Nonlinear optical properties of a Pöschl-Teller quantum well

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I. INTRODUCTION

The nonlinear optical properties of quantum wells (QWs) and other low-dimensional systems have attracted an enormous interest in recent years. Especially second-order nonlinear optical properties, such as second-harmonic generation (SHG), optical rectification (OR), and electro-optic effect (EOE), and third-order optical properties, such as third-order absorption, and third-harmonic generation are extensively studied. This is because these nonlinearities have the potential for device applications in far-infrared laser amplifiers, photodetectors, and high-speed electro-optical modulators.

The linear intersubband absorption within the conduction band of a GaAs QW has been studied experimentally with and without an electric field. A very large dipole strength and a narrow band width have been observed, which suggest that the intersubband optical transition in QWs may have huge nonlinearities. On the theoretical side, Ahn and Chuang studied linear and nonlinear intersubband absorptions in QWs with and without an electric field. Yuen et al. and Shi and Pan studied a semiconductor superlattice. Zhang et al. considered electric-field-biased semiparabolic QWs. Results reveal that the linear and nonlinear intersubband absorptions significantly depend on the structure of the system and the applied electric field.

The second-order susceptibility is negligible except for the small contribution of the bulk susceptibility in symmetric QWs. However, when the inversion symmetry of the system is broken, it is possible to obtain a significant second-order susceptibility. Asymmetric QWs can be created in two ways: either by advanced material growing technology or by an external applied electric field. Results reveal a significant enhancement of both properties with the increasing electric field. They obtained one and six orders of magnitude higher values for OR and EOE than those in the bulk GaAs, respectively. Also, Zhang et al. calculated EOE and the SHG susceptibility and they found about two orders of magnitude larger EOE than that in the parabolic QW with an applied electric field.

In this work, QWs having the Pöschl-Teller potential are considered. This potential has not been studied extensively in the literature and to the best of our knowledge only Radovanovic et al. used the modified Pöschl-Teller potential to calculate intersubband absorption based on bound-bound, bound-free, and free-free transitions in QWs. The Pöschl-Teller potential has tunable asymmetry degree and the corresponding Schrödinger equation is analytically solvable.

The organization of this paper is as follows. In Sec. II, the exact wave functions and eigenenergies are given and the expressions for linear and nonlinear absorption coefficients, SHG and OR, are derived under the density matrix formalism. Numerical results for a typical GaAs QW are presented. The resulting SHG and OR coefficients are much larger than their values for bulk GaAs.

II. THEORY

The effective-mass Hamiltonian for the electrons in a potential well, $V(z)$ is

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

where


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Here $z$ represents the growth direction. The Pöschl-Teller potential\textsuperscript{26,28} $V(z)$ is governed by three parameters: $\kappa$, $\eta$, and $\beta$. This potential has singularities at $z=0$ and at $z=\pi/2\beta$. The parameters $\kappa$ and $\eta$ tune the degree of the asymmetry, and the potential profile is perfectly symmetric for $\kappa=\eta$.

The eigenfunctions $\psi_{n,k}(r)$ and eigenenergies $E_{n,k}$ are given, respectively, by

\begin{equation}
\psi_{n,k}(r) = \phi_n(z) \exp(i k_0 \cdot r),
\end{equation}

\begin{equation}
E_{n,k} = \frac{\hbar^2}{2m} \left( \kappa + \eta + 2n \right)^2 n = 0,1,2, \ldots,
\end{equation}

where $k_0$ and $r$ are the wave and position vectors in the $xy$ plane. $\phi_n(z)$ and $E_n$ are the envelope wave function and transverse energy of the $n$th subband, respectively, and are the solutions of the Schrödinger equation

\begin{equation}
H \cdot \phi_n(z) = E_n \phi_n(z),
\end{equation}

where $H_z$ is the $z$ component of the Hamiltonian $H$. $\phi_n(z)$ and $E_n$ are given by\textsuperscript{28}

\begin{equation}
\phi_n(z) = C_n \sin^n(\beta z) \cos^n(\beta z) \times z \left( \frac{\pi}{2} - n, \kappa + \eta + n, \kappa + \eta + 2n \right)^2.
\end{equation}

The one-electron density matrix equation with intraband relaxation is

\begin{equation}
\frac{\partial \rho_{ij}}{\partial t} = \frac{i}{\hbar} \left[ H_0 - qzE(t), \rho \right]_{ij} - \Gamma_{ij}(\rho - \rho^{(0)})_{ij},
\end{equation}

where $H_0$ is unperturbed Hamiltonian. The $\Gamma_{ij}$ elements are taken to be one to equal one value $\Gamma_0$ only. Equation (9) is solved via the iterative method,\textsuperscript{29,30} by noting that

\begin{equation}
\rho(t) = \sum_n \rho^{(n)}(t),
\end{equation}

with

\begin{equation}
\frac{\partial \rho^{(n+1)}_{ij}}{\partial t} = \frac{i}{\hbar} \left[ H_0, \rho^{(n+1)} \right]_{ij} - \Gamma_{ij}\rho^{(n+1)}_{ij} - \frac{1}{\hbar} \left[ qz, \rho^{(n)} \right]_{ij} E(t).
\end{equation}

The electron parameter $\mu$ and the density matrix as\textsuperscript{29,30}

\begin{equation}
P(t) = \chi(\omega) E e^{-i\omega t} + \chi(-\omega) E^* e^{i\omega t} = \frac{1}{V} \text{Tr}(\rho \mu),
\end{equation}

where $V$ is the volume of the system and Tr stands for the trace.

The absorption coefficient and the susceptibility are related by\textsuperscript{31}

\begin{equation}
\alpha(\omega) = \frac{4 \pi \omega}{n_c} \text{Im}[\chi(\omega)],
\end{equation}

where $n_r$ is the refractive index of the system and the $c$ is the speed of the light. By using the density matrix formalism and the iterative procedure,\textsuperscript{3,29,30} the linear and the third-order absorption coefficients, $\alpha^{(1)}(\omega)$ and $\alpha^{(3)}(\omega)$, are derived for both symmetric and asymmetric potentials. We neglect the higher-harmonic terms and consider only the steady-state response. The first-order and third-order absorption coefficients are found to be

\begin{equation}
\alpha^{(1)}(\omega) = \frac{4 \pi \omega}{n_c} \frac{\sigma_{10}(|\mu_{10}|^2)^{1/2}}{(E_10 - \omega)^2 + (\hbar \Gamma_0)^2},
\end{equation}

\begin{equation}
\alpha^{(3)}(\omega) = -2 \omega \left( \frac{4 \pi}{n_c} \right)^2 \frac{1}{(E_10 - \omega)^2 + (\hbar \Gamma_0)^2} \times \left( 1 - \frac{|\mu_{11} - \mu_{00}|^2}{4 |\mu_{10}|^2} \right) \frac{(E_10 - \omega)^2 + E_{10}(E_10 - \omega)}{(E_10 + \hbar \Gamma_0)^2}.
\end{equation}

Here $I$ is the intensity of the incident field, $\sigma$ is the density of the electrons, $E_{10}=E_1-E_0$, and $\mu_{ij}$ is the matrix element of the dipole operator $\mu_{ij}(\phi_{ij}\phi_{ij})$, and $i,j=0,1, \ldots$. $\alpha^{(1)}(\omega)$ keeps its form, whether the potential is symmetric or not. However, the second term in Eq. (15) is zero when the potential is symmetric. We write the total absorption coefficient $\alpha(\omega,I)$ as

\begin{equation}
\alpha(\omega,I) = \alpha^{(1)}(\omega) + \alpha^{(3)}(\omega,I).
\end{equation}

Derivation of the second-harmonic generation requires the consideration of the higher-order terms,\textsuperscript{10} such as $(e^{2i\omega})$. We get the SHG which is observable only in the case of asymmetric potentials as

\begin{equation}
\chi^{(2)}_{2\omega} = \frac{\sigma_{10}(|\mu_{10}|^2)(\mu_{11} - \mu_{00})}{(2 \hbar \omega - E_{10} + i \hbar \Gamma_0)(\hbar \omega - E_{10} + i \hbar \Gamma_0)},
\end{equation}

where only the near-resonant term at $2h\omega \approx E_{10}$ is considered.

The coefficient of the constant term which contributes zero frequency in the SHG expression is the OR coefficient and it is given by\textsuperscript{13,17,19}

\begin{equation}
\chi^{(2)} = \frac{8 \sigma_{10}(|\mu_{10}|^2)(\mu_{11} - \mu_{00}) E_{10}^2}{[(\hbar \omega - E_{10})^2 + (\hbar \Gamma_0)^2][(\hbar \omega + E_{10})^2 + (\hbar \Gamma_0)^2]},
\end{equation}

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III. NUMERICAL RESULTS AND DISCUSSION

We use the following input parameters: $\sigma_s = 3 \times 10^{10}$ cm$^{-3}$, $\Gamma_0 = 1/0.14$ ps$^{-1}$, $n_r = 3.2$, $m^* = 0.067 m_0$. The length of the quantum well, $L$, and $\beta$ are taken to be 126.5 Å and $\pi/2L$, respectively.

In Fig. 1, the potential profile is shown for three different $\kappa$ values, i.e., $\kappa = 1.2$, $\kappa = 2$, and $\kappa = 3$, while $\eta$ equals to 2. For $\kappa = \eta$, the curve becomes symmetric around $\beta z = \pi/4$, for $\kappa > \eta$ it becomes oblique and its minimum is shifted to the right. However, for $\kappa < \eta$ minimum of the curve is shifted to the left.

The first three normalized wave functions for the same $\kappa$ and $\eta$ values are shown in Fig. 2(a)–2(c). It can be observed that the shapes of the wave functions are very similar to the shapes of the wave functions of the parabolic potential with and without the electric field. This is due to the behavior of the potential around its minimum value where it may approximately be replaced by a parabolic curve. 

FIG. 1. The Pöschl-Teller potential profiles for $\eta = 2$. The solid curve stands for $\kappa = 1.2$, the dashed curve for $\kappa = 2$, and the dotted curve for $\kappa = 3$.

FIG. 2. The normalized first three wave functions of the QW having the Pöschl-Teller confining potential. The solid curves stand for $\kappa = 1.2$, the dashed curves for $\kappa = 2$, and the dotted curves for $\kappa = 3$ in panels (a), (b), and (c).
The linear absorption coefficient

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ence between two successive energy levels is

quadratic form of eigenenergies [Eq. (7)] where the difference between two successive energy levels is

\[ \Delta E_{n+1,n} = \frac{2\hbar^2 \beta^2}{m} (\kappa + \eta + 2n + 1). \]

(19)

The linear absorption coefficient \( \alpha(\omega, I=0) = \alpha(1)(\omega) \) and the total absorption coefficient \( \alpha(\omega, I) \) as functions of the incident photon energy at \( I = 1.0 \) MW/cm\(^2\) are shown in Fig. 3. The peak position of the linear absorption coefficient has a blueshift with increasing \( \kappa \), because the energy difference between first-excited and ground states has a linear dependency on the \( \kappa \). However, the peak value does not grow but remains almost constant. The resonant peak value (i.e., \( h\omega = E_{10} \)) of the linear absorption coefficient is proportional to \( E_{10}^3 |\mu_{10}|^2 \). Our calculations show that this product is more or less constant when \( 1.2 \leq \kappa \leq 3 \) and \( 1.2 \leq \eta \leq 2 \). The total absorption coefficient in Fig. 3 increases with increasing \( \kappa \). The resonant peak value of the total absorption coefficient is shown as a function of \( \kappa \) and \( \eta \) in Fig. 4. We see that the higher the \( \eta \) the higher the peak value. The Eq. (15) is totally negative at resonance and it is proportional to

\[ E_{10} |\mu_{10}|^2 \left( \frac{|\mu_{10}|^2 + |\mu_{11} - \mu_{00}|^2 (h\Gamma_0)^2}{4E_{10}^3} \right). \]

(20)

The first term in the parentheses decreases with increasing \( \kappa \) and \( \eta \). This is because as asymmetry parameters increase, the potential well becomes narrower yielding smaller \( |\mu_{10}|^2 \). Although the symmetry is broken for \( \kappa \neq \eta \) and \( |\mu_{11} - \mu_{00}|^2 \) increases, the second term in Eq. (20) becomes smaller since it is inversely proportional to \( E_{10} \). \( \alpha(3)(\omega) \) decreases in magnitude and as a result the resonant peak value of the total absorption coefficient increases.

The SHG coefficient as a function of incident photon energy for the asymmetric Pöschl-Teller potential is shown in Fig. 5. In the figure, the solid line stands for \( \kappa = 1.2 \) and the dotted line for \( \kappa = 3 \). The curve for \( \kappa = 3 \) is multiplied by three for clarity. The increasing \( \kappa \) value yields reduction in both peaks up to \( \kappa = 2 \) for which the SHG is zero, but for \( \kappa > 2 \) the SHG peaks have nonzero values although smaller than the peaks for \( \kappa < 2 \). The peak positions have an obvious blueshift while their separation increases. These can be attributed to the linear \( \kappa \) dependence of the energy difference between two successive levels as in Eq. (19). The maximum value for the SHG coefficient is about 15 times larger than the one in bulk GaAs for \( \kappa = 1.1 \). However, when the other input parameters quoted in the literature\(^{15,16} \) are used, it is possible to obtain larger peak values. For example, if the density of the electrons is increased up to the order of \( 10^{17} \) cm\(^{-3} \) the SHG peak increases more than two orders of magnitude. The electrons are, apart from thermal generation, supplied by dopant atoms. However, this supply is limited by the solubility of the dopant atom in GaAs.\(^{13} \) At higher-electron densities, a good description of the optical properties of QWs must take

![Figure 3](image3.png)

FIG. 3. The linear and the total absorption coefficients as a function of photon energy for the optical intensity \( I = 1.0 \) MW/cm\(^2\) and for \( \eta = 2 \). The solid curve stands for \( \kappa = 1.2 \), the dashed curve for \( \kappa = 2 \), and the dotted curve for \( \kappa = 3 \).

![Figure 4](image4.png)

FIG. 4. The resonant peak value of the total absorption coefficient as a function of the parameter \( \kappa \) for various \( \eta \) values. \( I = 1.0 \) MW/cm\(^2\).

![Figure 5](image5.png)

FIG. 5. The SHG coefficient as a function of incident photon energy for the asymmetric Pöschl-Teller potential.
into account the interactions among those electrons. The peak value of the SHG tensor at $2\hbar\omega = E_{10}$ is displayed in Fig. 6 as a function of $\eta$ and $\kappa$. The SHG is zero at $\kappa = \eta$. The peak increases with $|\mu_{11} - \mu_{00}|$ as the asymmetry is introduced. But the $E_{10}^2$ in the denominator substantially reduces the peak value at higher values of the asymmetry parameters.

We also calculate the OR coefficient for the $\kappa$ values of 1.2 and 3.0. The results are shown in Fig. 7. The peaks have a blueshift with increasing $\kappa$. The peak value of the solid line corresponds to three orders of magnitude larger values than in bulk$^{32}$ GaAs. However, this number can be enhanced when the other electron densities and relaxation times are used as mentioned above. For example, with the $\tau_e$ of the order of $10^{17}$ cm$^{-3}$ and $1/\Gamma_0$ of 0.2 ps$^{-1}$, for $\kappa = 1.1$, we get four orders of magnitude larger values than in bulk GaAs. The relaxation time, however, is certainly governed by intrinsic mechanisms such as electron-electron scattering, impurity scattering, collisions among electrons, optical-phonon emission for an excitation energy higher than 35 meV, well inhomogeneities, and temperature of the system.$^{3,13,18}$ In Fig. 8, the peak value of the OR coefficient at resonance frequency, i.e., $\hbar\omega = E_{10}$, is showed. The peak exhibits the similar pattern with the peak value of the SHG coefficient, except that it is reduced with $E_{10}$.

IV. CONCLUSION

The nonlinear optical properties of QWs described by a Pöschl-Teller confining potential are studied. We have calculated the linear and third-order absorption coefficients, the second-order susceptibility, and the optical rectification for symmetric and asymmetric cases of the Pöschl-Teller potential under the density matrix formalism. We find that the total absorption is reduced by nearly 30% and this reduction decreases with increasing asymmetry parameters at $I = 1.0$ MW/cm$^2$. We calculate SHG and OR coefficients much larger than in the bulk GaAs. The peak positions

FIG. 5. The SHG coefficient $|\chi^{(2)}_{20}|$ as a function of photon energy for $\eta = 2$. The solid curve stands for $\kappa = 1.2$ and the dotted curve for $\kappa = 3$ (multiplied by three for a better view).

FIG. 6. The resonant peak value of the SHG coefficient as a function of the parameter $\kappa$ for various $\eta$ values.

FIG. 7. The OR coefficient $|\chi^{(2)}_{02}|$ as a function of photon energy for $\eta = 2$. The solid curve stands for $\kappa = 1.2$ and the dotted curve for $\kappa = 3$.

FIG. 8. The resonant peak value of the OR coefficient as a function of the parameter $\kappa$ for various $\eta$ values.
strictly depend on the asymmetry parameter. Our investigation of the peak value of the SHG and OR coefficients for various $\kappa$ and $\eta$ show that a feasible SHG or OR coefficient is possible only for $\kappa$ and $\eta<2$. The QWs represented by the Pöschl-Teller confining potential seem to be possible with the recent progresses in the nanofabrication technology. An electric-field-biased QW having a Pöschl-Teller type confining potential is expected to yield a larger SHG.

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