Rotating electrons in quantum dots: Quantum Hall liquid in the classical limit

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(Dated: today)

We solve the problem of a few electrons in a two-dimensional harmonic confinement using quantum mechanical exact diagonalization technique, on one hand, and classical mechanics, on the other hand. The quantitative agreement between the results of these two calculations suggests that, at low filling factors, all the low energy excitations of quantum Hall liquid are classical vibrations of localized electrons. The Coriolis force plays a dominant role in determining the classical vibration frequencies.

PACS numbers: 71.10.-w, 73.21.La, 71.10.Pm, 73.43.Lp

Spectroscopic studies of semiconductor quantum dots have shown that in zero magnetic field they behave like ‘artificial atoms’ showing electronic shell structure and obeying Hund’s rule\(^1\), while in a strong magnetic field they have properties of quantum Hall liquids\(^2\)\(^-\)\(^7\). The integer quantum Hall effect corresponds in a quantum dot geometry has mainly been theoretical, showing formation of fractional quantum Hall liquid (e.g. the Laughlin wave function\(^8\) and Jain construction\(^9\)).

The generic model of a semiconductor quantum dot is very simple: Electrons interacting with Coulomb interaction in a two-dimensional harmonic potential. The Hamiltonian is

\[
H = -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_i \frac{1}{2} \hbar \omega_i r_i^2 + \sum_{i<j} \frac{e^2}{4\pi\varepsilon_0 |r_i - r_j|} \tag{1}
\]

where \(N\) is the number of particles, \(m\) the electron mass, \(\mathbf{r} = (x, y)\) a two-dimensional position vector, and \(\omega_0\) the oscillation frequency of the confining potential. We solve the many-particle problem for a fixed angular momentum using the single particle basis of the lowest Landau level (LLL):

\[
\psi_\ell(r, \phi) = A_\ell e^{-r^2/4} e^{i\ell\phi}, \tag{2}
\]

where \(\ell\) is the single-particle angular momentum and \(A_\ell\) a normalization factor. We are interested in solutions for large total angular momenta. In this case the restriction of the basis in the LLL is a good approximation\(^10\). Note that we do not explicitly include magnetic field in our calculations: The only effects the magnetic field would have, were to polarize the electron gas due to the Zeeman effect and to increase the total angular momentum. We present our results in terms of angular momentum. The total angular momentum can be related to the filling factor of electrons with the relation \(\nu = N(N-1)/2L\), where \(N\) is the number of electrons and \(L\) the total angular momentum.

We solve the many-particle Schrödinger equation using the straightforward CI technique. The many-particle states are linear combinations of Slater determinants of single particle configurations. The number of configurations needed increases fast with \(N\) and \(L\), but for the results shown here a complete basis in the LLL could still be used. For determining the Coulomb matrix elements we used the method of Ref. \(^11\).

Classical electrons in a 2D harmonic trap form Wigner molecules, where the electrons arrange in consecutive circles\(^12\)\(^-\)\(^16\). The elementary excitations of the classical system consist of the center of mass vibrations with angular frequency \(\omega_0\), internal vibrations which can be solved from the dynamical matrix, and rigid rotations of
the Wigner molecule. Since we are interested in the excitations of a rotating system (with fixed angular momentum) we have to solve the internal vibrations in a rotating frame. Taking into account the Coriolis force turns out to be crucial in the case of electrons in a harmonic trap (although its effect in real molecules is small).

The equilibrium positions of the electrons depend on the angular velocity \( \omega_r \) or angular momentum \( L = I \omega_r \) of the molecule (\( I \) is the moment of inertia \( I = \sum m r_i^2 \)), and they can be solved by minimizing the classical energy

\[
E_{cl}^0(L) = \frac{1}{2} m \omega_0 \sum_i r_i^2 + \sum_{i<j} \frac{e^2}{4 \pi \epsilon_0 |r_i - r_j|} + \frac{L^2}{2m \sum r_i^2}.
\]

(3)

The eigenfrequencies of the vibrations can then be solved analytically from the equations of motion of the rotating frame (by linearizing the equations around the equilibrium positions of electrons). Results for classical vibrational frequencies for 2, 3 and 4 electrons are shown in Fig. 1. The eigenfrequencies are shown as a function of the angular velocity of the rotating \( \omega_r \). We notice that all frequencies approach to either 0 or 2 times \( \hbar \omega_0 \). In all calculations shown in this letter we have used atomic units \( (m = \hbar = e = \omega_0 = 1) \) and chosen \( \omega_0 = 0.5 \). We should note that in the LLL the results are independent of \( \omega_0 \), apart from the energy scale.

For each particle number the highest mode corresponds to the breathing mode where the molecule expands and shrinks without changing its shape. In a rotating frame, however, each electron moves along an ellipse around its equilibrium position. In the case of two electrons this mode is naturally the only vibrational mode. For 2, 3 and 4 particles the breathing mode energy is the same and its dependence of the angular velocity is similar \( \omega_{hm} = \sqrt{3 \omega_0 + \omega_r} \) (this is general result for a Wigner molecule where the electrons form one single ring).

In the case of 3 and 4 electrons the non-rotating system has degenerate vibrational modes. However, when the system is put in rotation the degeneracy will split. In the case of three electrons the ground state is an equilateral triangle. In the doubly degenerate vibrational mode the triangle stays isosceles, the base stretching and shrinking. In the non-rotating system we can choose any of the sides to be the base, but only two of them linearly independently. However, we can also choose a linear combination of the two modes in such a way that the base circulates around. In this pseudo-rotation the electrons move in circles around their equilibrium positions (as indicated in Fig. 4). The degeneracy then follows from the two possible direction of the pseudo-rotation. If the molecule is put in rotation, the Coriolis force splits this degeneracy. Similar analysis can be made for the degenerate mode in the case of four electrons. It is interesting to note that in the case of sodium trimer, where the Jahn-Teller effect opens the equilateral triangle, a related pseudo-rotation have been observed.

\[
E_{cl} = E_{cl}^0(L) + \sum_k \hbar \omega_k (n_k + \frac{1}{2}) + \hbar \omega_0 (n_0 + 1),
\]

(4)

where \( \omega_k \) are all the vibrational frequencies determined in the rotating frame and \( n_k = 0, 1, 2, \cdots \), and the last term corresponds to the center of mass excitations. These energies can now be compared with those obtained by solving the many-particle Schrödinger equation. However, we still have to note that the quantum state for
The interaction energy is shown as a function of the angular momentum. The black dots are results of the Schrödinger equation and the open squares the results from the classical model. The center of mass excitations are not shown as points but are indicated as dashed lines. The numbers indicate the vibrational state \((n_1, n_2)\).

Fermions has to be antisymmetric. This means that not all combinations of \(L\) and \(n_k\) are allowed (but any center-of-mass excitation is always possible). The symmetry analysis can be made with help of group theory and it shows, for example, that without any vibrational modes only every second angular momentum is allowed for two particles, every third for the triangle of three particles and every fourth for the square of four particles. The lowest energy of any other angular momentum value must have either a center of mass excitation or an internal vibration in addition of the internal rotation. This fact leads to the well known oscillations of the lowest energy as a function of the angular momentum.

Figures 2 and 3 show the lowest energies for three and four particles obtained using two different ways: Solving exactly the many-particle Schrödinger equation and by solving the vibrational modes using classical mechanics and determining the energy from Eq. (2). The figures show the ‘interaction energy’, the energy difference between the interacting and non-interacting electrons, \(E - (N + L)\hbar\omega\), where \(E\) is the solution of the Schrödinger equation of of Eq. (4). In this presentation the center-of-mass excitations become horizontal (the center-of-mass motion is independent of the interactions) and they are only indicated as dashed lines. The results show that spectra determined by quantizing the classical vibrations agree very well with those from the full quantum mechanical calculations. The error in the total interaction energy is less than 1 %. We note in passing that in the case of the frequently studied system of two electrons the low energy spectrum only consists of rigid rotations and center-of-mass excitations, since the only vibrations mode is high in energy.

In the case of three electrons the purely rotational state can occur at angular momenta \(L = 3n\), where \(n\) is an integer. For \(L = 3n + 1\) the lowest energy state has a center of mass excitation (the point not shown) and for \(L = 3n + 2\) the lowest energy state has vibrational mode \(\omega_1\). The excited states for any angular momentum show simple systematics consisting of center of mass excitations and multiplets of \(\omega_1\), as indicated in Fig. 3. In the case of four particles the energy spectrum is more complicated due to the two low energy vibrational modes. Nevertheless, Fig. 3 shows that also in this case the spectrum consists of periodic sequences, but the length of the period is now four.
In Figures 2 and 3 we have shown the spectra for large angular momenta, where the quantization of the classical energies give quantitatively accurately the energy differences. The angular momentum \( L = 54 \) for four particles and \( L = 27 \) for three particles corresponds to the filling factor \( \nu = 1/9 \) of a quantum Hall liquid, where the electrons are expected to be localized to a Wigner crystal. However, the excitation spectrum, when plotted as in Figs. 2 and 3 are qualitatively similar already from angular momenta corresponding to filling factor \( \nu = 1/3 \).

Finally, we want to show that the pair correlation functions determined from the full quantum mechanical calculation are consistent with the vibrational modes determined from classical mechanics. Figure 4 shows schematically the classical vibrational modes in the rotational frame compared to the pair correlation functions determined for different states shown in the spectra in Figs. 2 and 3. The pair correlation functions for the purely rotational states shows clearly the localization of the electrons, and their shape is in agreement with the semiclassical model of Matulis and Anisimovas\[17\]. However, the interpretation of the vibrational states is not so simple, because the structure of the pair correlation function depends on the reference point. In Fig. 4 the reference electron is chosen to be at the extreme point of the classical motion. In this case we can identify the classical extreme positions as shown as triangles and quadrangles drawn on top of the pair correlation functions. Note that the pair correlation function can capture the classical geometry in two different positions.

In conclusion, we have determined the classical rotational and vibrational modes of electrons in a two-dimensional harmonic trap using a rotational frame. Results of the quantized energies are compared with numerically exact solutions of the many-particle Schrödinger equation, and they indicate clearly that when the angular momentum of the system increases to the region which corresponds to the filling factor of 1/9 of the quantum Hall liquid, the whole low-energy excitation spectrum can be quantitatively described with the classical rotations and vibrations. The pair-correlation functions are consistent with the classically determined vibrational modes.

Acknowledgments. We would like to thank Ben Mottelson, Matti Koskinen and Stephanie Reimann for valuable discussions. This work was supported by the Academy of Finland.

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