots may be regarded as a 2D ‘molecule’ that consists only of electrons, as contrasted with the ordinary atoms where electrons are bound to nuclei. The quantum states in strong magnetic fields can in fact be treated with a molecular description, which has been developed by one of the present authors [3]. In this approach we start from the classical equilibrium configuration and make an expansion of the Hamiltonian to obtain anti-symmetrized wavefunctions. In a previous work [3] this approach has been tested for ground and excited states of three electrons, and was found to give energies as accurate as within 0.1% of the exact-diagonalization result for L ∼ 30 in a parabolic confining potential.

Here we extend the theory to four, five, and six electrons in search of features for larger number of electrons. All our results are for a GaAs dot with a typical experimental situation of 4meV confinement energy in a magnetic field of 20T.

II. MAGIC NUMBERS

The magic numbers are known to depend on the number of electrons, N, and total spin, S. For fully spin-polarized electrons, magic L’s are 3,6,9,12,... for N = 3 and L = 6,10,14,18,... for N = 4. Namely, the magic numbers occur with an interval of N, or more precisely L = N(N − 1)/2 + N × integer. Another sequence of magic numbers, having an interval N − 1 with L = N(N − 1)/2 + (N − 1) × integer, appears for six spin-polarized electrons. For five spin-polarized electrons, the main sequence has an interval N and the ground state for any the magnetic field belongs to the sequence. If one looks more closely at the L- dependence, however, there are weak cusps with an interval N − 1, and we can call these states excited magic-number states. It is known that an N-fold ring has the magic number states with interval N − 1, while an N − 1-fold ring with a particle at the center has an interval N − 1. If we look at the quantum mechanical density correlation function in Fig. 4, where we fix the position of one electron to plot the density of others, we can indeed identify both N- and N − 1-fold rings.
FIG. 1. Quantum mechanical density correlation with one electron fixed at the position indicated by a dot (upper panels) as compared with classical equilibrium point-charge configurations (lower panels) for typical magic-number states. For \( N = 5, 6 \), \( N\)-fold and \((N - 1)\)-fold symmetric states occur and give rise to two sequences of magic numbers with intervals \( N \) and \( N - 1 \), respectively.

III. ECKART-FRAME THEORY

The molecular description provides not only a way of understanding the magic numbers, but also a quantitatively accurate description of the ground-state energy in the strong field regime. The starting point is the remarkable correspondence between the quantum mechanical configurations (upper panels of Fig.1) and the classical equilibrium configurations (lower panels) of point charges interacting with the Coulomb repulsion. The physical picture of the system in the high field regime is then that of an ‘electron molecule’ which rotates with total angular momentum \( L \) and vibrates around its classical equilibrium configuration. We can first harmonically expand the Hamiltonian around the classical configuration. The vibration is treated in a similar way to that of chemical molecules, and this is facilitated by the use of a molecular-fixed reference frame called the Eckart frame in which the rotational and vibrational motions decouple to first order. We then diagonalize the Hessian matrix for the harmonically expanded Hamiltonian and obtain the effective potential. Using the effective potential and taking account of Coriolis coupling, we find the rotational and vibrational motions decouple to first order. We called the Eckart frame in which the rotational and vibrational motions decouple to first order [3]. We then diagonalize the Hessian matrix for the harmonically expanded Hamiltonian and find the rotational and vibrational states. The final important ingredient is the anti-symmetrization of the wavefunction.

When the classical equilibrium configuration has \( C_m \) symmetry, a group-theoretical consideration dictates that antisymmetrization enforces a wavefunction to have a factor

\[
\sum_{i=0}^{m-1} (\pm 1)^i \exp \left[ -\frac{2\pi i t}{m} \left( L_{RM} + k_s + \sum_{i=1}^{2N-3} n_i k_v(i) \right) \right],
\]

where \( n_i, k_v(i) \) are the quantum number and phase parameter corresponding to the \( i \)th normal mode, respectively, while \( k_s \) is the phase parameter for the spin wavefunction. It follows that the wavefunction vanishes unless

\[
L_{RM} + k_s + \sum_{i=1}^{2N-3} n_i k_v(i) \equiv \begin{cases} 0 \mod m, & m \text{ odd} \\ m/2 \mod m, & m \text{ even} \end{cases}
\]

This criterion reproduces the correlation between the \( N \)- and \((N - 1)\)-fold rings and the interval of magic numbers.

After quantum numbers that satisfy this condition have been found, the total energy can be written in the form

\[
E = E_{CM} + E_{cl} + E_{zp} + E_x(n_1, \cdots, n_{2N-3})
\]

where \( E_{CM} \) is the energy of center-of-mass motion, \( E_{cl} \) is that of the classical configuration, \( E_{zp} \) is the quantum zero-point energy and \( E_x(n_1, \cdots, n_{2N-3}) \) is the excitation energy of the vibrational state.

IV. FOUR ELECTRONS

We have calculated energies and density correlation functions for ground states against total angular momentum for all the spin configurations using both exact diagonalization and Eckart-frame theory. The energies for spin-singlet (\( S = 0 \)) states are plotted in figure which shows that the Eckart-frame theory produces accurate ground state energies. We have also checked that ground-state energies obtained by Eckart-frame theory for all the other spin configurations agree very well with those of the exact diagonalization. One can readily see from equation that the interval between magic numbers is affected by the total spin \( S \). For the spin-polarized case, \( S = 2 \) here, the magic numbers are \( L = 6, 10, 14, 18, \ldots \) and these are explained by equation with \( k_s = 0 \). In the case of \( S = 0 \) states magic numbers are \( L = 6, 8, 10, 12, 14, 16, 18, \ldots \). The spin-resolved correlation functions are displayed in fig. which show that there are two different sequences; one has \( L = 10, 14, \ldots \) while the other has \( L = 12, 16, \ldots \) in the Eckart-frame theory, these magic numbers are characterized by different \( k_s \). The former corresponds to \( k_s = 0 \) and the latter to \( k_s = 2 \). Except for a normalization, the spin wavefunctions are written as

\[
k_s = 0 : \begin{array}{c|c} \\
\end{array} - \begin{array}{c|c} \\
\end{array} \]

\[
k_s = 2 : \begin{array}{c|c} \\
\end{array} + \begin{array}{c|c} \\
\end{array} = \begin{array}{c|c|c} \\
\end{array}
\]

We can rewrite these in terms of spin-singlet pairs as

\[
k_s = 0 : \begin{array}{c|c|c} \end{array} - \begin{array}{c|c|c} \end{array} \]

\[
k_s = 2 : \begin{array}{c|c|c} \end{array} + \begin{array}{c|c|c} \end{array} = \begin{array}{c|c|c|c} \end{array}\]


where
\[ \equiv \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle). \]
These wavefunctions are the same as the RVB (resonating valence bond) states considered for the Hubbard model [8].
The configuration of the spin resolved density correlation in Fig. 3 is indeed explained from equations (4,5).

**FIG. 2.** (a) Lowest energies against the total angular momentum \( L \) for \( N = 4, S = 0 \).
(b) The same for \( N = 5, S = 5/2 \). Solid (open) arrows indicate the magic numbers with interval \( N \) (solid-down-arrows) and the interval \( N - 1 \) (open-up-arrows). In each figure, the solid line with filled circles represents the result of Eckart-frame theory while the dotted line with open circles gives the exact diagonalization result.

**FIG. 3.** Spin-resolved density correlation functions for \( N = 4, S = 0 \) magic-number states. We fix an up-spin at the position indicated with a filled circle to contour-plot the density of parallel spins (upper panels) and anti-parallel spins (lower panels).

**V. FIVE ELECTRONS**

In the case of five electrons, there are two different classical equilibrium configurations: a pentagon and a square with one particle at the center. These configurations are shown in Fig. 1. We have calculated lowest-energy states against \( L \) in the Eckart-frame theory for both of the configurations, and have plotted the lowest of these two energies in Fig. 2. The difference from the exact-diagonalization result is less than 0.2 % for \( L \sim 40 \).

In Fig. 2 we have indicated the magic numbers with the interval \( N \) (solid-down-arrows) and the interval \( N - 1 \) (open-up-arrows). If we look at in Fig. 1 the density correlation for the states belonging to the \( N \)-sequence \( (L = 30) \) or the \( (N - 1) \)-sequence \( (L = 22) \), the shape of the molecule does indeed possess the \( N \)-fold or \( (N - 1) \)-fold symmetries, respectively.

**VI. SIX ELECTRONS**

For the six electron system, we have again two kinds of classical equilibrium configurations: a six-fold ring and a pentagon with a center particle as shown in Fig. 1. If we more closely look at the six-fold ring, the classical configuration is distorted from the regular hexagon and there are doubly-degenerate three-fold equilibria, which would naively imply magic numbers with an interval of three.

The exact-diagonalization result for the magic numbers for six spin-polarized electrons, however, consists of a series having period of six \( (L = 21, 27, 33) \) along with another having period of five \( (L = 25, 30, 35, 40, 45, ...) \). The period of six may at first seem inconsistent with the three-fold classical configurations. However, this discrepancy can be resolved by noting that the six-fold symmetry is restored when a quantum mechanical mixture of the rotational-vibrational states centered at the two three-fold configurations is used to construct the approximate electron state. In Fig. 4, the classical energy of a rotating configuration \( L = 33 \), no vibration) is plotted against the distortion (see Fig. 4 B) that couples the three-fold rings. The saddle point is the regular hexagon while the two minima are the rings distorted in staggered directions. The height of the barrier (about 0.0001meV) is much smaller than the typical lowest quantum vibrational energy (about 1.0 meV), so that they are almost completely mixed to result in a restored six-fold symmetry.

To calculate the energy of the hexagonal states we approximate the vibrational potential energy. A six-electron molecule has nine in-plane normal modes and the lowest has the same displacement pattern as distortion shown in Fig. 4. The vibrational potential depends on \( L \) and is almost parabolic for \( L \geq 15 \), but for the normal mode shown in Fig. 4 there is some small extra structure which originates from the double minimum in the energy without vibration.

There are two relevant normal modes that are Coriolis-coupled, and, because the curvature of the vibrational potential obtained by diagonalizing the Hessian matrix around the saddle point is small, one
of the solutions of the coupled equation of vibrational motion becomes unstable. However, this way (i.e., use of the Hessian matrix) of evaluating the potential is only valid in the immediate vicinity of the saddle point, while the wavefunction has a much larger extension, over which we should approximate the vibrational potential (inset in Fig. 4 a) by a parabola. We can then fit the curvature of the vibrational potential in the region of about 20% of the mean radius, which is a few percent larger than the curvature obtained by the Hessian matrix, and indeed makes the vibrational motion stable. This is how we find the ground state energy in the six-fold case.

For the five-fold configuration with a center electron, we have obtained the ground-state energy in the same way as for \( N = 3, 4 \). We compare the ground-state energies of six-fold and five-fold configurations at each value of \( L \). In Fig. 4 we have plotted the lowest of the two possible energies. The result agrees very well with the exact diagonalization and the difference between the ground-state energies is 0.4% or less around \( L = 60 \).

![Image of potential-energy surface](image)

FIG. 4. (a) The classical potential-energy surface for \( N = 6, S = 3, L = 33 \), plotted against the distortion in the lowest normal mode. Double minima correspond to doubly-degenerate, deformed classical equilibria indicated in insets A and C, while the saddle point B is a regular hexagon. In the inset of (a), the vibrational potential energy is plotted against the distortional vibration.

(b) Lowest energies against \( L \) for \( N = 6, S = 3 \). The solid line with filled circles is obtained in the Eckart-frame theory with the quantum mixing, while the dotted line with open circles the exact diagonalization result.

VII. CONCLUSION AND DISCUSSIONS

In this paper, we have confirmed the accuracy of the electron-molecule description of interacting electrons in a quantum dot in high magnetic fields for four, five and six electron systems. For four spin unpolarized electrons, there are two sequences of magic numbers that correspond to two RVB-like spin configurations. For five electrons, accurate ground state energies are obtained by considering both \( N \)-fold and \((N-1)\)-fold molecules. For six electrons, we have shown that the quantum mixing between states localized on classically distorted configurations leads to the symmetry expected from the exact diagonalization results.

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