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Optical-absorption spectra of quantum dots and rings with a repulsive scattering centre

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PACS. 73.20Dx – Electron states in low-dimensional structures (including quantum wells, superlattices, layer structures, and intercalation compounds).
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Abstract. – We have studied electron correlation effects in quantum dots and rings which include a repulsive scattering centre and are subjected to a perpendicular magnetic field. The results for the dipole-allowed absorption spectrum show good qualitative agreement with the observed magnetoplasmon dispersion in similar systems. This work provides a unified description of the electron correlations in quantum dots and quantum rings in a magnetic field. We also demonstrate that optical absorption is a direct route to explore the effects of impurity and interactions in a quantum ring.

Quasi–zero-dimensional electron systems, or quantum dots, in a magnetic field have been under intense investigations in recent years [1]-[6]. 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 [4], [5] have been generally in good agreement with the experimental results [6]. The electronic and optical properties of these systems are essential elements in developing the mesoscopic devices in the future [7]. Ever since the first theoretical work on interacting electrons in quantum dots subjected to a magnetic field was reported [4], a large number of papers on variations of such systems have been published in the literature [3], [5]. Almost all of these theoretical studies involve impurity-free quantum-confined few-electron systems. Here we report on the results of our work on dipole-allowed absorptions of a quantum dot and a quantum ring with a repulsive scatterer at the centre.

Experimental work on the magnetoplasma resonances in a two-dimensional electron system confined in a ring geometry has been reported recently [8], and transport properties of the quantum dots with an impurity which can be controlled independently are also under active investigations [9]. Interestingly, such systems are related to another system called antidot array —a two-dimensional electron system with a periodic array of scatterers, whose transport [10], [11] and optical properties [12] are also of much current interest. Finally, in a mesoscopic ring, the most common problem studied so far, both experimentally [13] as well as theoretically [14], [15] has been the persistent current. We have recently developed a model for a quantum ring [15] where in addition to the persistent current, other electronic properties can also be studied very accurately. The energy spectrum calculated earlier by us for such a system with and without an impurity can be used to explore the dipole-allowed absorption spectrum.

Our present work, therefore, unifies our understanding of electron correlations in two very interesting systems: a quantum dot with a repulsive scatterer and a quantum ring. We also demonstrate here that in optical-absorption studies one makes a direct probe of impurity and correlation effects in such systems.

We model the quantum dots and rings like in the earlier works [4], [5], [15]. We consider electrons of effective mass m^* moving in the (x, y)-plane confined by a parabolic potential and subjected to a perpendicular magnetic field. The single-electron Hamiltonian is written as

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

where r_0 is the radius of the ring ($r_0 = 0$ for the dot). We use the symmetric gauge and the vector potential is $\mathbf{A} = \frac{1}{2}(-By, Bx, 0)$. The impurity is modelled by a Gaussian potential

$$V^{\mathrm{imp}}(\mathbf{r}) = V_0 \exp[-(\mathbf{r} - \mathbf{R})^2/d^2], \tag{2}$$

where V_0 is the potential strength, d is proportional to the width of the impurity potential (the full width at half-maximum is $\approx 1.67d$), and $\mathbf{R}$ is the position of the impurity. In the present work the position of the impurity is located such that $|\mathbf{R}| = r_0$.

We apply the exact diagonalization method by constructing the basis using the single-particle wave functions of the Hamiltonian (1). These wave functions are of the form

$$\psi_{nl} = R_{nl}(r)\,\exp[il\theta], \qquad n = 0, 1, 2, \ldots,\ l = 0, \pm1, \pm2, \ldots, \tag{3}$$

where n and l are the radial and orbital angular-momentum quantum numbers, respectively. For parabolic quantum dots ($r_0 = 0$) the radial part can be expressed explicitly as

$$R_{nl}(r) = C \exp[-r^2/(2a^2)]r^{|l|}L_n^{|l|}(r^2/a^2), \tag{4}$$

where C is the normalization constant, $a = \sqrt{\hbar/(m^*\Omega)}$, $\Omega = \sqrt{\omega_0^2 + \omega_c^2/4}$, and $L_n^k(x)$ is the associated Laguerre polynomial. In our quantum ring model ($r_0 \neq 0$) the radial part R_{nl} has to be determined numerically.

Intensities of the optical absorption are calculated within the electric-dipole approximation. If the single-particle matrix elements are defined as

$$\begin{aligned} d_{\lambda\lambda'} &= \langle\lambda'|r\exp[i\theta]|\lambda\rangle \\ &= 2\pi\delta_{l+1,l'}\int_0^\infty r^2 R_{\lambda'}(r)R_\lambda(r)\,\mathrm{d}r\,, \end{aligned}$$

where λ represents the quantum number pair $\{n, l\}$, the dipole operators can be written as

$$\begin{cases} X = \frac{1}{2}\sum_{\lambda\lambda'}\left[d_{\lambda'\lambda} + d_{\lambda\lambda'}\right]a^\dagger_{\lambda'}a_\lambda\,, \\ Y = \frac{1}{2i}\sum_{\lambda\lambda'}\left[d_{\lambda'\lambda} - d_{\lambda\lambda'}\right]a^\dagger_{\lambda'}a_\lambda. \end{cases} \tag{5}$$

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

$$A = |\langle f|\mathbf{r}|0\rangle|^2 = |\langle f|X|0\rangle|^2 + |\langle f|Y|0\rangle|^2\,. \tag{6}$$

In the figures for the absorption spectra presented below, the areas of the filled circles are proportional to A.

Quantum dots. – In the numerical calculations that follow, we have used material parameters appropriate for GaAs, *i.e.* $\varepsilon = 13$ and $m^* = 0.067m_{\rm e}$. We have included spin in our quantum dot calculations but ignored the Zeeman energy. The confinement potential strength is chosen to be $\hbar\omega_0 = 4$ meV and the parameters for the repulsive Gaussian potential at the dot centre are $V_0 = 32$ meV and $d = 5$ nm. With these parameters the electrons are confined in a wide ring. Both the effective radius and the width of this ring are about 20 nm for a single electron.

Figure 1 shows electromagnetic absorption energies and intensities of the system with one, two and three electrons as a function of the magnetic field. The one-electron results reveal four distinct modes. The strongest of the upper two modes can be interpreted as a bulk magnetoplasmon mode according to its asymptotic behaviour, *i.e.* its energy approaches $\hbar\omega_{\rm c}$ as the magnetic field is increased. The origin of the discontinuities near 5 and 8 teslas can be traced back to the fact that the potential forming the ring, in our case, is highly asymmetric. We have a steep Gaussian potential near the centre of the dot and the outer edge is formed by a soft parabolic potential. For a symmetric potential we expect that the bulk magnetoplasmon mode is a smooth function of the magnetic field.

If we ignore the above-mentioned discontinuities, the two upper modes of the one-electron spectrum behave clearly the same way as seen in the experimental results of Dahl *et al.* [8]. However, the two lower modes behave quite differently (in the one-electron case) when compared with those experimental results. The lower modes, *i.e.* edge magnetoplasmon modes, reveal a periodic structure similar to the results of a parabolic ring [15] (see below). That is, however, true only for the one-electron system.

When the number of electrons in the system is increased, the periodic structure of the edge modes (the two lowest modes) starts to disappear. This is, of course, due to the electron-electron interaction. The Coulomb interaction is very important in wide rings. It should be emphasized that because the spin degree of freedom is also included in these calculations, the difference between the one- and two-electron results is entirely due to the Coulomb force. The model quantum rings we have studied so far [15] are extremely narrow and the interaction does not play an important role. The lowest mode (which is also the strongest) behaves (even only for three electrons) much the same way as does the lowest mode in the experiment [8] (where the system consists of the order of one million electrons). It is quite safe to speculate that the second lowest mode would be the same as the second lowest mode in that experiment. It is interesting to note that this mode is also similar to the observed magnetoplasma resonance in antidot arrays [12]. In the high-field regime, the upper mode observed in antidot systems is also qualitatively reproduced in the quantum dot case.

Quantum rings. – We have demonstrated earlier [15] that our model in the appropriate limit, correctly reproduces the behaviour of an ideal one-dimensional ring [13] and that of a two-dimensional electron gas. The energy spectrum in the case of non-interacting and interacting electrons, magnetization and the susceptibility have been studied earlier in this model. The two-body Coulomb matrix elements were evaluated numerically, with the result that in the lowest Landau level and for an impurity-free system, the Coulomb interaction simply shifts the non-interacting energy spectrum to higher energies [15]. There is no discernible effect of interaction on the magnetization which was explained as due to conservation of angular momentum in the system. The impurity potential is found to lift 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 even in the case of impurity interactions is, however, still insignificant [15].

In our ring model the length is measured in units of r_0 (radius of the ring). The energy and impurity strength V_0 are expressed in units of $h^2/2m^*\pi A$, where $A = \pi r_0^2$ is the area of the

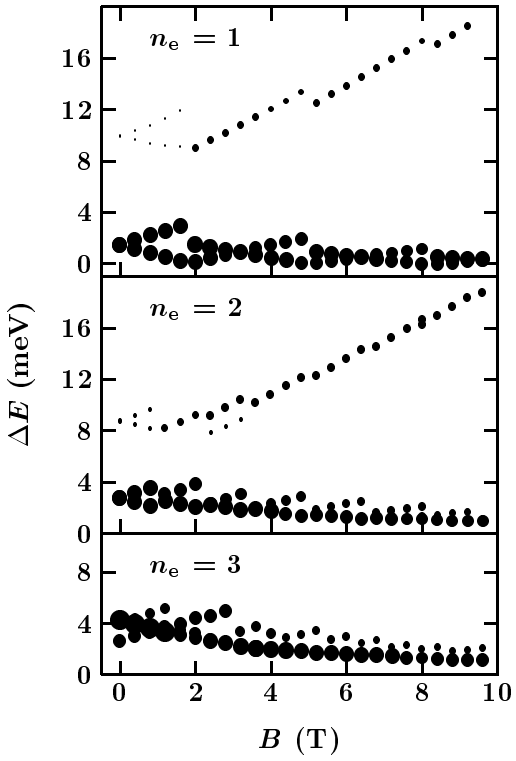

Fig. 1.

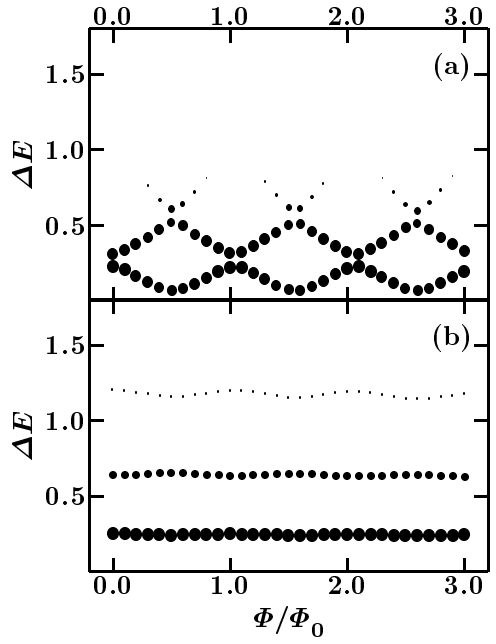

Fig. 2.

Fig. 1. – Absorption energies and intensities of a quantum dot including a repulsive scatterer with one, two and three electrons as a function of the magnetic field. The areas of the filled circles are proportional to the calculated absorption intensity.

Fig. 2. – Dipole-allowed absorption energies of a single electron in a quantum ring *vs.* Φ/Φ_0 for $\alpha = 20$ and *a*) $V_0 = 1.0,\ d = 0.2$; *b*) $V_0 = 4.0,\ d = 0.5$. The areas of the filled circles are proportional to the calculated absorption intensity.

ring [15]. In these units the confinement potential is

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

where $\alpha = \omega_0 m^* A/h$, $x = r/r_0$. The parameter α is related to the width of the ring. For $\alpha = 20$, the single-electron energy spectrum closely resembles that of an ideal one-dimensional ring, while for $\alpha = 5$, it has the characteristics of a two-dimensional electron gas [15]. In our present work we have used $r_0 = 10$ nm and $\alpha = 20$. Given these parameters, electrons are confined in a narrow ring whose radius is about four times its effective width. The other parameters are the same as in the quantum dot case, namely, $\varepsilon = 13$ and $m^* = 0.067m_e$.

In a pure one-electron ring the dipole-allowed absorption from the ground state can happen with equal probability to the first two excited states and all other transitions are forbidden. An impurity in the ring will mix the angular-momentum eigenstates of the pure system into new states between which dipole transitions are allowed. In the case of an impurity of medium

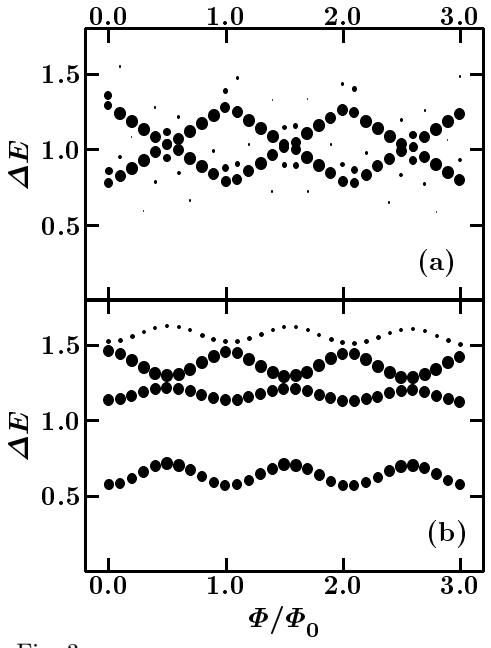

Fig. 3.

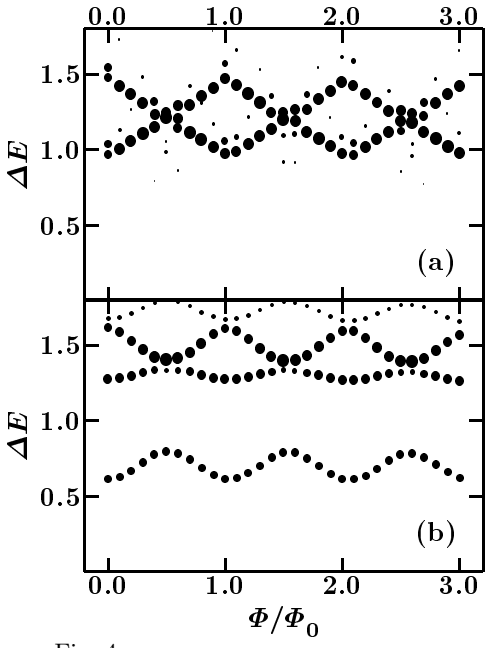

Fig. 4.

Fig. 3. – Dipole-allowed absorption energies for four non-interacting electrons in a quantum ring *vs.* Φ/Φ_0 and $\alpha = 20$, where only the impurity potential is included. The other parameters V_0 and d are the same as in fig. 2.

Fig. 4. – Same as in fig. 3, but with Coulomb and impurity potential included.

strength, as shown in fig. 2 *a*), an appreciable part of the transition probability still goes to the first two excited states while in the case of a strong impurity, absorptions taking the electron to the lowest excited state become more favourable (fig. 2 *b*)). One very important result here is that, *in a system with broken rotational symmetry the transition probability depends strongly on the polarization of the incident light.* That is, if instead of unpolarized light considered in this work we were to consider the case of light polarized for example along the diameter passing through the impurity (which is the case in [16]), the absorption would prefer the *second* excited state. Another prominent feature observed in fig. 2, *i.e.* the periodic behaviour of absorption energies as functions of the applied field, follows closely the behaviour of the persistent current. The blocking of this current caused by a strong impurity is reflected as the flat behaviour of absorption frequencies as a function of the magnetic field. Finally, as we pointed out earlier, the oscillatory behaviour in fig. 2 *a*) is indeed qualitatively similar to that seen in the quantum dot with the repulsive scatterer at the centre (fig. 1).

In order to study electron correlations, we consider rings with four spinless electrons. The main difference to the pure single-electron ring is that the dipole transitions to the first excited state are forbidden ($|\Delta L| > 1$). Just as in the one-electron ring discussed above, the introduction of an impurity will permit transitions to the previously forbidden states. In general, the effect of an impurity and the behaviour of the absorption spectrum as a function of the external magnetic field can be qualitatively explained by the single-particle properties. For example, when we compare fig. 3 *a*) and *b*) we notice that the lifting of the degeneracy in the

energy spectra of non-interacting electrons is reflected by a smoother behaviour as a function of the applied field. The sole effect of the Coulomb interaction on the energy spectrum is to shift it upwards and to increase the gap between the ground state and the excited states [15]. Consequently, as shown in fig. 4, the Coulomb interaction moves the absorption to higher frequencies. The intensities clearly show the effect of the electron-electron interaction: In the non-interacting system (fig. 3) the intensity of each absorption mode does not depend on the magnetic field at all, whereas in the interacting system (fig. 4) there is a strong variation of intensity as a function of the field.

In closing, we demonstrate here that the optical-absorption spectra in a quantum ring not only reflects the behaviour of the persistent current, but it also reveals the subtle effects of the interaction and broken symmetry caused by an impurity. Quite clearly, the magnetoplasma excitations in the quantum dots and rings with a repulsive scatterer in the middle provide an ideal ground for a detailed study of the impurity and correlation effects in low-dimensional electron systems.

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