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Impurity effects on energy levels and far-infrared spectra of nanorings

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Abstract

The effects of a positively charged impurity on the energy levels and far-infrared spectra of one and two electrons in semiconductor nanorings under magnetic fields are studied. The effects of the nanoring size and the impurity position are also discussed. It is shown that the electron–electron interaction and electron–impurity one in nanorings are strongly dependent on the nanoring size and the impurity position. Based on the studies of the impurity and field effects, the impurity-induced Aharonov–Bohm oscillations of the far-infrared spectra are found. The results predict a possibility of observing phenomena related to electron–impurity interaction in a nanoring in the future.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Rapid progress in the fabrication of semiconducting growth technology makes possible the fabrication of low-dimensional nanostructures exhibiting high quantum confinement, which leads to significant modifications of the electronic and optical properties. Recently several novel experiments on semiconductor nanorings have been reported [1–3]. These nanorings may be considered as the best candidates to display various pure quantum effects such as the Aharonov–Bohm (AB) effect [4], because they are in the scattering-free and few-particle limit [2]. Due to the ring geometry, the theoretical study of nanorings is also particularly interesting [5–13].

Understanding the impurity states in the confined systems is an important problem in semiconductor physics. The positively charged impurity (donor centre) with one electron or two electrons can form the neutral donor (D^0) or negative donor (D^-) centres in low-dimensional structures. There is a great interest in the electronic structure and properties of D^0 and D^- in various low-dimensional structures such as quantum dots [14, 15]. It can be

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believed that a fundamental study on the properties of the impurity in semiconductor nanorings is also important, because the dimensionality and the ring geometry often introduce unexpected physical phenomena. The positively charged impurity can make lower states strongly localized. Moreover, the variation of wavefunctions and energy levels, and then the related electronic and optical properties in nanorings, can be greatly changed by the attractive Coulomb potential. The impurity can cause the rotational-symmetry break of the confinement potential of a nanoring, and then it is possible to introduce some new phenomena related to the localization and the symmetry break. The AB effects of excitons or charged excitons in one-dimensional rings have been studied recently [16–18]. It is noted that the AB effects of an exciton in a one-dimensional ring are predicted, which is in contrast to the general belief that an exciton is a neutral entity and should not be sensitive to the applied flux [16, 17]. The D^0 or D^- can be viewed as an exciton or a charged exciton with an infinite hole mass. Then it is interesting to study the quantum behaviour such as the AB effects of D^0 and D^- in a more realistic two-dimensional nanoring with finite width.

To our knowledge, the positively charged impurity effects on FIR spectra of one and two electrons in nanorings have not been explored. The D^- represents the simplest system in which the electron–electron and electron–impurity interactions have significant effects on the electronic structures and related optical properties. In order to better understand the localization and the symmetry break induced by the impurity and to explore the AB oscillations of the FIR spectra, the energy levels and FIR spectra of D^0 and D^- in nanorings under magnetic fields have been calculated and the effects of the nanoring size and the impurity position are shown in this paper.

The organization of the remainder of this paper is as follows. In section 2, the model and Hamiltonian are described and the procedures to obtain the solutions are briefly outlined. The main results are shown and discussed in section 3, followed by a summary in section 4.

2. Model Hamiltonian

Our model includes one or two electrons with a positively charged impurity confined by a two-dimensional nanoring in a magnetic field. The magnetic field is along the \hat{z} axis, perpendicular to the plane of the ring. Within the effective-mass approximation, the Hamiltonian of D^- in a nanoring is given by

$$H(\vec{r}_1, \vec{r}_2) = \sum_{i=1}^2 \left([\vec{p}_i + \vec{A}(\vec{r}_i)]^2 - \frac{2}{|\vec{r}_i - \vec{D}|} + U(\vec{r}_i) \right) + \frac{2}{|\vec{r}_1 - \vec{r}_2|}, \quad (1)$$

and the Hamiltonian of D^0 in a nanoring is

$$H(\vec{r}) = [\vec{p} + \vec{A}(\vec{r})]^2 - \frac{2}{|\vec{r} - \vec{D}|} + U(\vec{r}). \quad (2)$$

$\vec{D} = (D, \varphi_D)$ defines the impurity position, and the impurity angular coordinate is taken as $\varphi_D = 0$, without any loss of generality due to the symmetry. The effective atomic units are used and the effective Rydberg Ry^* and Bohr radius a_B^* are taken to be the energy and length units, respectively. For the InGaAs nanorings, $Ry^* = 5.8$ meV and $a_B^* = 10$ nm. We choose the symmetric gauge vector potential $\vec{A}(\vec{r}) = \frac{1}{2} \vec{B} \times \vec{r}$ to describe a uniform magnetic field. To describe the ring geometry, we select the potential $U(\vec{r})$ as [5, 19]

$$U(\vec{r}) = \begin{cases} 0, & R_1 \leq r \leq R_2 \\ \infty, & \text{else,} \end{cases} \quad (3)$$

where R_1 and R_2 are the inner and outer radius of the nanoring. The mean radius and the width of the nanoring are $R_0 = (R_1 + R_2)/2$ and $W = R_2 - R_1$. This model can clearly describe the physical phenomena such as the AB oscillations related with the ring geometry like the harmonic confinement potential [6]. Furthermore, the infinite barriers make our calculations simple, and the model can give the credible results. The size of the nanoring is determined by R_0 and $\eta = W/R_0$. The mean magnetic flux through the ring is $\Phi = \pi R_0^2 B$, in units of the flux quantum $\Phi_0 = h/e$.

The Schrödinger-like equation is expressed as

$$H\Psi_n = E\Psi_n. \quad (4)$$

Because the radius and angle variables do not separate, equation (4) cannot be solved exactly. Therefore, approximation methods should be used. The Hamiltonian for D^- can be rewritten as [20]

$$H = H_0 + H', \quad (5)$$

with

$$H_0 = \sum_{i=1}^2 \left([\vec{p}_i + \vec{A}(r_i)]^2 - \frac{2}{r_i} + U(\vec{r}_i) \right), \quad (6)$$

and

$$H' = \sum_{i=1}^2 \left(\frac{2}{r_i} - \frac{2}{|\vec{r}_i - \vec{D}|} \right) + \frac{2}{|\vec{r}_1 - \vec{r}_2|}. \quad (7)$$

We can construct the basis through the two-electron wavefunctions $\psi(\vec{r}_1, \vec{r}_2)$ of H_0 , which can be obtained exactly using the method of series expansion [20]. The total spin S of the two electrons is included via the Pauli principle. Let us consider a linear variational function of the form

$$\Psi_n = \sum_{i=1}^f c_i \psi_i, \quad (8)$$

where ψ_i is the i th exact eigenstate of H_0 with eigenenergy E_{0i} . According to the variational principle, it is straightforward to obtain the equation

$$\sum_{i=1}^f [(E_{0i} - E_i)\delta_{ij} + H'_{ij}]c_i = 0, \quad i = 1, \dots, f, \quad (9)$$

with

$$H'_{ij} = \langle \psi_i | H' | \psi_j \rangle. \quad (10)$$

The condition that this set of equations has a nonzero solution leads to the secular equation of finite degree f ,

$$\det \|(E_{0i} - E_i)\delta_{ij} + H'_{ij}\| = 0, \quad i, j = 1, \dots, f. \quad (11)$$

By diagonalizing the secular equation (11), we can obtain the n th energy level E_n and the corresponding wavefunction Ψ_n . Similarly we can obtain the energy levels and wavefunctions for one electron and D^0 by the exact solutions and diagonalizing Hamiltonian of equation (2).

To analyse the properties of the solutions, two useful quantities can be extracted from Ψ_n : the electron density

$$N_n(\vec{r}) = \langle \Psi_n | \sum_i \delta(\vec{r} - \vec{r}_i) | \Psi_n \rangle; \quad (12)$$

and the conditional probability distribution

$$P_n(\vec{r}|\vec{r}_2 = \vec{r}_0) = \frac{\langle \Psi_n | \delta(\vec{r} - \vec{r}_1) \delta(\vec{r}_0 - \vec{r}_2) | \Psi_n \rangle}{\langle \Psi_n | \delta(\vec{r}_0 - \vec{r}_2) | \Psi_n \rangle} \quad (13)$$

for finding one electron at \vec{r} given that the second electron is at $\vec{r}_2 = \vec{r}_0$ [21]. The incident electromagnetic wave will induce transitions between the initial and the final states of the two-electron system. Using the electric dipole approximation, the corresponding absorption coefficient at low temperature is then given by [5]

$$\alpha(\omega) = c\omega \sum_f |\langle \Psi_f | \vec{e} \cdot \vec{d} | \Psi_0 \rangle|^2 \delta(\omega - \omega_{f0}), \quad (14)$$

where \vec{d} is the electric dipole operator, c is a constant factor, and ω_{f0} is the energy difference between the initial state $|\Psi_0\rangle$ and the final state $|\Psi_f\rangle$. For circularly polarized light, the complex polarization vector of the constant external electronic field $\vec{e}^\pm = (1/\sqrt{2})(1, \pm i)$ corresponds to right (+) and left (−) circularly polarized light, respectively.

3. Results and discussions

The impurity in the nanoring destroys the rotational invariance and makes different angular momentum eigenstates $|n, l\rangle$ mix to form new eigenstates without a fixed angular momentum. The ground state of D^0 in the nanoring is mainly composed of $|0, 0\rangle$, $|0, \pm 1\rangle$ and $|0, \pm 2\rangle$, with percentage 19.7%, 16.8% and 10.9%, respectively. And the first excited state is mainly composed of $|0, \pm 1\rangle$, $|0, \pm 2\rangle$ and $|0, \pm 3\rangle$, with percentage 40.4%, 7.9% and 1.2%, respectively. Thus the energy levels and wavefunctions are greatly changed by the impurity. The energy levels and electron densities of D^0 in a nanoring with different D are plotted in figure 1. The impurity position has a strong influence on the ground-state energy which has a minimum value near $D = R_0$ as shown in figure 1(a). This is a result of the coupling of the electron–impurity potential with the confinement one, which makes the electron–impurity interaction depend on the impurity position. Due to the stronger electron–impurity interaction, the ground state of D^0 is much more localized near $D = R_0$, which can be seen from the ground-state electron density in figure 1(b). However, the impurity position has less influence on the higher energy levels due to the more extended wavefunctions for excited states.

For two electrons and an impurity in a nanoring, there is both repulsive electron–electron interaction and attractive electron–impurity interaction. There exists a competition between the two Coulomb interactions, which makes the energy levels and the electron–electron correlation dependent on D . The energy levels and corresponding $P_n(\vec{r})$ with different D are clearly shown in figure 2. The lower energy levels have minimum values near $D = R_0$ as shown in figure 2(a). Due to the electron–electron interaction, the excited-state energies are also changed greatly by the impurity position, which are quite different from those of D^0 . The lowest singlet state is found to be more sensitive to the impurity position than the triplet one. As is shown in figure 2(b), the second electron is much more localized for $D = R_0$ at the singlet state due to the impurity-position effects as mentioned above. The differences between the $P_0(\vec{r})$ of the triplet state for $D = R_0$ and R_1 or R_2 are much smaller, because the two electrons with the same spins cannot be at the same place. For one electron and a positive impurity in a nanoring, the impurity can bound the electron well to form a neutral donor in despite of the impurity position. However, for two electrons and a positive impurity in a nanoring, whether the second electron can be bound by the neutral donor well is strongly dependent on the impurity position because of the competition between the electron–electron interaction and the electron–impurity interaction that is strongly dependent on the impurity position. It is readily seen that $P_4(\vec{r})$ is

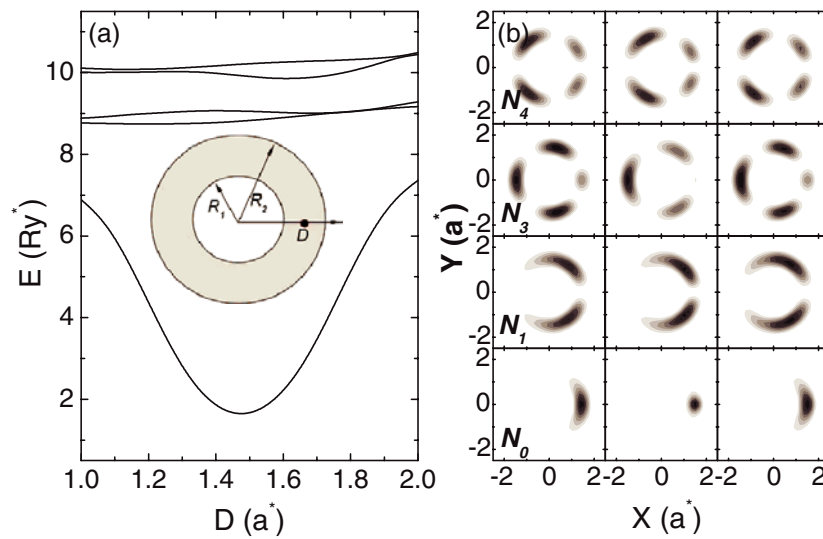


Figure 1. (a) Energy levels of D^0 in a nanoring with $R_1 = 1a_B^*$ and $R_2 = 2a_B^*$ as a function of D . The inset is the schematic geometry of a nanoring with inner radius R_1 and outer radius R_2 , and D shows the impurity position. (b) $N_0(r)$, $N_1(r)$, $N_3(r)$ and $N_4(r)$ for $D = R_1, R_0$ and R_2 , from left to right.

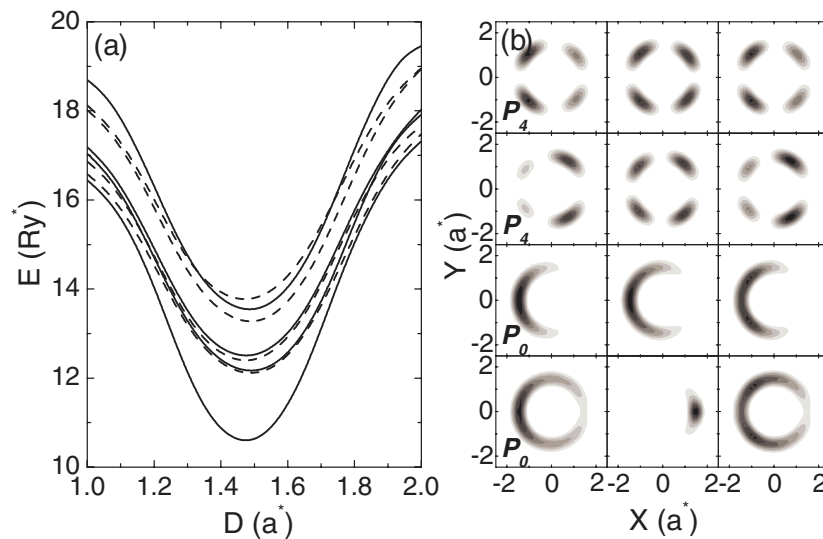


Figure 2. (a) Energy levels of D^- in a nanoring with $R_1 = 1a_B^*$ and $R_2 = 2a_B^*$ as a function of D . The solid and the dashed curves are for singlet and triplet states, respectively. (b) $P_0(r|\vec{r}_2 = \vec{D})$ and $P_4(r|\vec{r}_2 = \vec{D})$ for singlet (lower) and triplet (upper) states with $D = R_1, R_0$ and R_2 , from left to right.

more extended for both the singlet and triplet states, which means that the impurity position has less influence on excited states.

In nanoscale quantum rings, the electron–electron interaction can cause spin oscillations of the ground-state energy levels and peak splitting in far-infrared spectra. The size effects of

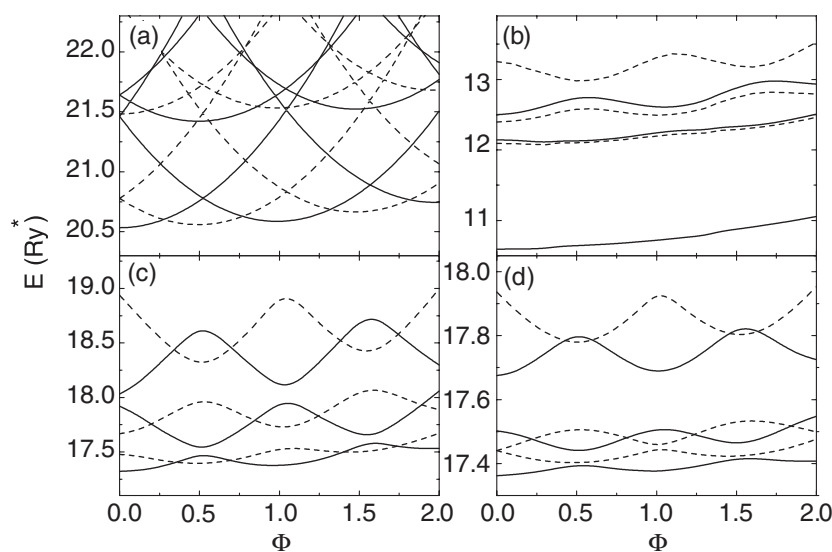


Figure 3. Energy levels as a function of Φ for (a) two electrons, (b) D^- of $D = R_0$ and (c) D^- of $D = R_2$ in a nanoring with $R_1 = 1a_B^*$ and $R_2 = 2a_B^*$. (d) is the same as (c) but in a nanoring with $R_1 = 2a_B^*$ and $R_2 = 3a_B^*$. The solid and the dashed curves are for singlet and triplet states, respectively.

nanorings have a great influence on the electron–electron and electron–impurity interactions, which are important in quantum phenomena of electronic states confined in nanorings. For a better understanding of the size effects on the two interactions, we have calculated the energy levels for two electrons and D^- as a function of magnetic field in nanorings with different sizes. As shown in figure 3(a), the spin oscillation appears for the ground-state energy of two electrons in a nanoring due to the electron–electron interaction. The impurity suppresses not only the AB oscillations but also the spin oscillations of the ground states. The spin oscillations of two-electron ground states disappear near $D = R_0$, but it still exists near $D = R_2$ as shown in figures 3(b) and (c), respectively. The spin oscillation reduction depends strongly not only on the impurity position but also on the size of the nanoring. For a narrower ring, the electron–impurity interaction plays a much more important role. There is no spin oscillation in a nanoring with a larger R_0 even for $D = R_2$, as shown in figure 3(d).

For one electron in a nanoring, the ground-state energy oscillates with magnetic fluxes and l changes as $0 \rightarrow -1 \rightarrow -2 \rightarrow \dots$. According to the selection rule, the dipole transition is from the ground state with l to the excited state with $l \pm 1$. As is shown in figure 4, the FIR spectra for one electron show the discontinuous drops with increasing magnetic fields due to the selection rule and the AB oscillations of the energy levels. Because of the rotational-symmetry break, the D^0 states are now a mixture of one-electron states with different l . The dipole transitions are changed by the state mixing and more peaks appear in the FIR spectra, and then the donor effects can be reflected by the optical properties. From the analysis of the components of the D^0 states as mentioned above, the dipole transition can exist between the ground state and the first excited state that oscillates with the magnetic fluxes, and the transition probabilities can be large enough. One of the most interesting features is that the impurity can induce the AB oscillations in the FIR spectra. The AB oscillations in the FIR spectra are much clearer for $D = R_0$ due to the impurity-position effects. It can be expected that the FIR spectra of D^0 approach those of one electron at $D \rightarrow \infty$. Due to the similarity

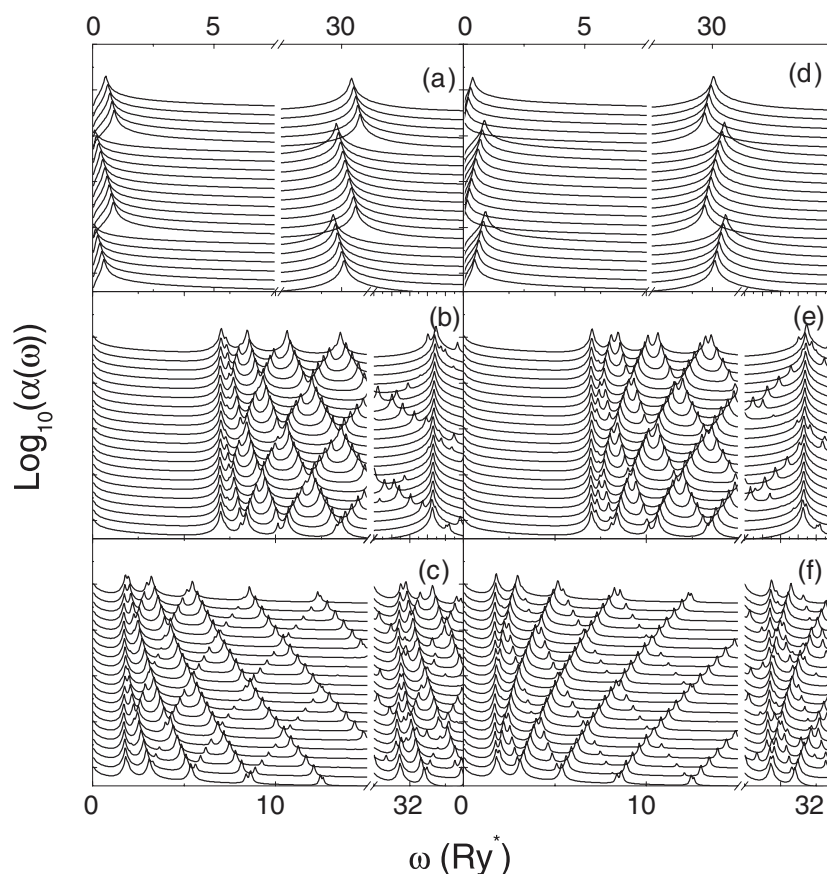


Figure 4. FIR spectra of left circularly polarized light as a function of ω for (a) one electron, (b) D^0 of $D = R_0$ and (c) D^0 of $D = R_2$ in a nanoring with $R_1 = 1a_B^*$ and $R_2 = 2a_B^*$ in different Φ . (In each subplot, from bottom to top, Φ (0–2) is increased in steps of 0.1.) (d)–(f) are the corresponding FIR spectra of right circularly polarized light.

between D^0 and the exciton, the results support the existence of the AB oscillations for the exciton in a one-dimensional nanoring [16, 17]. And even in a two-dimensional nanoring with finite width, the AB oscillations can still exist.

In order to compare the FIR spectra of two electrons with those of D^- in a nanoring, we have plotted the corresponding FIR spectra of two electrons and D^- in nanorings with different R_1 and R_2 in figure 5. Due to the electron–electron interaction, the peaks in the FIR spectra for two electrons and D^- split into two or more smaller ones. As is shown in figure 5(a), there are discontinuous drops in the FIR spectra of two electrons with increasing magnetic fields because of the spin oscillations of two-electron ground states as mentioned above. No AB oscillations appear in the two-electron FIR spectra. However, the FIR spectra of D^- clearly show the AB oscillations. In general, the influence of the electron–impurity interaction in a nanoring with larger R_0 and smaller η becomes stronger and makes the ground-state wavefunction more localized, which makes the dipole-transition probabilities smaller and then the AB oscillation strength weaker. This is the reason why the AB oscillations in figure 5(b) are clearer than those in figure 5(c). Therefore, it is better to choose a nanoring with a small size to observe the AB oscillations in the FIR spectra.

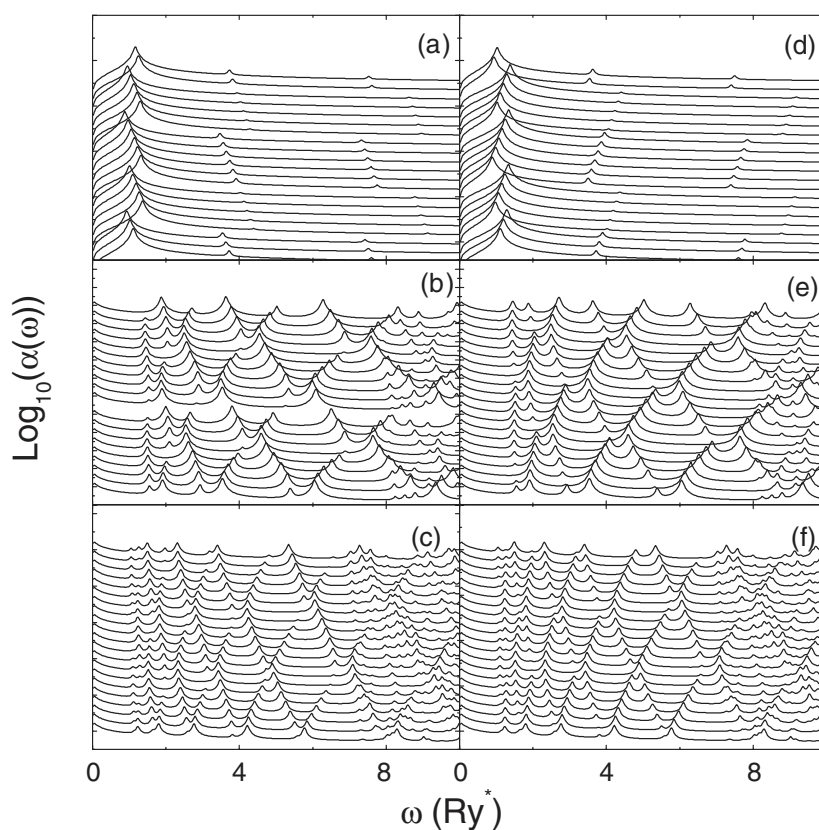


Figure 5. FIR spectra of left circularly polarized light as a function of ω for (a) two electrons in a nanoring with $R_1 = 1a_B^*$ and $R_2 = 2a_B^*$, (b) D^- of $D = R_0$ in a nanoring with $R_1 = 1a_B^*$ and $R_2 = 2a_B^*$, and (c) D^- of $D = R_0$ in a nanoring with $R_1 = 2a_B^*$ and $R_2 = 3a_B^*$ in different Φ . (In each subplot, from bottom to top, Φ (0–2) is increased in steps of 0.1.) (d)–(f) are the corresponding FIR spectra of right circularly polarized light.

4. Summary

The energy levels and FIR spectra of D^0 and D^- in a nanoring have been studied. The localization of the ground state is stronger if the impurity is near the mean radius of the nanoring. The D^0 states can be formed in a nanoring, but whether a second electron can be bound well by the neutral donor depends on the impurity position. The suppression of the spin oscillation of the ground states caused by the impurity depends not only on the impurity position but also on the nanoring size, and the suppression is much greater in a larger and narrower nanoring.

Due to the strong localization and the symmetry break, one of the most interesting phenomena is that the FIR spectra of D^0 and D^- in the nanoring clearly show AB oscillations. In general, an additional potential in a nanoring which destroys the rotational symmetry may induce AB oscillations in the FIR spectra. The attractive Coulomb potential of an impurity placed near the mean radius of the nanoring shows the oscillations more clearly. Furthermore, the effects of the electron–electron and electron–impurity interactions on the FIR spectra are sensitive to the size of a nanoring. Such a spectroscopic characterization of nanorings is useful for better exploring the effects of electron–impurity interaction.

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