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The nonlinear optical rectification coefficient of quantum dots and rings with a repulsive scattering center

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ABSTRACT

By using the matrix diagonalization method within the effective-mass approximation, we have investigated the second-order nonlinear optical rectification coefficient associated with intersubband transitions in quantum dots and rings which include a repulsive scattering centre and are subjected to a perpendicular magnetic field. Based on the computed energies and wave functions, we have studied the effects of impurity and magnetic field in quantum dots and rings on this coefficient. The results show that the nonlinear optical properties of quantum dots and rings are strongly affected by the external magnetic field, the quantum size and the impurity. Also we find that the second-order nonlinear optical rectification coefficient of quantum rings shows the Aharonov–Bohm oscillation as the external magnetic field is increased.

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1. Introduction

Semiconductor quantum dots are one kind of useful quantum structures which can be fabricated by directly self-organized growth [1]. 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. The electronic and optical properties of these systems are essential elements in developing the mesoscopic devices in the future [2]. A quantum ring is a quantum dot structure with a ‘hole’ in its middle. Compared with quantum dots, quantum rings belong to another kind of topological structures in which more rich phenomena can be clearly shown [3–5]. Quite different from the conventional submicron mesoscopic structures, the nanoscopic rings are in the true quantum limit. The weak electron–electron interaction in these rings makes them most suitable for the observed state transitions can be well explained with the single-electron spectrum of a parabolic ring [6]. In addition, the ringlike confinement breaks down the generalized Kohn theorem so that, unlike in quantum dots, the excitation spectrum of quantum rings may reveal electron–impurity interaction effects [7].

External perturbations such as the application of a magnetic field, can provide much valuable information about the confined systems [8]. Therefore the effect of a magnetic field on the electric and optical properties of confined quantum systems is of great interest for fundamental physics and device application. Since Maksym and Chakraborty first reported the theoretical work on interacting electrons in quantum dots subjected to a magnetic field [9], a large number of

papers on variations of quantum dots [10–16] and rings [17–20] have been published. However, most of these theoretical studies involve impurity-free quantum-confined few-electron systems. It is well known that impurities play an essential role in semiconductor devices. Shallow impurity increases the conductivity of a semiconductor by several order of magnitude. Hence, in the recent years, the impurity effects of low-dimensional semiconductors have increased considerably mainly because of the great interest in the physics and technological applications. Recently, Pujari et al. studied impurity effects on the electronic structure of quantum dots [21].

As compared in bulk semiconductors, the nonlinear optical properties are greatly enhanced in the low-dimensional semiconductors, which have been investigated both experimentally and theoretically [22–27]. Among the nonlinear optical properties, the second-order nonlinear optical property plays an essential role. This is because it is the simplest and the lowest-order nonlinear effects. Thus, it is interesting to investigate the second-order nonlinear optical rectification coefficient (ORC) in low-dimensional semiconductors in the presence of an external magnetic field. In 2006, Baskoutas et al. investigated the exciton effects on the nonlinear ORC in semiparabolic quantum dots [28]. Very recently, Rezaei et al. have investigated the nonlinear ORC of a two-dimensional quantum pseudodot system [29]. Also, Karabulut et al. studied the combined effects of applied electric and magnetic fields and hydrostatic pressure on the nonlinear ORC and optical absorption in asymmetric double quantum wells [30]. In the present work, we will focus on studying the second-order nonlinear ORC in quantum dots and rings which include a repulsive scattering centre and are subjected to a perpendicular magnetic field. To the best of our knowledge, the second-order nonlinear ORC of quantum dots and rings with a repulsive scattering centre has not been studied extensively in the literature.

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2. Theory

The system we study is one electron of effective mass m_e moving in the (x, y) plane confined by a parabolic potential and subjected to a perpendicular magnetic field. We model the quantum dots and rings as they are realized in the laboratory [3,4] by a potential of the form $V(r) = \frac{1}{2}m_e\omega_0^2(r-r_0)^2$ where r_0 is the radius of the ring ($r_0 = 0$ for the dot). For such a system the Hamiltonian can be written in the effective-mass approximation as

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

where e is the electric charge of an electron, c is the speed of light, and ϵ is the dielectric constant. \vec{r} (\vec{p}) is the position vector (the momentum vector) of the electron, r_0 is the radius of the ring ($r_0 = 0$ for the dot), and ω_0 defines the strength of the confinement potential [4]. With the symmetric gauge for magnetic field $\vec{A} = (B/2)(-y, x, 0)$, the Hamiltonian then reads

$$H = \frac{p^2}{2m_e} + \frac{1}{2}m_e\omega^2r^2 - m_e\omega_c^2r_0 + \frac{1}{2}m_e\omega_0^2r_0^2 - \frac{1}{2}L_z\omega_c, \quad (2)$$

where $\omega^2 = \omega_0^2 + \omega_c^2/4$, $\omega_c = eB/cm_e$ is the cyclotron frequency, and L_z is the z -component of the angular momentum. The impurity is modelled by a Gaussian potential

$$V_{imp}(r) = V_0 \exp[-(r-R)^2/d^2], \quad (3)$$

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 \vec{R} is the position of the impurity. In the present work the position of the impurity is located such that $|\vec{R}| = r_0$.

The Hamiltonian has cylindrical symmetry which implies the orbital momentum L is a conserved quantity, i.e., a good quantum number. Hence, the eigenstates of this system can be classified according to the orbital angular momentum L . To obtain the eigenfunction and eigenenergy, the Hamiltonian is diagonalized in the model space spanned by two-dimensional harmonic states

$$\Psi_L = \sum_i c_i \phi_i^{\omega'}(\vec{r}), \quad (4)$$

where $\phi_i^{\omega'}(\vec{r}) = R_{n_i \ell_i}(r) \exp(-i\ell_i\theta)$ is i th eigen-state of the two-dimensional harmonic oscillator with a frequency ω' and an energy $(2n_i + |\ell_i| + 1) \hbar\omega'$. $R_{n\ell}(r)$ is the radial wave function, given by

$$R_{n\ell}(r) = N \exp(-r^2/(2a^2)) r^{|\ell|} L_n^{|\ell|}(r^2/a^2), \quad (5)$$

in which N is the normalization constant, $L_n^\ell(x)$ is the associated Laguerre polynomial, $a = \sqrt{\hbar/(m_e\omega')}$ and \hbar is the reduced Plank constant. The radial and orbital angular momentum quantum numbers can have the following values:

$$n = 1, 2, \dots, \ell = 0, \pm 1, \pm 2, \dots \quad (6)$$

Here ω' is an adjustable parameter, and is, in general, not equal to ω .

Let $N = 2n + \ell$. Let $\{\Psi_K\}$ denote the set of basis functions including all the Ψ_K having their N smaller or equal to an upper limit N_{\max} . It is obvious that the total number of basis functions of the set is determined by N_{\max} . After the diagonalization we obtain the eigenvalues and the eigenvectors. Evidently, the eigenvalues depend on the adjustable parameter ω' . In our calculation, ω' serves as a variational parameter to minimize the low-lying state energy. The matrix diagonalization method consists in calculating the matrix elements with the given basis and extracting the lowest eigenvalues of the matrix generated. The better the basis describes the Hamiltonian, the faster the convergence will be.

It is obvious that the wave functions in perturbative calculation are not orthogonal states. Hence, our calculation is suitable only for

that the first-order corrections to the eigenfunctions should be very small. This is sufficient in the regime of strong confinement. Based on the density matrix approach and the perturbation expansion method, the second-order nonlinear ORC is given by [28–31]

$$\chi_0^{(2)} = \frac{4\sigma_s M_{fi}^2 \delta_{fi} \left\{ E_{fi}^2 \left(1 + \frac{T_1}{T_2} \right) + \left[(h\nu)^2 + \left(\frac{\hbar}{T_2} \right)^2 \right] \left(\frac{T_1}{T_2} - 1 \right) \right\}}{\epsilon_0 \left[(E_{fi} - h\nu)^2 + \left(\frac{\hbar}{T_2} \right)^2 \right] \left[(E_{fi} + h\nu)^2 + \left(\frac{\hbar}{T_2} \right)^2 \right]}, \quad (7)$$

where σ_s is the electron density and ϵ_0 is the vacuum permittivity. T_1 and T_2 are the longitudinal and the transverse relaxation times, respectively. And $h\nu$ is the photon energy. $M_{fi} = e\langle\Psi_f|r|\Psi_i\rangle$ is the electric dipole moment of the transition from the Ψ_i state to the Ψ_f state, and $\delta_{fi} = |e\langle\Psi_f|r|\Psi_f\rangle - e\langle\Psi_i|r|\Psi_i\rangle|$. E_{fi} is the transition energy from the Ψ_i state to the Ψ_f state. In this work, for simplicity, we only consider the transition between the $L=0$ and the $L=1$ states.

3. Results and discussion

Our numerical computation is carried out for one of the typical semiconducting materials, GaAs, as an example with the material parameters shown in the following: $m_e = 0.067m_0$ (where m_0 is the single electron bare mass), and $\epsilon = 12.53$. In addition, the relaxation times are set to $T_1 = 1$ ps, $T_2 = 0.8$ ps, and the electron density is taken $\sigma_s = 5.0 \times 10^{24} \text{ m}^{-3}$. The confinement potential strength is chosen to be $\hbar\omega_0 = 4.0$ meV and the parameters for the repulsive Gaussian potential are $V_0 = 32.0$ meV and $d = 5.0$ nm [32]. With these parameters the electrons are confined in a wide ring. Both the effective radius and the width of this ring are about 20.0 nm for a single electron.

In Fig. 1, we set $r_0 = 0$ (quantum dots) and plot the nonlinear ORC in a quantum dot with a repulsive scattering centre as a function of the incident photon energy for four different values of the external magnetic field, i.e., $B = 4.0, 6.0, 8.0,$ and 10.0 T, respectively. From this figure we can find that the magnetic field effect on the second-order nonlinear ORC is significant. We find that all peak positions of ORC shift to higher energies (blue shift) with increasing B . This blueshift occurs because the energy difference E_{fi} between the Ψ_f and Ψ_i states will increase with increasing B . As seen in Fig. 1, we find that the nonlinear ORC first increases with B up to a critical magnetic field value, $B = 8.0$ T, and for further large B value it begins to decrease. Therefore, the

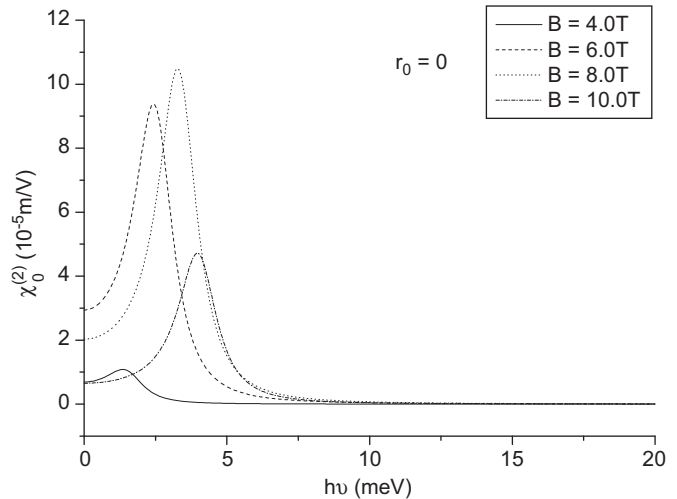


Fig. 1. Variations of the second-order nonlinear ORC $\chi_0^{(2)}$ as a function of the incident photon energy $h\nu$ for a quantum dot ($r_0 = 0$) including a repulsive scattering center for four different values of the magnetic field.

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