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Electron correlations in quantum ring and dot systems

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Abstract

A model for a quantum ring in magnetic fields is introduced where various electronic properties viz., the single- and many-electron energy spectrum, magnetization (persistent current) and the dipole-allowed absorption energies can be studied very accurately. The impurity potential lifts the degeneracies in the energy spectrum and the persistent current is then reduced from the impurity-free value. The effect of the Coulomb interaction on the persistent current is, however, insignificant. The dipole-allowed absorption energies in a quantum ring are presented. Similar studies for a quantum dot with a Gaussian impurity in the middle reveal quite rich structures in the absorption spectrum.

1. Introduction

Recent studies of quantum confined systems have made it increasingly clear that electron correlations play a major role in these mesoscopic systems [1]. Recent experimental observations of the persistent current in a mesoscopic ring [2] and the magnetoplasmon resonances in quantum ring arrays [3] clearly require theoretical understanding of the role of electron correlations in a quantum ring. While the single-electron results are fairly well established [4], no reliable quantitative theory exists, as yet, in the case of many-electron systems. Based on some intuitive arguments, Leggett [5] recently conjectured that, for arbitrary electron–electron interactions and an arbitrary external potential, the maxima and minima of the energy curves for even and odd number of electrons would be the same as for the noninteracting systems.

We have recently introduced a model of quantum ring to study the energy spectrum where impurity and Coulomb interactions are included explicitly [6] in the Hamiltonian. In our model the electron is confined in a parabolic potential and subjected to a perpendicular magnetic field. The single-electron Hamiltonian is written as

$$\mathscr{H} = \frac{1}{2m^*}\left(p - \frac{e}{c}A\right)^2 + \frac{1}{2}m^*\omega_0^2(r - r_0)^2,$$

where we use the symmetric gauge vector potential $A = \frac{1}{2}(-By, Bx, 0)$. We have demonstrated earlier [6] that our model, in the appropriate limit, correctly reproduces the behavior of an ideal one-dimensional ring [4] and that of a two-dimensional electron gas. The energy spectrum in the case of non-interacting and interacting electrons, magnetization [6] and the susceptibility [7] have been studied earlier in this model. The two-body Coulomb matrix elements are evaluated numerically, with the result that, in the lowest Landau level and for an impurity-free system, the Coulomb interaction simply shifts the noninteracting energy spectrum to higher energies. There is no discernible effect of interaction on the magnetization. This is explained as due to conservation of angular momentum in the system: all close-lying states in the lowest Landau level belong to different angular momentum and the Coulomb force cannot couple them.

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Weidenmüller et al. reached at a similar conclusion independently [8]. Influence of inter-electron interaction on the persistent current has also been studied in one-dimensional (1D) disordered discrete-lattice ring model [9]. In this model, exact results from numerical diagonalization of the Hamiltonian are available for small ring sizes. In the case of long-range Coulomb interactions, it was found that, depending upon the disorder, interaction can increase or decrease (mostly decrease) the current.

Electronic properties of quasi-zero-dimensional electron systems (quantum dots) in a magnetic field have been under intense investigations in recent years [10–13]. These systems exhibit phenomena reminiscent of atoms (and are therefore commonly called artificial atoms) and yet their size, shape, etc. can be controlled in the experiments. Theoretical results on the electronic properties of these quantum-confined few-electron systems [10–12] have been generally in good agreement with the experimental results [13]. Ever since the first theoretical work on interacting quantum dots in a magnetic field was reported [10], a large number of papers on variations of such systems have been published in the literature [11]. Almost all of these theoretical studies involve impurity-free quantum-confined few-electron systems. Here we describe the properties of a quantum dot which includes a repulsive scatterer. Such a system can alternatively be thought of as a quantum ring depending upon the magnetic-field strength and the strength of the impurity. Experimental work on the magnetoplasma resonances in quantum dots with repulsive impurity at the center has been reported recently [3].

2. Quantum ring model

In our quantum ring model, the wave functions are of the form

$$\psi_\lambda = R_{nl}(r)e^{il\theta}, \quad n = 0, 1, 2, \ldots, \quad l = 0, \pm 1, \pm 2, \ldots,$$

and λ represents the quantum number pair $\{n, l\}$. The impurity interaction is chosen to be of the form:

$$V^{\text{imp}}(r) = V_0 e^{-(r-R)^2/d^2}, \tag{1}$$

where V_0 is the potential strength and d is the width. The impurity matrix element can then be written as

$$T_{\lambda,\lambda'} = 2\pi V_0 e^{im\theta_0} \int R_\lambda(r) R_{\lambda'}(r) e^{-(R^2+r^2)/d^2} I_m\left(\frac{2rR}{d^2}\right) r\,dr \tag{2}$$

where $m = l' - l, (R, \theta_0)$ is the impurity position and I_m is the modified Bessel function. The two-body interaction matrix elements [6] are

$$V_{\lambda_1\lambda_2\lambda_3\lambda_4} = \delta_{l_1+l_2,l_3+l_4} 2\pi \int_0^\infty dq\, qV(q) \times \int_0^\infty dr_1\, r_1 J_{|l_1-l_4|}(qr_1) R_{\lambda_1}(r_1) R_{\lambda_4}(r_1) \times \int_0^\infty dr_2\, r_2 J_{|l_2-l_3|}(qr_2) R_{\lambda_2}(r_2) R_{\lambda_3}(r_2), \tag{3}$$

where J_m is the Bessel function of order m. We have used the Coulomb interaction in a plane: $V(q) = 2\pi\kappa/q$, where $\kappa = e^2/4\pi\varepsilon_0\varepsilon$. Let r_0 be the radius of the ring and $A = \pi r_0^2$ its area. The length is measured in units of r_0 and the energy in units of $h^2/2\,m^*\pi A$ [6]. In these units the confinement potential is

$$U(r) = \tfrac{1}{2}m^*\omega_0^2(r - r_0)^2 = 4\alpha^2(x-1)^2,$$

where $\alpha = \omega_0 m^* A/h$, $x = r/r_0$. This is to be compared with the Coulomb interaction which in the present case takes the form

$$\frac{e^2}{\varepsilon r} = 9.45\, m^*\left(\frac{r_0}{1\text{ nm}}\right)\frac{1}{\varepsilon x}.$$

In our present work we used $r_0 = 10$ nm, $\varepsilon = 12.9$ as the background dielectric constant, and the effective mass was chosen to be $m^* = 0.067$, appropriate for GaAs. In the impurity potential given above, the strength V_0 is expressed in this energy unit. For $\alpha = 20$, the single-electron energy spectrum closely resembles that of an ideal 1D ring, while for $\alpha = 5$, it has the characteristics of a 2D electron gas [6, 7]. In what follows, we present the numerical results for these two values of α. Once the energy spectrum is obtained from numerical diagonalization of the Hamiltonian, the magnetic moment is calculated from the derivative of energy with respect to the magnetic field. The persistent current is found to decrease drastically in the presence of strong disorder, but the role of Coulomb interactions on the persistent current is almost insignificant.

3. Dipole-allowed transitions

The effect of the impurity on the optical absorption spectrum was studied in the dipole approximation. Defining the single particle matrix elements

$$d_{\lambda\lambda'} = \langle\lambda'|re^{i\theta}|\lambda\rangle = 2\pi\delta_{l+1,l'}\int_0^\infty r^2 R_{n'l'}(r) R_{nl}(r)\,dr,$$

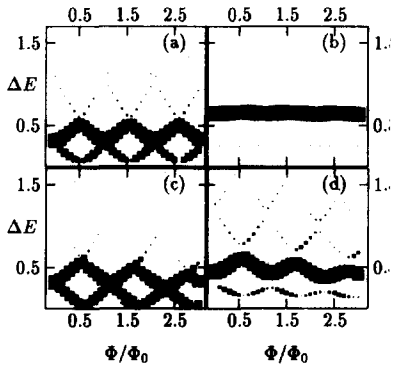

Fig. 1. Dipole-allowed absorption energies of a single electron in a quantum ring versus Φ/Φ_0 for: (a) $\alpha = 20$, $V_0 = 1.0$, $d = 0.2$; (b) $\alpha = 20$, $V_0 = 4.0$, $d = 0.5$; (c) $\alpha = 5$, $V_0 = 0.5$, $d = 0.2$ and (d) $\alpha = 5$, $V_0 = 1.0$, $d = 0.5$.

the dipole operators can be written as

$$X = \frac{1}{2}\sum_{\lambda\lambda'}[d_{\lambda'\lambda} + d_{\lambda\lambda'}]a^{\dagger}_{\lambda'}a_{\lambda},$$

$$Y = \frac{1}{2i}\sum_{\lambda\lambda'}[d_{\lambda'\lambda} - d_{\lambda\lambda'}]a^{\dagger}_{\lambda'}a_{\lambda}.$$

The probability of the absorption from the ground state $|0\rangle$ to an excited state $|f\rangle$ will then be proportional to the quantity

$$W = |\langle f|\boldsymbol{r}|0\rangle|^2 = |\langle f|X|0\rangle|^2 + |\langle f|Y|0\rangle|^2. \quad (4)$$

In the figures, where we display absorption spectra, the areas of the filled points are proportional to W.

In impurity free one-electron rings the dipole-allowed absorption from the ground state can happen only to the first two excited states. Furthermore, in a pure ring the transition probabilities to both of these states are equal as can be seen in Fig. 1(c) which exhibits a practically impurity free system (low values of the impurity potential strength). When the strength of the impurity increases; the ground state and the first excited state will mix and most of the transition probability will shift to the second excited state. This is clearly demonstrated by comparing Fig. 1(a) and (b).

In Figs. 2 and 3, we have plotted some of the lowest absorption energies in four-electron rings. In an impurity-free ring, the transition to the first excited state is not dipole-allowed ($|\Delta L| > 1$). The stronger the impurity gets, there will be more mixing of different angular momenta and the previously forbidden transitions will be allowed. In the parameter range we have used for the impurity, most of the transition probabilities will still go to the modes allowed in impurity-free systems. The lifting of the degeneracy in the energy spectra is reflected in the absorption spectra by a smooth behavior as a function of the applied magnetic field.

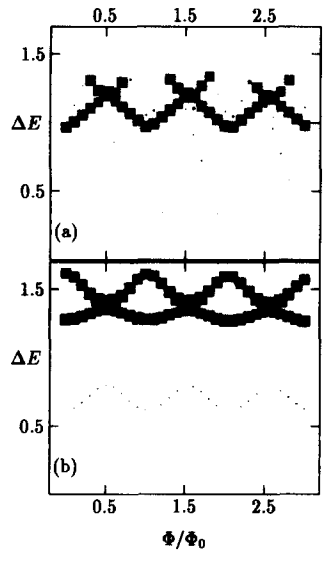

Fig. 2. Dipole-allowed absorption energies for four electrons in a quantum ring versus Φ/Φ_0 at $\alpha = 20$ with Coulomb interaction and impurity potential (a) $V_0 = 1.0$, $d = 0.2$ and (b) $V_0 = 4.0$, $d = 0.5$ included.

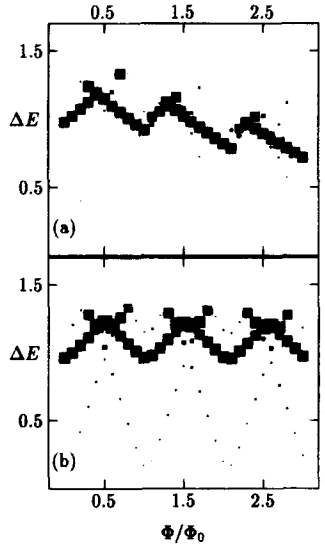

Fig. 3. Same as in Fig. 2 but for $\alpha = 5$, and (a) $V_0 = 0.5, d = 0.2$ and (b) $V_0 = 1.0$, $d = 0.5$.

4. Quantum dots

We consider electrons of effective masses m^* moving in the $z = 0$ plane and confined by a parabolic potential

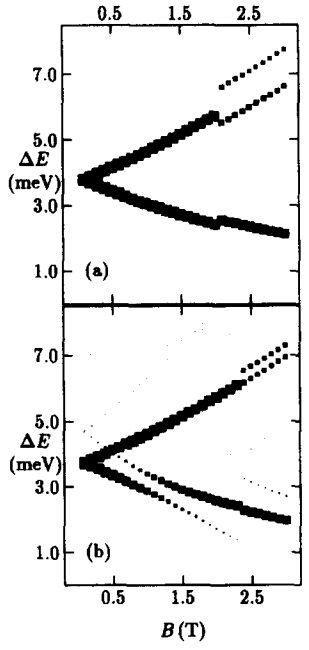

Fig. 4. Dipole-allowed transition energies of a two-electron (interacting) quantum dot with $\hbar\omega_0 = 4$ meV, $V_0 = 4$ meV, $d = 5$ nm and the impurity position (a) $R = 0$ nm and (b) $R = 5$ nm.

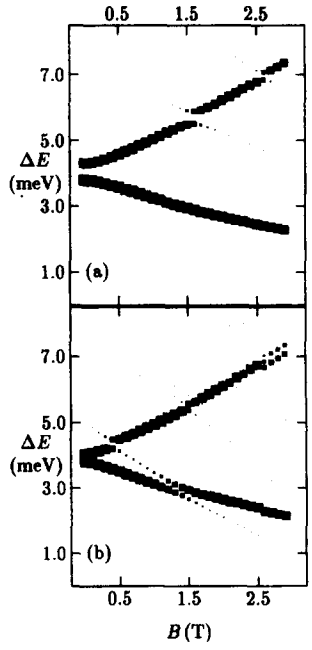

Fig. 5. Same as in Fig. 4, but for $R = 10$ nm and (a) non-interacting and (b) interacting electrons.

$\frac{1}{2}m^*\omega_0^2(x^2 + y^2)$. We model the impurity by a Gaussian potential [Eq. (1)], and apply the exact diagonalization method by constructing the basis using the single-particle wave functions of a perfect parabolic quantum dot [10]. In the actual calculations the spin of the electrons is taken into account but the Zeeman energy is ignored. Intensities of the optical absorption are calculated within the electric-dipole approximation [Eq. (4)].

Electromagnetic absorption of a parabolic quantum dot (without impurities) has two well-known branches, viz., edge and bulk magnetoplasmon modes. For a moderately strong Gaussian impurity at the dot center (Fig. 4a), the continuous modes of the impurity-free case are broken at about 2 T. This discontinuity is a combined effect of the impurity and of the Coulomb force. At about 2 T the ground state changes from $L = 0$ to $L = 1$ (L is the total orbital angular momentum). Without the impurity this transition happens at about 2.5 T (singlet–triplet transition). The upper mode also splits into two weaker modes.

When the impurity is moved slightly away from the center (Fig. 4(b)), the above mentioned discontinuity is still present. It is just moved a little bit to 2.2 T. Now we can see another combined effect of the impurity and the Coulomb force: there is a strong anticrossing in the lower mode near 1 T. This anticrossing is due to the coupling between states with different total orbital angular momenta, i.e. the circular symmetry is broken.

As the impurity is moved further away from the center (Fig. 5), but still remain well inside the dot (radius of the dot is ≈ 25 nm), there is a mode starting at about 5 meV at $B = 0$ T that goes through both the absorption modes. The coupling of these modes is seen as anticrossings in the upper and lower absorption modes. There are also other anticrossings in the upper mode. The degeneracy at $B = 0$ T is clearly lifted. A comparison of Fig. 5(a) and (b) shows clearly the effect of the Coulomb force. Without Coulomb interaction there are no discontinuities in the lower mode. The upper mode has clear anticrossings but not at the same magnetic field values as when the interaction is on. The gap between the two modes at $B = 0$ T is bigger when the interaction is off [14].

5. Conclusion

We have studied the effect of an impurity in a quantum ring subjected to an external magnetic field. The impurity lifts the degeneracy in the energy spectrum, reduces the persistent current, and allows the dipole transitions forbidden in a impurity-free system. In a few-electron quantum ring, the role of the Coulomb interaction is found to be insignificant. In the quantum dot, however, the combined effect of the Coulomb interaction and an impurity

results in anticrossings in the excitation energies which are absent in noninteracting or impurity-free systems.

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