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Quantum dot version of topological phase: half-integer orbital angular momenta

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We show that there exists a topological phase equal to π for circular quantum dots with an odd number of electrons. The non-zero value of the topological phase is explained by axial symmetry and two-dimensionality of the system. Its particular value (π) is fixed by the Pauli exclusion principle and leads to half-integer values for the eigenvalues of the orbital angular momentum. Our conclusions agree with the experimental results of T. Schmidt et al., Phys. Rev. B **51**, 5570 (1995), which can be considered as the first experimental evidence for the existence of the new topological phase and half-integer quantization of the orbital angular momentum in a system of an odd number of electrons in circular quantum dots.

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It is known for a long time already [1, 2], see also [3], that in certain cases half-integer quantization of the orbital angular momentum occurs in molecules. In Ref. [2] half-integer values of the orbital angular momentum are associated with the Berry's geometrical phase π that the nuclear wave function acquires under a pseudo-rotation around the equilateral configuration of the molecule Na_3. This was apparently the first experimental verification of the Berry's phase in high-resolution molecular spectroscopy. For reviews on Berry's phase [4, 5] in more general context see Refs. [6, 7].

In this paper we show that the half-integer quantization of the orbital angular momentum may occur also in circular quantum dots with odd numbers of electrons. In these systems the electron motion may be considered as being restricted to two dimensions. 2D geometry and the assumption of axial symmetry of the confining potential results in the existence of loops that are not deformable to a point [8]: the topology of the system is equivalent to that of a once-punctured plane, cf., [9]. Hence, there exists a topological phase. Since this topological phase defines a one-parametric set of self-adjoint generators of rotations, it determines the rotational dynamics of the electronic system, cf., [10]. Its particular value follows from the Pauli exclusion principle. In circular quantum dots with an odd number of electrons the topological phase of the ground state wave function takes the value π. Below we demonstrate that our conclusions agree with the experimental results [11]. Based on our analysis presented in this paper, we believe that Ref. [11] may be considered as the first experimental observation of half-integer orbital angular momenta in a system of an odd number of electrons in circular quantum dots.

According to [12] (see also [13]) the oscillatory model with the parabolic confinement

$$V_{cf} = \sum_{a=1}^{N} m_* \Omega^2 \mathbf{r}_a^2/2 + V^{(0)}, \tag{1}$$

is a good approximation for low-lying levels in real circular N-electron quantum dots [14, 15]. Here m_* is the effective mass, $\mathbf{r}_a$ is the two-dimensional coordinate of an electron, and the effective confining frequency Ω and the reference energy level $V^{(0)}$ are phenomenological parameters. In general Ω and $V^{(0)}$ depend on the number of particles in a quantum dot (cf., Ref. [12]) and the quantum numbers describing the state of the electronic system. Within this approach the Schrödinger equation can be written in dimensionless variables as [16]

$$\left\{-\frac{1}{4Q^2}\sum_{a=1}^{N}\frac{\partial^2}{\partial \boldsymbol{\rho}_a^2} + \sum_{a=1}^{N}\rho_a^2 + \frac{1}{2}\sum_{a\neq b}^{N}|\boldsymbol{\rho}_a - \boldsymbol{\rho}_b|^{-1}\right\}\Psi_N = \\ = \varepsilon(N)\Psi_N. \tag{2}$$

Here,

$$Q = \frac{1}{\hbar}\left(\frac{m_* e^4}{2\epsilon^2\Omega}\right)^{1/3} = \left(\frac{\mu}{\epsilon^2}\right)^{1/3}\left(\frac{E_B}{\hbar\Omega}\right)^{1/3} \tag{3}$$

is the dimensionless parameter [17] which is determined by the ratio of the characteristic Coulomb energy of electron-electron interaction to the mean level spacing in

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the confining potential. We employ the following notations: ϵ is the effective dielectric constant, $\mu = m_*/m_e$, a_B is the Bohr radius, $E_B = m_e e^4/2\hbar^2$, $-e$ and m_e are charge and mass of a bare electron. The reduced energy $\varepsilon(N) = [E(N) - V^{(0)}(N)]/E_0$ and the dimensionless coordinate $\boldsymbol{\rho}_a = \mathbf{r}_a/a_0$ are determined by the characteristic energy and the characteristic size of the system

$$E_0 = Q\hbar\Omega = \frac{\mu E_B}{\epsilon^2 Q^2},\ a_0 = \left(\frac{2e^2}{\epsilon m_* \Omega^2}\right)^{\frac{1}{3}} = \frac{2\epsilon}{\mu}\, Q^2 a_B. \tag{4}$$

In virtue of the axial symmetry of the problem, the reduced energy $\varepsilon(N) = \varepsilon_M(N)$ can be numbered by values of the conserved total orbital momentum M, which is an eigenvalue of generator of rotations $\hat{L} = -i\partial/\partial\varphi$, φ is the angle of rotation of the system as a whole, $0 \le \varphi < 2\pi$.

It is well known that the differential operator $\hat{L}$ becomes self-adjoint, i.e. determines an observable, if it is defined on the Hilbert space of wave functions obeying boundary conditions, which in their most general form read [10],

$$\Psi(2\pi) = e^{i\theta}\Psi(0), \quad 0 \le \theta < 2\pi \tag{5}$$

(see also a recent paper [9]). The topological phase θ arises as a result of rotation of the system around the axis of symmetry by 2π. Unlike the Berry's phase [4, 5] which is acquired by a wave function in the process of evolution of a system determined by a Hamiltonian, the topological phase θ itself determines an operator $\hat{L}_\theta$ from a one-parameter family of self-adjoint operators and, hence, the unitary operator $\hat{U}_\theta$ which describes the rotational dynamics of the system similarly to the evolution operator,

$$\Psi(\varphi + \tau) = \hat{U}_\theta(\tau)\Psi(\varphi) = \exp(i\tau\hat{L}_\theta)\Psi(\varphi).$$

In virtue of Eq. (5), the eigenvalues of the generator $\hat{L}_\theta$ are given by

$$M = \gamma + m,\ m = 0, \pm 1, \ldots,\ \theta = 2\pi\gamma\,, 0 \le \gamma < 1\,, \tag{6}$$

and its eigenfunctions

$$\Psi_M(\varphi) = \exp(iM\varphi)/\sqrt{2\pi} \tag{7}$$

implement an irreducible representation of the two-dimensional rotation group $SO(2)$.

The specific value of γ is determined by additional physical reasons. If we require that the wave function remains unaltered after the rotation of the system by 2π, then $\gamma = 0$ and the eigenfunctions (7) implement a single-valued representation of $SO(2)$. In this case the orbital angular momentum eigenvalues are (up to the factor of $\hbar$) integers. In cases where γ is a rational number the representation is multiple-valued [8] and the angular momentum quantization may be fractional. However, if the system is invariant with respect to time inversion, only two cases $\gamma = 0$ or $\gamma = 1/2$ can be realized [9].

We will show now that the choice between two possible values of γ for our problem is fixed by the Pauli exclusion principle. Formally, Eq. (2) is equivalent to the Schrödinger equation for N particles with masses $2Q^2$. We are interested in the case of an odd number of electrons $N \ge 3$. In the limit $Q \to \infty$ the ground state is realized by a rigid configuration of electrons minimizing the potential energy. This configuration is invariant under the 2π rotation around the symmetry axis. This may be used to understand the quantization of the angular momentum operator. Indeed, the overall phase acquired by the ground state wave function after the rotation is determined by the total momentum J. The 2π rotation of a two-dimensional system is obviously the identity element of the symmetric group S_N and thus belongs to the alternating group A_N of even permutations of the set $\{1, ..., N\}$. Hence, the 2π rotation of the system is equivalent to an even number of pairwise transpositions, and according to the Pauli exclusion principle the wave function do not change:

$$\exp(i2\pi J) = 1\,, \quad J = M + \Sigma = 0, \pm 1, \pm 2, \ldots \tag{8}$$

Here the total momentum J is represented by the sum of the orbital and spin angular momenta. For the odd number of electrons the spin quantum number Σ is half-integer. Thus the orbital angular momentum M must also take a half-integer value. According to Eq. (6) this implies that $\gamma = 1/2$ or that the system is characterized by the topological phase $\theta = \pi$.

Consider now the case of three electrons. If the total spin number $\Sigma = \pm 1/2$, then M can take any half-integer value. However, the situation is different if $\Sigma = \pm 3/2$. Then there is an additional symmetry in the problem. The symmetry group of such system is C_{3v} which is isomorphic to the symmetric group S_3. The group C_{3v} consists of rotations about the symmetry axis by multiples of the angle $2\pi/3$ (the C_3 group) and reflections in the three bisectrices of the triangle. C_3 is isomorphic to A_3 and thus the wave function of the system at $Q \to \infty$ does not change also if it is subjected to a rotation by $2\pi/3$. Thus,

$$\exp(iJ2\pi/3) = 1\,, \quad J = M + \Sigma = 0, \pm 3, \pm 6, \ldots \tag{9}$$

This means that M can take the values $M = \pm(3 + 6k)/2$, $k = 0, 1, 2, \ldots$.

To arrive to these conclusions we have considered the classical limit $Q \to \infty$. However, if one varies the parameter Q adiabatically, the quantum numbers M and Σ cannot change. Therefore our result is valid also at $Q \sim 1$ which is typical for real quantum dots. Moreover, it can be easily shown that this is true in the limit $Q \to 0$ also. Indeed, the variables in the Schrödinger equation can be separated exactly in this case. Then, taking proper account of the Pauli exclusion principle one arrives after not complicated calculation to the following result for a three-electron quantum dot: minimal energy corresponds to the state with $M = 1/2, \Sigma = 1/2$.

Now we show that our conclusions are in excellent agreement with the experiment of T. Schmidt et al. [11]. The authors of Ref. [11] measured the ground state energy $E(N)$ of N-electron circular quantum dots in GaAs-based heterostructures in a perpendicular magnetic field $0 \le H \le 16\,\mathrm{T}$ for $N = 1 \div 30$. To explain the data, we should modify the calculation of the spectrum of a quantum dot in order to take into account the magnetic field. For this purpose it is enough to make the changes in Eqs. (2)-(4): (i) $\Omega(N) \to \Omega_L(N)$, where $\Omega_L = \sqrt{\Omega^2 + \omega_L^2}$ and $\omega_L = eH/2m_*c$ is Larmor frequency; (ii) $Q \to Q_L = (\mu/\epsilon^2)^{1/3}(E_B/\hbar\Omega_L)^{1/3}$; and (iii) take into account the Zeeman shift (we use the symmetric gauge for vector potential $\mathbf{A} = 1/2\,[\mathbf{H} \times \mathbf{r}]$). This way we find for the energy of a quantum dot

$$E_{M\Sigma}(N;H) = \varepsilon_M(N;H)Q_L\hbar\Omega_L(N) - (M + \mu g\Sigma)\hbar\omega_L + V^{(0)}_{M\Sigma}(N), \tag{10}$$

where g is the effective Lande factor and $\varepsilon_M(N;H)$ replaces $\varepsilon_M(N)$ in Eq. (2) after the change $Q \to Q_L$.

It is very important that the first term in the RHS of Eq. (10) depends on H^2. Therefore, in a weak field, $\omega_L \ll \Omega(3)$, the derivative of the energy with respect to magnetic field is determined for the most part by the Zeeman energy

$$\left.\frac{dE_{M\Sigma}}{dH}\right|_{H=0} = -\frac{e\hbar}{2m_*c}(M + \mu g\Sigma), \tag{11}$$

and does not depend on the shape and parameters of the confining potential. In the experiment of Ref. [11] the typical values of the parameters are $\epsilon = 12.5$, $\mu = 0.067$, and $g = 0.44$. Thus the coefficient in the RHS of Eq. (11) is equal to 0.864 (measuring $E_{M\Sigma}$ in meV and H in T). On can see from Eq. (10) that at $H \approx 0.5\,\mathrm{T}$ the quadratic term in the expansion of $E_{M\Sigma}$ becomes of the order of the Zeeman energy. Therefore the weak-field interval is $0 \le H < 0.5\,\mathrm{T}$.

The results of calculation of the effective Coulomb energy $E(3,H) - 3E(1,H)$, which was measured in the experiment [11], are shown in Fig.1 for the weak-field limit. For the energy of a one-electron quantum dot we adopt the expression $E(1,H) = \hbar\Omega_L(1) - \mu g\hbar\omega_L/2$, where $\hbar\Omega_L(1)$ is the Fock-Darwin energy and $\hbar\Omega(1) = 3.60\,\mathrm{meV}$ [11]. The experimental points are taken from Ref. [11]. The diameter of the circles corresponds to the size of experimental points in Fig.3 of Ref. [11] and reflects experimental error of approximately $0.025\,\mathrm{meV}$. Two direct lines in Fig.1 show the slope of $E(3,H) - 3E(1,H)$ at $H \to 0$ calculated according to Eq. (11). For the solid line $M = 1/2$ and for the dotted one $M = 1$. It is clear from Fig.1 that, unlike the value $M = 1$ for the orbital angular momentum considered by the authors of Ref. [11], the value $M = 1/2$

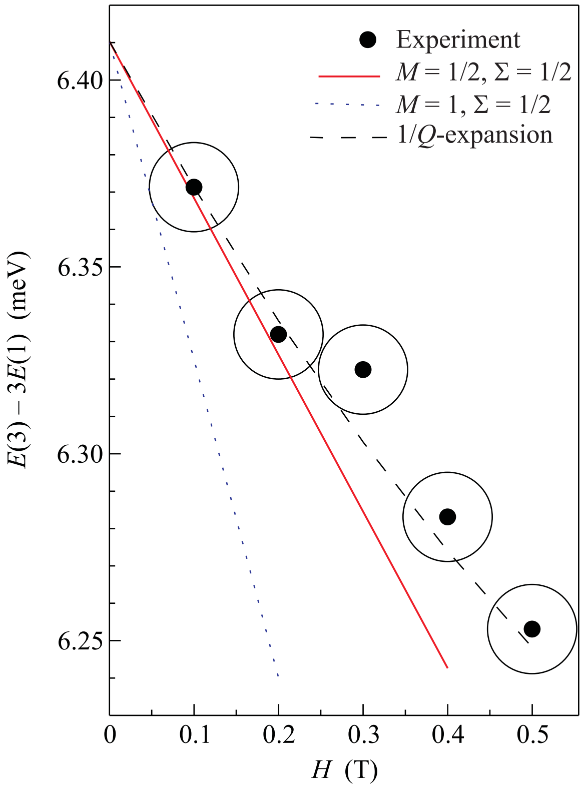

Fig.1. The effective Coulomb energy $E(3) - 3E(1)$ versus magnetic field H for weak field, $\omega_L \ll \Omega(3)$. The solid and the dotted lines show the slope of $E(3,H) - 3E(1,H)$ at $H \to 0$ calculated according to Eq. (11) for $M = 1/2$ and $M = 1$ respectively. The experimental points are taken from Ref. [11]. The size of the circles corresponds to the size of experimental points in Fig.3 of Ref. [11] and reflects experimental error of approximately $0.025\,\mathrm{meV}$. The dashed line gives the results of calculations according to Eq. (10) in approximation (12) with parameters $\hbar\Omega(3) = 5.21\,\mathrm{meV}$, $V^{(0)}(3) = -24.0\,\mathrm{meV}$ and $\hbar\Omega(1) = 3.60\,\mathrm{meV}$

agrees with the data quite well. Deviation of the experimental points from the linear law (11) at $H > 0.2\,\mathrm{T}$ is explained by the influence of the quadratic term in the weak field expansion of $E_{M\Sigma}$.

The solution of Eq. (2) valid for a more broad range of magnetic fields H can be obtained in the form of an expansion over the small parameter $1/Q_L$ ("$1/Q$-expansion" method [16]). The first three terms of this expansion for the energy of the ground state and the nearest excited state read

$$\varepsilon_{Mm_1}(3) = 3.9311 + (3.0908 + |m_1|)Q_L^{-1} + \\ + \big[0.1908(M+m_1)^2 + 0.2435\big]Q_L^{-2}. \qquad (12)$$

Here $m_1 = \pm M$[2)] is the eigenvalue of the orbital angular momentum of the center of mass of the 3-electron system. The results of calculations for the ground state $m_1 = -M = -1/2$ according to Eq. (12) are shown in Fig.1 by the dashed line.

The agreement between the data and our calculations leads us to believe that the results of the experiment [11] unambiguously specify the quantum numbers of the ground state of a three-electron quantum dot right up to the point of the first crossing, or up to such value of magnetic field $H^{(cr)}$ when the symmetry of the ground state is changed [18]. Quantum numbers of the ground state after the first crossing cannot be chosen *a priori* because of the unknown dependence of the phenomenological parameters Ω and $V^{(0)}$ in Eq. (1) on the quantum numbers. Varying these parameters we can obtain an excellent fit of the experimental data [11] by the results of the $1/Q$-expansion. Certainly, in the experiment [11] $Q \sim 1$, or are even slightly less than 1. However, it was shown in Ref. [16] that for the case of two-electron dots the first three terms of $1/Q$-expansion provide 3%-accuracy even at $Q \lesssim 1$. Since the relative contribution of the Coulomb repulsion for three-electron quantum dots is greater than for two-electron dots, we believe that the accuracy of approximation (12) in the region $Q \sim 1$ is of the same order at least up to the first crossing.

The result of the fitting procedure is shown in Fig.2. The experimental points are taken from Ref. [11]. We have found the locations of three crossings in the range $0 < H < 8\,\mathrm{T}$ at $H_1^{(cr)} = 2.5\,\mathrm{T}$, $H_2^{(cr)} = 4.3\,\mathrm{T}$ and $H_3^{(cr)} = 6.2\,\mathrm{T}$. Quantum numbers M and Σ are chosen according to condition (8) everywhere except the region between the first and the second crossings, $H_1^{(cr)} < H < H_2^{(cr)}$, where the condition (9) was used. The values of effective confining frequencies $\hbar\Omega(3)$ are given

2) This equality follows from the requirement of the wave function invariance with respect to an even number of pairwise transpositions.

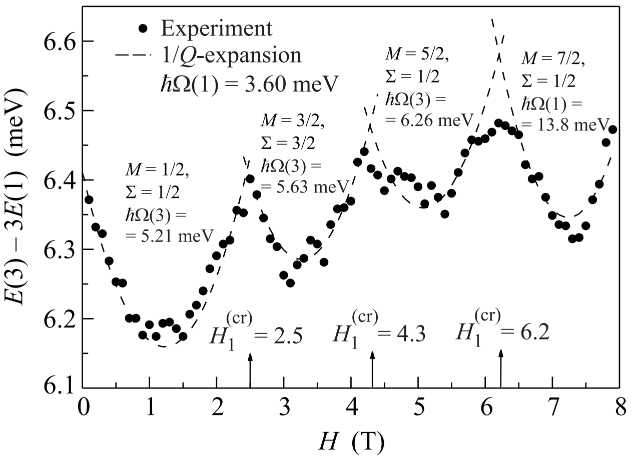

Fig.2. Comparison of the experimental data (solid circles) of T. Schmidt at el. [11] for $E(3) - 3E(1)$ with the results of calculations according to Eq. (10) in approximation (12)(the dashed line). The numbers give the values of the total electron spin and orbital angular momenta, and the effective confining frequencies. Arrows indicate the crossing points

in Fig.2, and the values of the parameter $V^{(0)}(3)$ in meV for successive intervals between the crossing points are -24.0, -30.4, -37.9, -126.8. One can see that the theoretical curve is in a very good agreement with the experiment.

We believe that the results shown in Figs.1, 2 represent convincing evidence in favor of our interpretation of the experiment [11]. Therefore, we regard the data presented in Ref. [11] as the first experimental demonstration of the existence of theoretically admissible half-integer values of the orbital angular momentum in two-dimensional quantum systems. It is worth emphasizing that the choice between the integer and the half-integer variants of quantization of orbital angular momentum in our problem is dictated by the Pauli exclusion principle.

However, there is a question whether our result contradicts the fundamental laws of quantum mechanics. Whatever is the motion of electrons in the quantum dot, the whole system is three-dimensional, and thus its orbital angular momentum must be integer. The question is where the extra half-integer orbital angular momentum is concentrated in this system.

Certainly, the additional half-integer orbital momentum belongs to the macroscopic subsystem of the whole heterostructure not relating to the system of electrons in the quantum dot. This problem is akin to the back-reaction problem for motion of a system of microscopic particles in a classical background. In our case, just the heterostructure, which is a macroscopic device, creates the two-dimensional classical background for the electrons of the quantum dot. In the standard situation when the whole structure is fixed, the half-integer orbital angular momentum which arises in the subsystem of electrons after tunneling of an odd electron into the dot is compensated by the momentum transferred to the macroscopic device. The device is at rest with respect to the Earth and therefore the transferred momentum is unobservable. If an exotic experiment with a quantum dot immersed in a pendent heterostructure could be held on, then the device would start rotating upon loading an odd electron into the quantum dot. The total orbital angular momentum would be of course integer but the angular momentum transferred to the macroscopic subsystem would stay unobservable.

It is worth noting that half-integer quantization of the orbital angular momentum in molecules [2, 3] is bound up with the existence of the topological Berry phase and was observed only for the slow subsystem of a molecule. Clearly, the total momentum of the molecule remained integer. In our case the quantum dot also is a subsystem of the whole heterostructure which in contrast to the molecule is a macroscopic object.

In conclusion, we have predicted the existence of a new topological phase along with half-integer quantization of the orbital angular momentum for 2D axially symmetric systems with an odd number of confined electrons. We argue that the experimental data for circular quantum dots in a strong magnetic field [11] is in agreement with this statement.

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