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A theoretical study of third-harmonic generation in semi-parabolic plus semi-inverse squared quantum wells

^a Optics
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ABSTRACT

A theoretical study of third-harmonic generation is performed by using the compact-density-matrix method. An electron is confined in semi-parabolic potential plus semi-inverse squared potential quantum wells. Our calculations show that the absolute value, the imaginary part and the real part of third-harmonic generation coefficients are greatly influenced by the parabolic confinement frequency and the characteristic parameter of the inverse squared potential. The relationship between the absolute value and the imaginary part as well as the relationship between the absolute value and the real part is discussed. It is found that the resonant peaks of the absolute value originate from the imaginary part and are not related to the real part.

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1. Introduction

Recently, studies of electronic and optical properties in lowdimensional semiconductor quantum systems, such as quantum wires, quantum wells and quantum dots, have been of great interest due to their potential applications in electronic and optoelectronic devices. For instance, due to potential applications of nonlinear optical effects in far-infrared laser amplifiers [\[1\],](#page--1-0) photo detectors [\[2\]](#page--1-0) and high-speed electro-optical modulators [\[3\],](#page--1-0) nonlinear optical properties such as optical rectification, second and third harmonic generation, optical absorption, refractive index changes, Raman scattering and optical Kerr effects in lowdimensional semiconductor quantum systems [4–[26\]](#page--1-0) have been intensively studied. Besides, with the immense technological progress in nanofabrication techniques, it is possible to fabricate high precision semiconductor quantum systems with strong confinement of electrons. Electron confined in strong confinement quantum systems has discrete energy levels and quantum states, which will greatly enhance nonlinear optical effects [\[27](#page--1-0)-30].

Two dimensional quantum systems, called quantum wells (QWs), are also usually used to give a study of nonlinear optical effects. Not only based on strong quantum confinement, engineering the electronic structure of quantum wells by controlling size and shape offers the possibility of tailoring the energy spectrum to produce desirable

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nonlinear optical effects. Therefore, nonlinear optical effects in QWs have been investigated by many researchers [\[12](#page--1-0)-18]. For example, Zhang et al. studied the second-order nonlinear optical properties in parabolic and semi-parabolic QWs with applied electric field [\[12\].](#page--1-0) Liu et al. investigated linear and nonlinear intersubband optical absorption and refractive index changes in asymmetrical semiexponential QWs [\[13\]](#page--1-0). Wang et al. reported nonlinear optical rectification in asymmetric coupled quantum wells by changing the structure parameters [\[14\].](#page--1-0) Chen et al. discussed linear and nonlinear intersubband optical absorption in double triangular quantum wells by changing the structure parameters [\[15\].](#page--1-0) Chen et al. also discussed second-order nonlinear optical susceptibilities in asymmetric coupled quantum wells [\[16\].](#page--1-0) Yesilgul analyzed linear and nonlinear intersubband optical absorption coefficients and refractive index changes in symmetric double semi-V-shaped quantum wells [\[17\].](#page--1-0) Keshavarz analyzed linear and nonlinear intersubband optical absorption in symmetric double semi-parabolic quantum wells [\[18\].](#page--1-0) The research above shows that by controlling the size of QWs, we can obtain dynamic characteristics of nonlinear optical coefficients. For example, changing the parabolic confinement frequency [\[12\],](#page--1-0) changing σ and U_0 [\[13\]](#page--1-0) and changing the widths of the barrier and the well [\[14](#page--1-0)–18] can induce blue or red shift of nonlinear optical coefficients and decrease or increase of nonlinear optical coefficients. The research above also shows that based on factual physical conditions, the shape of QWs is different, which will help us to know more nonlinear optical effects. For quantum wells made of parabolic potential plus inverse squared potential, related work has been done to study the electronic and optical properties [19–[22\].](#page--1-0) For

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example, Liu et al. give a detailed study of linear and nonlinear optical absorption in two dimensional quantum system with parabolic potential plus inverse squared potential in a static magnetic field [\[19\].](#page--1-0) Based on Liu et al.'s [\[19\]](#page--1-0) model, Duque et al. investigated linear and nonlinear optical absorption and refractive index changes with applied electric and magnetic field [\[20\]](#page--1-0). Based on Liu et al.'s [\[19\]](#page--1-0) model, Duque et al. also investigated second and third harmonic generation with applied magnetic field [\[21\]](#page--1-0). Besides, nonlinear optical rectification and second harmonic generation in semiparabolic potential plus semi-inverse squared potential quantum wells were discussed by Hassanbadi et al. Hassanbadi et al. point out that with the increase of the parabolic confinement frequency, the second harmonic generation exhibits a blue shift and becomes small. Hassanbadi et al. also point out that with the increase of the characteristic parameter of the inverse squared potential, the second harmonic generation does not shift and increases. In our paper, we will give a theoretical study of third-harmonic generation (THG) in semi-parabolic potential plus semi-inverse squared potential quantum wells.

This paper is organized as follows. In Section 2, theory model is built and eigenvalues and eigenfunctions are given. The expressions for third harmonic generation are presented. In Section 3, the numerical results and detailed discussions are performed. Finally, conclusion is made in [Section 4](#page--1-0).

2. Theory

Suppose that an electron is confined in semi-parabolic and semi-inverse squared quantum wells. In the effective mass approximation, the Hamiltonian of the system can be written as

$$
H = -\frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(z),\tag{1}
$$

with

$$
V(z) = \begin{cases} \frac{1}{2} m^* \omega_0^2 z^2 + \frac{\hbar^2 \beta}{2m^* z^2}, & z \ge 0\\ \infty, & z < 0, \end{cases}
$$
 (2)

Here, \hbar is the Planck constant, m^* is the electron effective mass, ω_0 is the confinement frequency associated with the parabolic potential, and β is the characteristic parameter with the inverse squared potential. The eigenfunctions of the system can be obtained as [\[22\]](#page--1-0)

$$
\psi_{n,\mathbf{k}}(\mathbf{r}) = \phi_n(z) u_c(\mathbf{r}) e_{\parallel}^{\mathbf{i}\mathbf{k}} \cdot \mathbf{r}_{\parallel},
$$
\n(3)

with

$$
\phi_n(z) = N_n z^{2s} e^{-z^2/2} L_n^{\gamma}(z^2),\tag{4}
$$

where $s = (\sqrt{1/4 + \beta} + 1/2)/2,$ $\gamma = 2s \gamma = 2s - \frac{1}{2}$ $\frac{1}{2}$ and $N_n = \sqrt{2n!/\Gamma(2s+n+1/2)}$. $L_n^{\gamma}(z^2)$ is associated with the Laguerre polynomials. \mathbf{k}_{\parallel} and \mathbf{r}_{\parallel} are the wave vector and coordinate in the $x-y$ plane, respectively. $u_c(\mathbf{r})$ is the periodic part of the Bloch function in the conduction band at $\mathbf{k} = 0$. The energy eigenvalues of the system can be obtained as [\[22\]](#page--1-0)

$$
\varepsilon_{n,\mathbf{k}} = E_n + \frac{\hbar^2}{2m^*} \mathbf{k}_\perp^2,\tag{5}
$$

where

$$
E_n = (2n+1+\sqrt{\beta+1/4})\hbar\omega_0.
$$
\n⁽⁶⁾

With the compact density matrix approach and the iterative procedure, the analytical expressions for the THG can be written as [\[23\]](#page--1-0)

$$
\chi_{3\omega}^{(3)} = \frac{e^4 \sigma}{\varepsilon_0 \hbar^3} \frac{M_{01} M_{12} M_{23} M_{30}}{(\omega - \omega_{10} + i\Gamma_{10})(2\omega - \omega_{20} + i\Gamma_{20})(3\omega - \omega_{30} + i\Gamma_{30})}
$$
(7)

Here, σ is the electronic density, $\omega_{nm} = (E_n - E_m)/\hbar$ the transition frequency and $M_{nm} = |\langle \psi_{n,0} | z | \psi_{m,0} \rangle|$ the off-diagonal matrix element. The THG susceptibility has a resonant peak in the energy position of triple resonance, i.e., $\hbar \omega = \hbar \omega_{10} = \hbar \omega_{20}/2 = \hbar \omega_{30}/3$, given by [\[23\]](#page--1-0)

$$
\chi_{3\omega,\text{max}}^{(3)} = \frac{e^4 \sigma M_{01} M_{12} M_{23} M_{30}}{\epsilon_0} \tag{8}
$$

where the off-diagonal relaxation rate $\Gamma = \Gamma_{10} = \Gamma_{20} = \Gamma_{30}$.

3. Results and discussions

Next, third-harmonic generation coefficients in semi-parabolic and semi-inverse squared quantum wells will be discussed. The parameters used in our calculations are adopted as [19–[22\]](#page--1-0) $\sigma = 5.0 \times 10^{18}$ cm⁻³, $\Gamma = 1/0.2$ ps, $m^* = 0.067 m_0$ (where m_0 is the electron mass).

The THG coefficients $|\chi_{3\omega}^{(3)}|$ as a function of the incident photon energy $\hbar \omega$, with $\beta = 1$, for three different values of the confinement frequency ω_0 are plotted in Fig. 1. From the figure, we can see that the confinement frequency ω_0 has great influence on the THG coefficients $|\chi_{3\omega}^{(3)}|$. Fig. 1 shows three resonant peaks which occur at $\omega = 2.0 \times 10^{13} / s$, $\omega = 2.4 \times 10^{13} / s$ and $\omega_0 = 2.8 \times 10^{13} / s$. The result above shows that with the increase of the confinement frequency ω_0 , $|\chi_{3\omega}^{(3)}|$ moves toward the higher energy region. The physical origin is that the larger the confinement frequency ω_0 is, the stronger the quantum confinement is, and the larger the energy interval between different quantum states is. The features above are also in agreement with the results obtained in Refs. [19-[22\]](#page--1-0). Besides, Ref. [\[21\]](#page--1-0) shows that for each confinement frequency ω_0 , $\chi_{3\omega}^{(3)}$ have three resonant peaks, whereas our results show that for each confinement frequency ω_0 , there is only one peak. This can be explained as follows. Ref. [\[21\]](#page--1-0) gives a study of third-harmonic generation in a quantum ring made of parabolic potential plus inverse squared potential. The energy eigenvalues of the system are distributed unequally. Thus the energy differences between adjacent levels are not constant. Ref. [\[21\]](#page--1-0) points out that three peaks belong to $\hbar \omega_{10}$, $\hbar \omega_{20}/2$ and $\hbar \omega_{30}/3$. It is due to $\hbar\omega_{10} \neq \hbar\omega_{20}/2 \neq \hbar\omega_{30}/3$ that there are three peaks about the THG in Ref [\[21\]](#page--1-0). Our present work focuses on semi-parabolic potential plus semi-inverse squared potential quantum wells. The energy eigenvalues of our present system are distributed equally. Therefore, $\hbar\omega_{10} = \hbar\omega_{20}/2 = \hbar\omega_{30}/3$ leads to only one resonant peak. From the figure, it is also clearly noted that the resonant peaks of the THG

Fig. 1. The THG coefficients $|\chi_{3\omega}^{(3)}|$ as a function of the incident photon energy $\hbar \omega$, with $\beta = 1$, for three different values of the confinement frequency ω_0 .

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