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The nonlinear optical rectification in asymmetrical and symmetrical Gaussian potential quantum wells with applied electric field

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ABSTRACT

A detailed investigation of nonlinear optical rectification (OR) of asymmetrical and symmetrical Gaussian potential quantum wells (QWs) under the influence of applied electric field by using the compact-density-matrix approach is presented. We find that the approximation of the asymmetrical Gaussian potential QWs is extremely unreasonable in the previous works, some new and reliable results are obtained by us. The energy eigenvalues and their corresponding eigenfunctions of the asymmetrical and symmetrical Gaussian potential QWs are calculated with the differential method. According to the results obtained from the present work, we find that the applied electric field and the geometry factors have great influence on the nonlinear OR in these system.

1. Introduction

In recent years, there has been considerable interest in the nonlinear optical properties of the dimensionality semiconductor system, which have been utilized widely for optoelectronic device applications, such as light emitting diodes, laser diodes, and detectors. Due to the rapid development of the crystal growth technique like the molecular beam epitaxy, liquid phase epitaxy and chemical vapor deposition has become possible to produce a variety of dimensionality semiconductor nanostructures [1–3]. The larger-band-gap of semiconductor QWs, they are well known to be more advantageous to grow, process, and fabricate into devices than are small-band-gap semiconductors. And the intersubband transitions between quantized electron levels in semiconductor QWs provide a promising route to the fabrication of novel infrared detectors and lasers. Much attention has been paid to the nonlinear optical properties of low-dimensional semiconductor QWs structure [4–8].

The nonlinear OR in semiconductor QWs structures have been investigated by a number of researchers. As we know that the second-order nonlinear susceptibility is negligible except for a small contribution from the bulk susceptibility in a symmetric QW structure, but as the symmetry is broken by applying an electric field to the symmetric QW, nonvanishing contributions to the second-order nonlinear optical susceptibilities are expected to appear. For instance, the applied electric field on the nonlinear OR in parabolic QWs has been studied by Guo and Gu in 1993. They found the OR is six orders of magnitude higher than in bulk GaAs using a compact density-matrix approach [9]. In 2012, Hassanabadi et al. investigated nonlinear OR and second-harmonic generation in semi-parabolic and semi-inverse squared QWs [10]. As the same time, the intersubband nonlinear OR in asymmetric rectangular QWs has been studied and the results show that the asymmetry effect of the potential profile has an important influence on the OR coefficient [11]. In 2013, Niculescu et al. have studied the heterointerface effects on the nonlinear OR in a laser-dressed graded QW using a finite difference method with the effective mass approximation. The numerical results show that the peak values and positions of the nonlinear OR coefficient can be controlled by both the applied electric field and the laser field [12].

It is known that the Gaussian potential is perfectly suitable to describe the experimental results. Based on the Gaussian potential, there are a number of works that have been reported to investigate the optical properties. Guo and Du have reported their results for linear and nonlinear optical absorption coefficients and refractive index changes in asymmetrical Gaussian potential QWs with applied electric field [13]. After this moment, the other optical properties in this system are investigated, such as nonlinear OR and second-harmonic generation [14,15]. But we find both energy and wavefunction for the low-lying state in this model are

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chosen wrongly to be applied in these works above [16]. Until now, the nonlinear OR has not been discussed in symmetrical Gaussian potential QWs. Therefore, it is very necessary to investigate the nonlinear optical properties for electron confined in the asymmetrical and symmetrical Gaussian potential QWs in the presence of electric field.

In the present work, we will investigate the effects of the applied electric field and structural parameters on the nonlinear OR coefficients of the asymmetrical and symmetrical Gaussian potential QWs. In Section 2, the eigenfunctions and eigenenergies of electron states are obtained using finite difference method, and the analytical expression for the nonlinear OR coefficients is derived by means of the compact-density-matrix approach and an iterative method. In Section 3, the numerical results and discussions are presented for asymmetrical and symmetrical Gaussian potential QWs with applied electric field. A brief summary is given in Section 4.

2. Theory

We are concerned with the asymmetrical and symmetrical Gaussian potential QWs system with an applied electric field. Within the effective-mass approximation, the Hamiltonian of this system can be written as

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

with

$$V(z) = -V_0 \exp(-z^2/2L^2), \quad -\infty < z < \infty \tag{2}$$

for the symmetrical Gaussian potential QWs, and

$$V(z) = \begin{cases} -V_0 \exp(-z^2/2L^2), & z \ge 0 \\ \infty, & z < 0 \end{cases} \tag{3}$$

for the asymmetrical Gaussian potential QWs [13–15,17,18]. Here z represents the growth direction of the QWs. F is the strength of the applied electric field parallel to z direction, q is the absolute value of the electric charge. And V_0 and L are the height of the Gaussian potential QWs and the range of the confinement potential, respectively.

Taking the potential (2) and (3) into account, the eigenstates in asymmetrical and symmetrical Gaussian potential QWs are the solutions of the following equation:

$$\left[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} + V(z) + qFz\right]\phi_{n_z}(z) = E_{n_z}\phi_{n_z}(z). \tag{4}$$

Due to the potential function $V(z)$ and the presence of the applied electric in the Hamiltonian (Eq. (1)), it is impossible to find self-energy analytic eigenfunctions that correspond to the exact solution of one electron confined in asymmetrical and symmetrical Gaussian potential QWs. To obtain the eigenvalues and eigenvectors of the time-independent Schrödinger equation (Eq. (4)), we have adopted the finite difference method [19,20]. This is a numerical method for solving the partial differential equation based on discretization of the Hamiltonian on a spatial grid. The time-independent Schrödinger equation (Eq. (4)) in the presence of applied electric field under finite difference method can be written as follows:

$$-\frac{1}{2m^*}\left[\frac{\Psi(z_{j+1}) - 2\Psi(z_j) + \Psi(z_{j-1})}{h^2}\right] + V(z_j)\Psi(z_j) + qFz_j\Psi(z_j) = E\Psi(z_j), \tag{5}$$

where $V(z)$ is well potential, $h = z_{j+1} - z_j$ is the spacing between the two neighboring discrete points. The matrix (Eq. (5)) is diagonalized to obtain the eigenvalues and the wavefunctions of asymmetrical and symmetrical Gaussian potential QWs. Next we used the compact-density-matrix method and the iterative procedure to calculate the nonlinear OR coefficients for the asymmetrical and symmetrical Gaussian potential QWs [21,22]. The system is excited by electromagnetic field $\vec{E}(t) = \tilde{E}e^{i\omega t} + \tilde{E}e^{-i\omega t}$. Let us denote ρ as the one-electron density matrix for this regime. Then the evolution of density matrix ρ obeys the following:

$$\frac{\partial \rho_{ij}}{\partial t} = \frac{1}{\hbar}[H_0 - qz\vec{F}(t), \rho]_{ij} - \Gamma_{ij}(\rho - \rho^{(0)})_{ij}, \tag{6}$$

where H_0 is the Hamiltonian for this system without the electromagnetic field $\vec{E}(t)$, $\rho^{(0)}$ is the density matrix and Γ_{ij} is the relaxation rate.

Eq. (6) is calculated by the following iterative method:

$$\rho(t) = \sum_n \rho^{(n)}(t), \tag{7}$$

with

$$\frac{\partial \rho_{ij}^{(n+1)}}{\partial t} = \frac{1}{i\hbar}\left\{[H_0, \rho^{(n+1)}]_{ij} - i\hbar\Gamma_{ij}\rho_{ij}^{(n+1)}\right\} - \frac{1}{i\hbar}[qz, \rho^{(0)}]_{ij}\vec{E}(t). \tag{8}$$

The electric polarization of the QWs due to $\vec{E}(t)$ can be expressed as

$$p(t) = (\varepsilon_0\chi^{(1)}\tilde{E}e^{i\omega t} + \varepsilon_0\chi_{2\omega}^{(2)}\tilde{E}^2e^{2i\omega t}) + c.c. + \varepsilon_0\chi_0^{(2)}\tilde{E}^2, \tag{9}$$

where $\chi^{(1)}$, $\chi_0^{(2)}$ and $\chi_{2\omega}^{(2)}$ are the linear susceptibility, OR and second-harmonic generation, respectively. ε_0 is the vacuum dielectric constant. The electronic polarization of the nth order is given as

$$p^{(n)} = \frac{1}{V}\mathrm{Tr}(\rho^{(n)}ez) \tag{10}$$

where V is the volume of interaction and Tr denotes the trace or summation over the diagonal elements of the matrix $\rho^{(n)}ez$. In our paper, the OR coefficients per unit volume is given as

$$\chi_0^{(2)} = \frac{4e^3\sigma_\nu}{\varepsilon_0\hbar^2}\mu_{01}\delta_{01}\frac{\omega_{01}^2\left(1 + \frac{T_1}{T_2}\right) + \left(\omega^2 + \frac{1}{T_2^2}\right)\left(\frac{T_1}{T_2} - 1\right)}{\left[(\omega_{01} - \omega)^2 + \frac{1}{T_2^2}\right]\left[(\omega_{01} + \omega)^2 + \frac{1}{T_2^2}\right]}, \tag{11}$$

where σ_ν is the density of electrons in the QWs, T_1 is the longitudinal relaxation time of system, T_2 is the transversal relaxation time of system, $\mu_{01} = |\langle\Psi_0|z|\Psi_1\rangle|$ is the off-diagonal matrix element, $\delta_{01} = \mu_{11} - \mu_{00}$, ω_{01} is the transition frequency. The OR coefficients have a resonant peak for $\omega = \omega_{01}$ obtained by

$$\chi_0^{(2)} = 2\frac{T_1T_2e^3\sigma_\nu}{\varepsilon_0\hbar^2}\mu_{01}^2\delta_{01}. \tag{12}$$

3. Results and discussions

In this study, we have theoretically investigated the OR coefficients $\chi_0^{(2)}$ in asymmetrical and symmetrical Gaussian potential QWs under an applied electric field. The values of physical parameters used in our calculations are $m^* = 0.067m_0$ (where m_0 is the electron mass), $\varepsilon_0 = 8.85 \times 10^{-12}Fm^{-1}$, T_1=0.2 ps, $T_2 = 1$ ps, $\sigma_\nu = 5 \times 10^{24}m^{-3}$ [23–25].

In Fig. 1(a) and (b), the effects of applied electric field on the confinement potential profile of asymmetrical and symmetrical Gaussian potential QWs as a function of the position are plotted