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Classical Nature of Quantum Dots in a Magnetic Field

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A quasiclassical theory of few-electron quantum dots in a strong magnetic field is developed. The ground state energy and the corresponding many-electron wave function are obtained and used to derive a universal relation of critical magnetic fields and calculate the currents and the density--current correlation function.

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1. Introduction

Computation of the electronic structure of strongly correlated quantum dots is not an easy task [1]. One sure way to attack this problem is by employing the exact numerical diagonalization of the few-particle Hamiltonian

$$H = \frac{1}{2}\sum_{n=1}^{N}\left[\left(-\mathrm{i}\nabla_n + \frac{1}{2}[\boldsymbol{B}\times\boldsymbol{r}_n]\right)^2 + r_n^2\right] + \sum_{n>m}^{N}\frac{\lambda}{|\boldsymbol{r}_n-\boldsymbol{r}_m|}, \tag{1}$$

which we were able to carry out for quantum dots containing a small number of electrons [2]. In Eq. (1), energies are measured in units $\hbar\omega_0$ and coordinates in $l_0 = \sqrt{\hbar/m^*\omega_0}$, with ω_0 being the confinement frequency. The magnetic field is expressed in $\Phi_0/2\pi l_0^2$ ($\Phi_0 = hc/e$). The exact numerical work provides a complete piece of information about the system (the many-body wave function) in terms of numbers but will not arrive at any analytical relations. An alternative route to proceed is by developing simpler analytical approaches based on guessed or known basic ingredients of the physical problem or a visualizing idea [2, 3].

It is known, for example, that in the presence of a strong electron–electron interaction (which is further enhanced by the application of a strong magnetic field), the electrons in the quantum dots tend to crystallize into Wigner molecules [4] which for $2 \div 5$ electrons in a parabolic confinement consists of a single ring with

the electron equilibrium positions arranged equidistantly. Assuming the formation of such a structure we base our theory on the notion of a rotating and vibrating classical Wigner molecule (electron ring). In this way, we are able to calculate the ground state energy, construct the many-electron wave function and obtain the density-current correlators.

We also uncover a strikingly simple law describing the critical magnetic fields, i.e., the magnetic field strengths at which the ground state changes its angular momentum. Consideration of currents in the dot reveals the formation of persistent and local currents circulating around the electron density lumps. Trustworthiness of our theory is confirmed by comparison with the exact numerical results.

2. Model

We consider a 2D parabolic quantum dot containing up to $N = 5$ electrons in a perpendicular magnetic field $\boldsymbol{B}$. In the $B \to \infty$ limit the electrons form a ring of radius $a_n = a$ with electrons located at angular positions αn ($\alpha = 2\pi/N$) as shown in Fig. 1 for the case of three electrons. This figure also introduces the local coor-

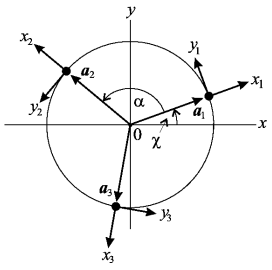

Fig. 1. Local coordinates for three electrons on a ring.

dinates x_n (y_n) counted in the radial (azimuthal) direction from the equilibrium positions. Due to the azimuthal symmetry the electronic ring may rotate; also, at high but not infinite magnetic fields harmonic vibrations of electrons around the classical equilibrium positions have to be taken into account. Coupling of these vibrations to the rotation of the system as a whole complicates the construction of a quantum-mechanical description. The situation can be managed by introducing a frame rotating with a constant angular velocity $\dot{\chi}$ in which the electron system has zero total angular momentum.

Let us briefly outline the solution while leaving the details of the procedure to a separate publication [5]. We follow Maksym [6] and start with the classical Lagrangian which is easily transformed into the rotating frame and recast in terms of normal modes obtained by Fourier-transforming the local coordinates. This makes it easy to deal with the condition of zero total angular momentum and we further employ the standard procedure to obtain the vibrational Hamiltonian

in the harmonic approximation. This Hamiltonian is a collection of independent 1D and 2D oscillators, thus its ground state is a product of the corresponding Gaussians. Transforming the result back into the laboratory frame we get the final expression for the wave function as

$$\Psi = \exp\left(\mathrm{i}M\chi - BK/4\right), \tag{2}$$

$$\chi = \frac{1}{Na}\sum_{n=1}^{N} y_n \left(1 - \frac{1}{Na}\sum_{n=1}^{N} x_n\right), \tag{3}$$

$$K = \sum_{n=1}^{N}(x_n^2 + y_n^2) + \frac{1}{N}\left[\left(\sum_{n=1}^{N} x_n\right)^2 - \left(\sum_{n=1}^{N} y_n\right)^2\right]. \tag{4}$$

3. Critical fields

The corresponding energy of the lowest state of angular momentum M is

$$E(M,B) = \frac{|M|}{B} + \lambda f_N \sqrt{\frac{NB}{2|M|}}. \tag{5}$$

Here, $f_N = 1/2, \sqrt{3}, 1+2\sqrt{2}, \ldots$ for $N = 2, 3, 4, \ldots$ is a geometric factor, and we have taken into account the fact that states of *negative* angular momenta have the lowest energies. As a matter of fact, the absolute angular momentum $|M|$ is monotonically increasing with increasing magnetic field. From our result (5) it is easy to find the critical field values B_M at which the absolute value of the ground state angular momentum jumps from $-|M|$ to $-(|M|+1)$

$$B_M = \frac{2|M|+1}{(Nf_N^2)^{1/3}}\lambda^{-2/3}. \tag{6}$$

Thus, our quasiclassical treatment predicts a strikingly simple and universal power--law dependence of the critical fields on the Coulomb interaction strength. Numerical studies [2] confirm that this law is indeed fulfilled even at quite small values of $|M|$ where quantum-mechanical effects are expected to be important.

4. Persistent currents

In order to visualize the electron motion in a strongly correlated quantum dot we consider the electrical currents. Left panel of Fig. 2 shows the charge and current density profiles for a three-electron quantum dot in the ground state of angular momentum $M = -18$. We see that an electron ring is formed and the currents flow in opposite directions on the inner and outer circumference of the ring. Although the current density profile looks almost ideally antisymmetric, its integral does not vanish indicating that there is a small symmetric component and

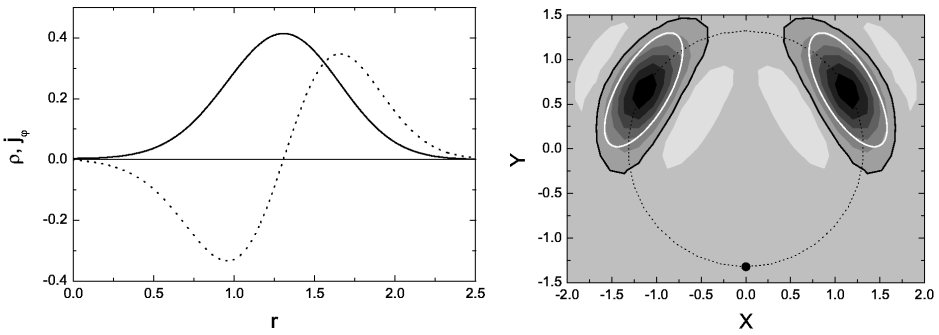

Fig. 2. Currents in a three-electron dot. The left panel shows the density (full line) and current (dotted line) profile, and right one shows the conditional currents arising when one electron is pinned at the position indicated by the dot.

a net current crossing the dot radius. This component of the current expresses the rotation of the crystallized ring as a whole and is akin to persistent currents flowing in small-scale electron rings [7]. However, we stress that in quantum dots the appearance of persistent currents is a truly many-body effect. Firstly, the ring itself is formed due to the Coulomb repulsion, and moreover, it is this repulsion that precludes the exact compensation between the paramagnetic and vector-potential components of the current [5].

5. Local currents

We find that the ring rotation accounts only for a small (symmetric) part of the large currents seen in Fig. 2. In order to understand the character and the role of the remaining current we must filter away the global rotation. This can be done by considering the density-current correlation function, in other words, the conditional currents — the currents flowing in the system, given that one electron is pinned at a certain position. We were able to show that in the quasiclassical limit such conditional currents are conserved and thus physically well defined. The right panel of Fig. 2 shows the vorticity (curl) of the conditional currents when one electron is fixed at a point on the classical radius. Dark (light) areas correspond to positive negative vorticity as obtained from an exact numerical diagonalization, and the zero-vorticity level is marked by a full black line. The results obtained quasiclassically are qualitatively similar but predict more strong localization, with the corresponding zero-vorticity level shown by the white line. We see that the two free electrons are performing a cyclotron-like motion along elliptic trajectories elongated in the azimuthal direction. That is, the Wigner crystal in a high magnetic field can be visualized as an ordered system of current vortices rather than just charge density lumps.

6. Conclusion

In conclusion, we see that the obtained quasiclassical description is capable of capturing the essential physics such as the ground state angular momentum transitions and Wigner crystallization. It provides us with a simple and transparent picture while being able to compete with the accuracy of a full quantum-mechanical calculation.

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