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Acoustic polaron in free-standing quantum wells

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The numerical results of the ground-state energy and the derivate of the acoustic polaron in free-standing quantum wells are performed by using the Huybrechts-like variational approach. The criterion for the self-trapping transition of the acoustic polaron in free-standing quantum wells is determined quantitatively. It is found that the critical coupling constant corresponding the discontinuous transition from a quasi-free state to a trapped state of the acoustic polaron in free-standing quantum wells tends to shift toward the weaker electron-phonon coupling with the increasing cutoff wave-vector. Detailed numerical results confirm that the self-trapping transition of acoustic polaron is expected to realize in the free-standing quantum wells of wide-band-gap semiconductors.

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1. Introduction

The electron mobility is important because it is a parameter which associates microscopic electron motion with macroscopic phenomena such as current-voltage characteristics. The mobility will be changed markedly if electron state transforms from the quasi-free to the self-trapped. Moreover, many physical properties of photoelectric material are also influenced by the electron state. Furthermore, the self-trapping of an electron is due to its interaction with acoustic phonons. Therefore the problems of acoustic polaron had been maintained interest of many scientists in the past decades [1-17].

Modern micro-fabrication techniques such as Electron beam evaporation [18], molecular beam epitaxy [19], and standard lithographic techniques [20] had allowed the creation of free-standing quantum well (FSQW) structures. The feature of free-standing structure is that the electrons (holes) in this structure are quantized. This attribute gives rise to interesting physical phenomenons and opens many possibilities for application. The phonons subsystem will undergo modification and quantization of the acoustic phonons spectrum in a way similar to the electron quantization should occur[21].

Various calculations for the ground-state energy of the acoustic polaron as a function of the e-p coupling strength have leaded to a discontinuous transition from a quasi-free state to a trapped state[6,8,9]. It is well known that the e-p coupling effects will be substantially enhanced in confined structure, such as FSQW systems, so that the self-trapping transition should be easier to realize.

As mentioned in above, the FSQW belongs to a confined structure of quasi-2D system, so that the self-trapping transition of the acoustic polarons will be easier to realize than that in body systems. In following section, we will carry out the numerical calculation for the ground-state energies and its derivates of the acoustic polaron in FSQW structures. The possibility of the self-trapping transition of the acoustic polaron in the FSQW structures will be discussed by using the characteristic curve of the ground-state energies and its derivates.

2. The e-LA-p interaction Hamiltonian and the ground state energy

The Hamiltonian of the electron-longitudinal acoustic phonon (e-LA-p) interactions through the deformation potential in a FSQW is given by [21]

$$H_{int} = D\vec{\nabla}\cdot\vec{u}\ . \tag{1}$$

Where D is the dimensionless deformation potential constant, and $\vec{u}$ is the displacement vector of the acoustic phonon.

The displacement vector $\vec{u}$ can be expressed through the eigenmode $W_n(\vec{q},z)$ and the corresponding creation and annihilation operators $a_n^{\dagger}(\vec{q})$ and $a_n(\vec{q})$, by the following formula[21]

$$u(\vec{r}) = \sum_{\vec{q},n}\sqrt{\frac{\hbar}{2A\rho w_n(\vec{q})}}[a_n(\vec{q}) + a_n^{\dagger}(\vec{q})]\times W_n(\vec{q},z)e^{i\vec{q}\cdot\vec{r}}\ . \tag{2}$$

Where $\vec{r}$ is the coordinate vector in *x-y* plane, w_n is the set of frequency of vibrations. $\vec{q}$ is wave-vector of the phonon modes. It may be conveniently done if we direct the axis x of the coordinate system along vector $\vec{q}$, so that $\vec{q} = (q_x, 0)$.

Specifying the axis z is perpendicular to the semiconductor quantum well slab and the width of the well is L, the interaction Hamiltonian of the e-LA-p in quantum well can be obtained as the following form by solution of the $u(\vec{r})$ in the boundary conditions of the stress tensor $\sigma_{x,z} = \sigma_{y,z} = \sigma_{z,z} = 0$ at $z = \pm(L/2)$ form Ref.(21)

$$H_{\text{int}} = \sum_q e^{i\vec{q}\cdot\vec{r}} \Gamma(\vec{q}, z)(a_q + a_q^\dagger) , \tag{3}$$

Where

$$\Gamma(\vec{q}, z) = F\sqrt{\frac{\hbar D^2}{2A\rho w_q}} \times [(q_t^2 - q_x^2)(q_l^2 + q_x^2) \cdot \sin(\frac{Lq_t}{2})\cos(q_l z)]. \tag{4}$$

Here $w_q = cq$ is the linear dispersion for the frequency of acoustic phonons with a finite cut-off wave vector q_0 , and c is the velocity of sound. A is area of the 2D plane. ρ is the mass density of the crystal, F is a normalization constant.

Parameters q_l and q_t are corresponding the longitudinal and transverse wave vector and determined from the system of two algebraic equations,[21]

$$\frac{\tan(q_t L/2)}{\tan(q_l L/2)} = -\frac{4q_x q_l q_t}{(q_x^2 - q_t^2)^2} , \tag{5}$$

$$s_l^2(q_x^2 + q_l^2) = s_t^2(q_x^2 + q_t^2) . \tag{6}$$

Here we have given a relation of q_l and q_t from Ref.(31)

$$|\vec{q}_l| = \sqrt{\frac{\mu}{\lambda + 2\mu}} |\vec{q}_t| . \tag{7}$$

where λ and μ are the Lame constants.

Introducing the dimensionless bulk e-p coupling constant α , which is given by

$$\alpha = \frac{D^2 m^2}{8\pi\rho\hbar^3 c} , \tag{8}$$

the e-p coupling function can be presented as

$$S_q = F\sqrt{\frac{4\pi c\alpha}{Aw_q}\frac{\hbar^2}{m}} \times [(\frac{\lambda + 2\mu}{\mu} q_l^2 - q_x^2)(q_l^2 + q_x^2) \cdot \sin(\sqrt{\frac{\lambda + 2\mu}{\mu}}\frac{Lq_l}{2})\cos(q_l z)]. \tag{9}$$

Consider the electron in a FSQW is confined in the z direction and free in the x-y plane. The e-LA-p system Hamiltonian in a FSQW is then written as

$$H = \frac{p_z^2}{2m} + \frac{p_{x-y}^2}{2m} + \sum_q \hbar w_q a_q^\dagger a_q + \sum_q (S_q a_q e^{i\vec{q}\cdot\vec{r}} + h.c.). \tag{10}$$

where $p_z^2/2m$ and $p_{x-y}^2/2m$ denote the kinetic energy of the electron in the z direction and x-y plane, respectively. The acoustic phonon contribution is given by $\sum_q \hbar w_q a_q^\dagger a_q$.

Using a method similar to Huybrechts-like variational approach [22] for 3D optical polaron problems and by some standard treatments, the variational energy of the polaron ground-state in FSQW can be obtained as

$$E_0(\lambda') = \frac{1}{2}\hbar\lambda'(1-a)^2 + \frac{1}{2}\hbar\lambda' - 2\alpha\int_0^{q_0}\int_0^{q_0}\int_{-\frac{L}{2}}^{L} \frac{F^2 Q}{\left(1 + a^2 q_x^2/2\right)} \cdot \exp[-\frac{q_x^2(1-a)^2}{2\lambda'}] dq_x dq_l dz, \tag{11}$$

Where

$$Q = [(\frac{\lambda + 2\mu}{\mu} q_l^2 - q_x^2)^2 (q_l^2 + q_x^2)^2 \cdot \sin^2(\sqrt{\frac{\lambda + 2\mu}{\mu}}\frac{Lq_l}{2})\cos^2(q_l z)], \tag{12}$$

Here a and λ' are variational parameters.

3. Numerical results and discussions

The variational calculations for the ground-state energies of the acoustic polaron in FSQW are numerically performed for different width of well L and cut-off wave vector q_0, by using Eq.(11). To compare with the previous results in Refs.(6), (8) and (9), we have also expressed the energy in units of mc^2 and the phonon vector in units of $mc/\hbar$ in the calculations. The width of a FSQW in this paper will be taken as 0.03 and 0.3.

As can be seen in Fig. 1(a), in case of the width of the well L is 0.03 and the cutoff wave vector is 150, the ground-state energy appears a knee with respect to α at $\alpha_c \approx 0.0051$, where the derivative of the ground-state energy has a catastrophe point, which is called “phase transition” critical point, where the polaron state transforms from the quasi-free to the self-trapped. When q_0 = 180 and 200, the critical points are at $\alpha_c \approx 0.0045$ and 0.004, respectively, where one can find knees in the ground-state energies, and catastrophe points in the derivatives with respect to α in Fig. 1(b) and (c). It is obviously that the critical point α_c shifts toward the weaker e-p coupling with the increasing cutoff wave-vector q_0. Fig. 2 exhibits the results of ground-state energies and derivatives of the acoustic polarons in FSQW for L = 0.3. One can find in Fig. 2 that the critical coupling constants are around 0.0074, 0.0063 and 0.0057, for q_0 = 150, 180 and 200, respectively. It is also found that the position of the critical point is sensitive to the cutoff wave-vector q_0 and shifts toward the direction of smaller e-p coupling with the increasing cutoff wave-vector. The character of the critical coupling constant varying with the cutoff wave-vector q_0 is consistent with the previous papers [6,7,9].

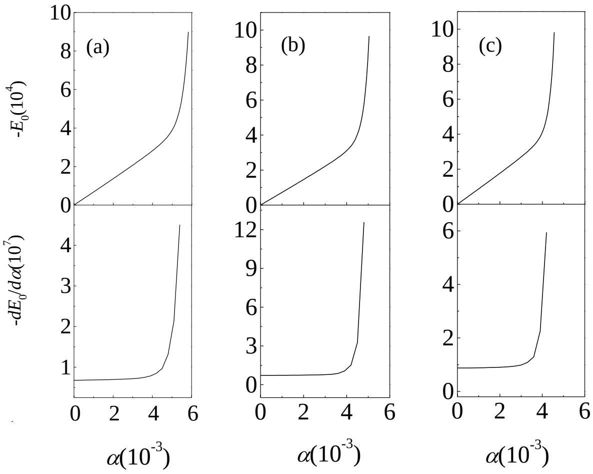

Fig. 1. Ground-state energies and their numerical derivatives of the acoustic polarons in a free-standing quantum well with the L = 0.03, as functions of the e-p coupling constant α for (a) $q_0 = 150$, (b) $q_0 = 180$ and (c) $q_0 = 200$, respectively.

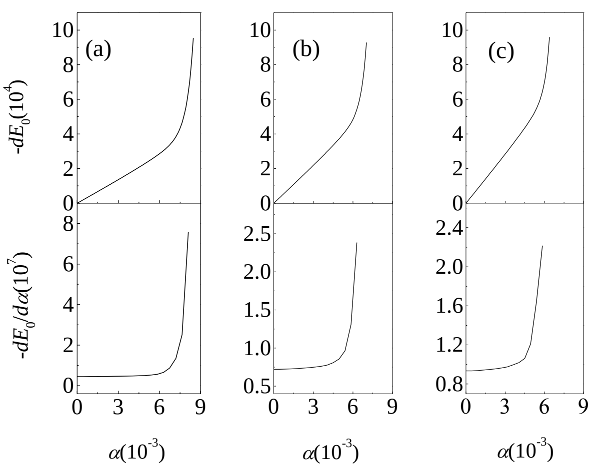

Fig. 2. Ground-state energies and their numerical derivatives of the acoustic polarons in a free-standing quantum well with the L = 0.3, as functions of the e-p coupling constant α for (a) $q_0 = 150$, (b) $q_0 = 180$ and (c) $q_0 = 200$, respectively.

It is worth noting the critical values of the e-p coupling constant increase with the increasing width of the well. For example, when the cutoff wave-vector q_0 equals to 180, the critical coupling constant, α_c, is around 0.0045 for the width is 0.03 (Fig. 1), whereas $\alpha_c \approx 0.0063$, when the width is 0.3 (Fig. 2). Which we thought the e-p coupling strength weakened with the increasing width of quantum well.

The $\alpha_c q_0$ had been used as a criterion for the self-trapping transition quantitatively. It is obviously that the $\alpha_c q_0$ for different values of cut-off wave-vectors almost tend to a given value of 0.8, when the width of a FSQW is 0.03. Similarly result had also been obtained in a quantum well with width of 0.3. The products of $\alpha_c q_0$ are all close to 1.1. Therefore, $\alpha_c q_0$ can then be used as a quantitative criterion for the presence of the self-trapping transition of the acoustic polaron in FSQW. Acoustic polaron in FSQW systems can be self-trapped if the material's αq_0 larger than the criterion $\alpha_c q_0$.

Now we use the criterion of the $\alpha_c q_0$ to judge the possibility of self-trapping transition for the acoustic polaron in FSQW materials. Firstly, we consider the semiconductors of GaN and AlN. In our previous work, it was indicated that the holes in GaN and both the electrons and holes in AlN are expected to have the self-trapping transition in 2D systems [8]. In present work, even the electron's αq_0 (0.24 for GaN and 0.57 for AlN) can get the same order of magnitude as $\alpha_c q_0$ (0.8), the self-trapping transition is still difficult to be observed. Which we thought the e-p coupling strength in FSQW is weaker than that in 2D system for the weakening of confined dimension in the vertical plane direction.

Holes have larger effective masses than electrons and must be easier to be self-trapped. For GaN, which has the light and heavy-hole masses 0.37 and 0.39 respectively [8], the corresponding product $\alpha q_0 \approx 0.91$ and 1.01 are both large enough to have self-trapping transition in FSQW systems for the quantum well width is 0.03. Similarly the light-hole mass in AlN is 0.47 [8] and the product $\alpha q_0 \approx 1.16$ is smaller than the critical value (2.6) in 3D system but larger than that (0.8 and 1.1) in FSQW. Therefore the light-hole in AlN can be self-trapped in FSQWs with L = 0.1 and 0.3. Furthermore, the heavy-hole mass in AlN is 0.73 [8] and the product $\alpha q_0 \approx 2.79$ (> 1.1) is sufficiently large to have self-trapping in the FSQW with width greater than 0.3.

4. Summary

The critical coupling constant for the self-trapping transition of the acoustic polarons in FSQW systems is determined by calculating the ground-state energies and the derivatives of the acoustic polaron. The value of the criterion $\alpha_c q_0$ of the acoustic polaron in FSQW systems is smaller than that in 3D system. Nevertheless, the $\alpha_c q_0$ value for FSQW is over that in 2D system [8]. Therefore, the self-trapping transition of the acoustic polaron in FSQW is a little more difficult to be realized than that in 2D system. It is still worth someone's attentions, for which the transition of the acoustic polaron in FSQW is easier to be realized than that in 3D system. In order to validate the criterion $\alpha_c q_0$ in this work, the close attention should be payed to the progress of the related experimental researchs in future.

Acknowledgments

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