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The energy-level and vibrational frequency properties of a polaron weak-coupled in a quantum well with asymmetrical Gaussian confinement potential

Wei Xiao[1] and Jinglin Xiao[2, †]

[1]Department of Basic Sciences, University of Informational Science and Technology of Beijing, Beijing 100101, China

[2]Institute of Condensed Matter Physics, Inner Mongolia University for the Nationalities, Tongliao 028043, China

Abstract: The vibrational frequency (VF), the ground state (GS) energy and the GS binding energy of the weak electron-phonon coupling polaron in a quantum well (QW) with asymmetrical Gaussian confinement potential are calculated. First we introduce the linear combination operator to express the momentum and coordinates in the Hamilton and then operate the system Hamilton using unitary transformation. The results indicate the relations of the quantities (the VF, the absolute value of GS energy and the GS binding energy) and the parameters (the QW barrier height and the range of Gaussian confinement potential in the growth direction of the QW).

Key words: quantum well; Gaussian confinement potential; polaron; vibrational frequency

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1. Introduction

Quantum structures in low-dimensional materials (LDM) have been employed powerfully in the last twenty years due to their fundamental physical properties[1, 2] and wide applications[3]. There are many forms of these quantum structures such as quantum dots, quantum wires, quantum rods, superlattices and quantum wells[4–8] in LDMs. Among the quantum structure forms, there has been great interest in the physics properties of quantum wells (QWs). QWs with very small dimensions have been manufactured using advanced experimental technologies. The size, shape and other physical and chemical properties can be controlled well in the experiments. Ambacher *et al.*[9] experimentally observed pyroelectric effects in the Al(In)GaN/GaN structures and QWs. Makino *et al.*[10] discussed mainly experimentally the exciton optical properties in ZnO-based multiple quantum well (MQW) heterostructures. Aumer *et al.*[11] reported on the luminescence properties of the tensile and compressive strain in the AlInGaN/InGaN QW. From these experiments, controlling the QW physical properties is interesting and has meaning for not only the fundamental physics, but also for potential application because of the special physical properties in these semiconductor LDM devices. In recent years, the electron and polaron properties in the QW have been widely studied using various methods. The confinement potentials play an important role in electronic and polaronic properties in a variety of QWs. It is noteworthy that the confinement potential is more important for the theoretical investigations of the polaron in the material quantum wells. It is known that the confinement potential is usually chosen as a parabolic potential. The previous works concentrated on the use of parabolic potential in the QWs. So, the QWs should be considered in other different potential forms (such as cylindrical, hyperbolic, Gaussian and spherical). However, the form of Gaussian potential is closer to the actual circumstances in the QWs.

Recently, using a Gaussian potential, many researchers have studied the electronic and polaronic properties. For example, Nandi *et al.*[12] discussed the different features of a potential in the form of a Gaussian well. Wu *et al.*[13] studied the effects of the nonlinear optical rectification polaron in QWs with asymmetrical Gaussian confinement potential (AGCP) and electric field. Xiao[14] investigated that the hydrogen-like impurity and temperature influence on the bound strongly-coupled polaron's state levels and transition frequency in AGCP QWs using the Pekar variation.

Based on these investigations, we found that a new confining potential is proposed as the Gaussian potential. The new potential, which contains AGCP, is practical for calculating GS energy and the GS binding energy. However, considering AGCP to study the VF, the GS energy and the GS binding energy isn't investigated.

In the present article, we use simple methods (linear combination operator and twice unitary transformation) to investigate the polaron's VF, GS energy and GS binding energy in the AGCP QWs. Our results provide a theoretical basis for low dimensional nanomaterials.

2. Theory model

An electron is confined in the QW with AGCP. The electron is moving in a GaAs semiconductor crystal and interacting with bulk longitudinal optical (LO) phonons. The system Hamiltonian has the following forms:

$$H=\frac{p^2}{2m}+V(z)+\sum_{\boldsymbol{q}}\hbar\omega_{\rm LO}a_{\boldsymbol{q}}^{+}a_{\boldsymbol{q}}+\sum_{\boldsymbol{q}}\left(V_q a_{\boldsymbol{q}}\exp(i\boldsymbol{q}\cdot\boldsymbol{r})+h\cdot c\right), \tag{1}$$

Correspondence to: J L Xiao, xiaojlin@126.com
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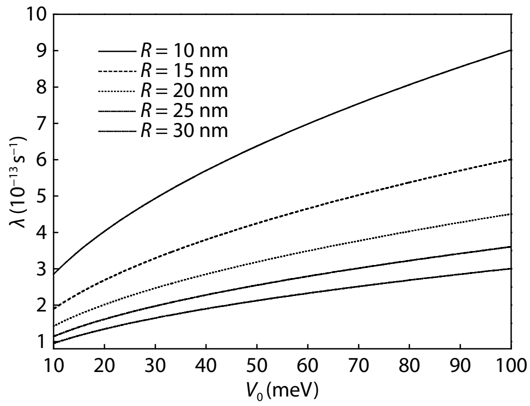

Fig. 1. Relational curves of the vibrational frequency (VF) λ with the barrier height of the quantum well (QW) V_0 and the range of the asymmetrical Gaussian confinement potential R.

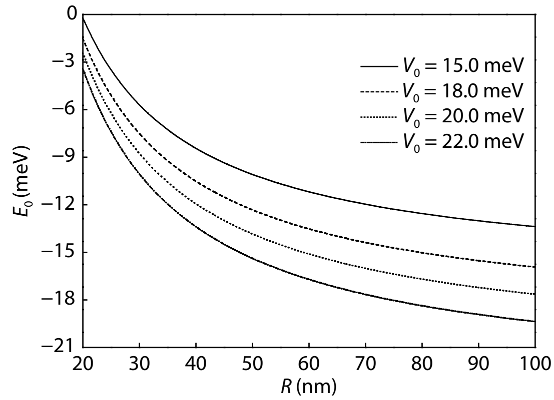

Fig. 2. Relational curves of the GS energy E_0 with the barrier height of the QW V_0 and the range of the AGCP R.

where

$$V(z)=\begin{cases}-V_0\exp\left(-\dfrac{z^2}{2R^2}\right), & z\geqslant 0,\\ \infty, & z<0.\end{cases} \tag{2}$$

In the above equation, m is the electron band mass, $a_{\boldsymbol{q}}^{+}\left(a_{\boldsymbol{q}}\right)$ denotes the creation (annihilation) operator of the bulk LO phonon. $\boldsymbol{q}$, $\boldsymbol{p}$ and $\boldsymbol{r}$ are the wave vector, momentum and position vector of the electron, respectively. $V(z)$ is the z-directional AGCP that represents the growth direction of the QWs[15]. V_0 and R are the QW's barrier height and the range of the AGCP, respectively. V_q and α in Eq. (1) are

$$V_q=i\left(\frac{\hbar\omega_{\rm LO}}{q}\right)\left(\frac{\hbar}{2m\omega_{\rm LO}}\right)^{\frac14}\left(\frac{4\pi\alpha}{v}\right)^{\frac12},$$
$$\alpha=\left(\frac{e^2}{2\hbar\omega_{\rm LO}}\right)\left(\frac{2m\omega_{\rm LO}}{\hbar}\right)^{\frac12}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right). \tag{3}$$

We operate the twice unitary transformations to the Hamiltonian in Eq. (1)[16]:

$$U_1=\exp\left(-i\sum_{\boldsymbol{q}}\boldsymbol{q}\cdot\boldsymbol{r}a_{\boldsymbol{q}}^{+}a_{\boldsymbol{q}}\right), \tag{4a}$$

$$U_2=\exp\left[\sum_{\boldsymbol{q}}\left(a_{\boldsymbol{q}}^{+}f_q-a_{\boldsymbol{q}}f_q^{*}\right)\right], \tag{4b}$$

$f_q\left(f_q^{*}\right)$ is the variational function, then we introduce the linear combination operator b_j^{+} and b_j[17]:

$$p_j=\left(\frac{m\hbar\lambda}{2}\right)^{\frac12}\left(b_j+b_j^{+}\right),$$
$$r_j=i\left(\frac{\hbar}{2m\lambda}\right)^{\frac12}\left(b_j-b_j^{+}\right), \tag{5}$$

where λ is the variational parameter. The GS wave function is expressed as

$$|\psi_0\rangle=|0\rangle_{\rm a}|0\rangle_{\rm b}, \tag{6}$$

where $|0\rangle_{\rm b}$ is the vacuum state of b and $|0\rangle_{\rm a}$ is the unperturbed zero-phonon state. The expectation value of the system Hamiltonian can be denoted as

$$F_0\left(\lambda,f_q\right)=\langle\psi_0|\,U_2^{-1}U_1^{-1}HU_1U_2\,|\psi_0\rangle. \tag{7}$$

The variation of $F_0(\lambda,f_q)$ with respect to λ is given as

$$\lambda=\left(\frac{V_0}{3mR^2}\right)^{1/2} \tag{8}$$

where λ is VF. The GS energy and the GS binding energy are obtained by

$$E_0=\frac32\hbar\left(\frac{V_0}{3mR^2}\right)^{1/2}-V_0-\alpha\hbar\omega_{\rm LO}, \tag{9}$$

$$E_{\rm b}=2\alpha\hbar\omega_{\rm LO}+V_0-\frac34\hbar\left(\frac{V_0}{3mR^2}\right)^{1/2}. \tag{10}$$

3. Results and discussions

The effective mass of GaAs is taken to be a value of $0.0675m_0$, the strength of electron-LO-phonon coupling is set to 0.068, and the phonon energy is $\hbar\omega_{\rm LO}$ = 36.184 meV[18].

Fig. 1 depicts the VF of the polaron changing with the barrier height of the QW V_0 and the range of the AGCP R. The five lines correspond to the range of the different values of the AGCP: R = 10 nm, R = 15 nm, R = 20 nm, R = 25 nm and R = 30 nm. From Fig. 1 one can easily see that the VF increases with increasing barrier height of the QW, whereas it decreases with increasing range of the AGCP. Fig. 2 plots the GS energy as a function of the barrier height of the QW and the AGCP. The four lines correspond to the barrier height of the QWV_0 = 15.0 meV, V_0 = 18.0 meV, V_0 = 20.0 emV and V_0 = 22.0 emV.

In Fig. 3, we illustrate the GS binding energy varying with the barrier height of the QW and the range of the AGCP. The four lines correspond to the barrier height of the QW: V_0 = 15.0 meV, V_0 = 18.0 emV, V_0 = 20.0 meV and V_0 = 22.0 meV. It turns out that the absolute value of GS energy $\left|E_0\right|$ and the GS binding energy $E_{\rm b}$ increase with the barrier height of the QW V_0 and the range of the AGCP, R.

From Figs. 1, 2 and 3 one can easily find that the VF decreases with the range of the AGCP, whereas the absolute value of GS energy and the GS binding energy increase with it

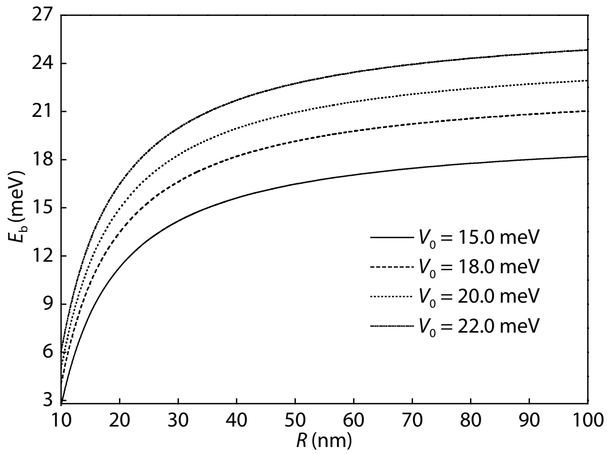

Fig. 3. Relational curves of the GS binding energy E_b with the barrier height of the QW V_0 and the range of the AGCP R.

because the electron motion is confined by the AGCP. The decrease of the confinement potential and z results in the reduction of the particle motion range, the electron energy and the interaction of the electron with the phonons around it are enhanced. So, the VF is increased. These physics properties contribute to the interesting quantum confining effect.

However, from the first term in Eq. (9), due to the range of the AGCP term, the GS energy is a positive value, whereas the total GS energy is negative. Moreover, from the last term in Eq. (10), due to the range of the AGCP term, the GS binding energy is a negative value. It is clear that the absolute values of GS energy and the GS binding energy increase with range of the AGCP. Here we can find that the VF, the GS energy and the GS binding energy in the QW can be adjusted by changing the barrier height of the QW and the range of the AGCP .

In summary, it is well known that the barrier height of the QW and the range of AGCP in the growth direction of the QW are vital factors for polaron research in the QW with AGCP.

The asymmetric Gaussian type QW is a new type of low-dimensional nano-quantum system. Due to its special properties, this new structure has attracted the attention of many scholars. This structure is characterized by the existence of a limited potential in the direction of growth z of the QW in which electrons can't exist at all. The limited potential in the range of $z \geqslant 0$ is the Gaussian function potential. We can see that the restricted potentials on both sides of $z = 0$ are asymmetrical, so it is called the asymmetric Gaussian restricted potential. Since the Gaussian function itself is characterized by a rapid decrease to zero as z increases from 0, which shows that the Gaussian function has a strongly restricted property in the z direction. This point indicates that there is a strongly restricted characteristic in the growth direction of the QW, that is, in the z-axis direction. This is why we call this new type of low-dimensional nano-quantum system an asymmetric Gaussian type QW.

Through the above discussions, we find that the QW barrier height and the range of Gaussian confinement potential in the growth direction of the QW are important physical quantities for studying the properties of the energy-level and vibrational frequency of weak -coupling polarons in a QW with AGCP.

4. Conclusions

In conclusions, the VF, the GS energy and the GS binding energy of the polaron weakly-coupled in the QW with AGCP are investigated by the above-mentioned methods. They have the following properties: (1) The VF, the absolute value of GS energy and the GS binding energy will increase with the barrier height of the QW. (2) The VF will decrease with the range of the AGCP in the QW, whereas the absolute value of GS energy and the GS binding energy increase with it. Here we can find that changing the barrier height of the QW and the range of the AGCP can adjust the three physics quantities in the special QW.

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