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Self-trapping transition of acoustic polaron in free-standing square quantum dots

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The interaction of the electron and acoustic phonon in free-standing square quantum dot systems is investigated theoretically. The electron-acoustic phonon interaction Hamiltonian is derived by taking the displacement vector's divergence of the acoustic phonon. The variational ground-state energies and their derivatives of the acoustic polaron in square quantum dot structures are numerically computed for different cutoff wave-vectors. The discriminating standards for the self-trapping transition of the acoustic polaron in square quantum dots are confirmed quantitatively. The results indicate that the self-trapping transition of the electron in wide-band-gap semiconductors and alkali halides square quantum dot structures might be occured.

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1. Introduction

As a parameter which associates microscopic electron motion with macroscopic phenomena such as current-voltage characteristics, the electron mobility plays a key role in material sciences. The mobility will be changed dramatically if electron state transforms from the quasi-free to the self-trapped. Moreover, many physical properties of photoelectric and electric material are also influenced by the electron state. Furthermore, the self-trapping of an electron stems from its interaction with acoustic phonons. Therefore the interest to the problem of acoustic polaron has been maintained in past few decades [1-18].

Due to the feature of confined zero dimensional system, quantum dot (QD) is a good candidate for optoelectronic device [19-23]. An electron is strongly confined and the optical emission of QD device should be greatly enhanced over the bulk device [19]. The electron-phonon (e-p) interaction in QD plays a critical role for construing the time evolution and dephasing mechanism after optical excitation [24]. The self-trapping transition of the acoustic polaron in QDs is necessary to be clarified.

Different approaches to the calculation of the ground-state energy of the acoustic as function of e-p coupling strength exhibited a discontinuous transition from a quasi-free state to a trapped state [6,8,9]. The e-p coupling effects shuold be substantially enhanced in confined structures, such as QD systems, so that the self-trapping transition will be easier to be realized.

In this paper, the possibility of the self-trapping transition of the acoustic polaron in free-standing square QDs will be studied. The numerical results of ground-state energies and their derivatives of the acoustic polaron in square QDs will be calculated by using Huybrechts-like variational approach.[25] Finally, we apply the theory to GaN, AlN and alkali halides.

2. The Ground-state energy

The interaction Hamiltonian of the electron and longitudinal acoustic phonon (e-LA-p) in nanoscale rectangular quantum dots can be given by [26]

$$H_{e-p} = E_a \nabla \cdot u(r). \tag{1}$$

Here the E_a is deformation potential constant, and $u(r)$ is the displacement vector of acoustic phonon.

Alexandrov suggested that the plane wave description of the electron is not fully adequate in nanoscale structures.[27] The phonons are modified here in QD systems due to the abrupt changes of the material properties at the interface between the QD and the surrounding material. The electron wave functions are also modified come from the variations in electron and hole band energies near the boundaries of the QD. For acoustic phonons, the changes in elastic properties near the QD boundaries cause the modifications in the displacement amplitude.

By using McSkimin's approximate solution for a rectangular quantum dot with flexural thickness mode, the *x*-, *y*-, and *z*-directed displacements had been written as [26, 28]

$$u(k,x,y,z) = A\left[\sin l_1 y + \alpha' \sin l_2 y + \beta' \sin l_2 y\right] \cdot \sin mx \cos nz, \tag{2}$$

$$v(k,x,y,z) = A\left[\frac{-l_1}{m}\cos l_1 y - \frac{\alpha' l_2}{m}\cos l_2 y + \frac{\beta'(m^2+n^2)}{l_2 m}\cos l_2 y\right]\cos mx\cos nz, \quad (3)$$

$$w(k,x,y,z) = A\left[\frac{n}{m}\sin l_1 y - \alpha'\frac{(m^2+l_2^2)}{nm}\sin l_2 y + \beta'\frac{n}{m}\sin l_2 y\right]\cos mx\sin nz. \quad (4)$$

In above the α' and β' are determined by applying boundary conditions of rectangular face. The indices of phonon mode in state k have been represented as m and n, respectively, for x- and z-components. The l_1 and l_2 for y-components express the subject mode index for the irrotational contribution and rotational contribution to the phonon displacement.

Due to the traction force on the rectangular surface should be vanished at $x=a$, $y=b$, $z=c$, the normalization constant A can then be obtained by [26, 28]

$$\frac{1}{abc}\int_{-a/2}^{a/2}dx\int_{-b/2}^{b/2}dy\int_{-c/2}^{c/2}dz\, u^*(k,x,y,z)u(k,x,y,z) = \frac{}{2M\omega_k}.$$

The e-p interaction Hamiltonian can be obtained as the following

$$H_{e-p} = \sum_k (V_k a_k + h.c.), \quad (5)$$

Here the V_k express the e-p coupling function that given by

$$V_k = \frac{E_a S}{\sqrt{N}}\cdot 3k\cos kx\sin ky\cos kz. \quad (6)$$

In case of square QD, $a=b=c=D$, the S can be represented as

$$S = \frac{1}{\left\{\left(1+\frac{\sin kD}{kD}\right)\left(3-\frac{2\sin kD}{kD}+\frac{3\sin^2 kD}{k^2D^2}\right)\right\}}. \quad (7)$$

Due to the electron in the nanoscale square QD systems is confined in three dimensional boxes. The e-LA-p system Hamiltonian can be written as

$$H = \frac{p^2}{2m} + \sum_k \omega_k a_k^\dagger a_k + \sum_k (V_k a_k + h.c.). \quad (8)$$

Where the $\sum_k \omega_k a_k^\dagger a_k$ is acoustic phonon contribution.

Carrying out two unitary transformation as following equations

$$U_1 = \exp\left(-ia\sum_k k\cdot r a_k^\dagger a_k\right). \quad (9a)$$

$$U_2 = \exp\sum_k\left(f_k a_k^\dagger - f_k^* a_k\right). \quad (9b)$$

to Eq. (8) and introducing the linear combination operators of the position and momentum of the electron by the following relations

$$p_j = \left(\frac{m\ \lambda}{2}\right)^{1/2}\left(b_j^\dagger + b_j\right). \quad (10a)$$

$$r_j = i\left(\frac{}{2m\lambda}\right)^{1/2}\left(b_j - b_j^\dagger\right). \quad (10b)$$

The e-LA-p system Hamiltonian finally transforms to the following form:

$$\begin{aligned}H_1 = {} & \frac{\lambda}{2}\sum_j b_j^\dagger b_j + \frac{3\ \lambda}{4} \\ & + \sum_k\left(\omega_l + \frac{a^2\ {}^2k^2}{2m}\right)\left(a_k^\dagger a_k + f_k a_k^\dagger + f_k^* a_k + |f_k|^2\right) \\ & + \left\{\left(V_k^* a_k^\dagger + V_k^* f_k^*\right)\exp\left[-\frac{a^2k^2}{4m\lambda}\right]\right. \\ & \cdot\exp\left[-a\left(\frac{}{2m\lambda}\right)^{1/2}\sum_j k_j b_j^\dagger\right] \\ & \left.\cdot\exp\left[-a\left(\frac{}{2m\lambda}\right)^{1/2}\sum_j k_j b_j\right] + h.c.\right\} \\ & + \frac{a^2}{2m}\left(\sum_k k|f_k|^2\right)^2 - 2a\sum_{jk}\frac{k_j P_j}{2m}|f_k|^2.\end{aligned} \quad (11)$$

Here we have omitted the multi-phonon processes, which contribute less to the polaronic energy.

By some standard treatments, the variational energy of the polaronic ground-state in square QD can be obtained as

$$\begin{aligned}E_0 = {} & \frac{3\lambda}{4}(1-a)^2 - \alpha\int_0^{k_0}\frac{1}{D^3}18k^2\cdot\left(R+\frac{\sin 2kD}{2k}\right)^2 \\ & \cdot\left(R-\frac{\sin 2kD}{2k}\right) \\ & \cdot\frac{1}{\left\{\left(1+\frac{\sin kD}{kD}\right)\left(3-\frac{2\sin kD}{kD}+\frac{3\sin^2 kD}{k^2D^2}\right)\right\}^2} \\ & \cdot\frac{1}{1+a^2k/2}\cdot\exp\left[-\frac{a^2k^2}{2\lambda}\right]dk,\end{aligned} \quad (12)$$

Where the k_0 is the cutoff wave vector corresponding the boundary of the first Brillouin zone and the α is e-LA-p coupling constant that given by

$$\alpha = \frac{E_a{}^2 m^2}{8\pi\rho\ {}^3 v_l}. \tag{13}$$

Here ρ is the mass density of the square QD.

3. Numerical results and discussions

The ground-state energies of the acoustic polaron in square QD systems are numerically performed for different D and k_0, by using the formula (12). To facilitate comparison of the earlier research results, [6,8,9] we will also express the energy in units of mv_l^2 and the phonon vector in units of $mv_l/\hbar$ in the calculations.

It is obviously that the ground-state energy and its derivative vary continuously with the coupling constant α for k_0 = 40, in Fig. 1(a). But there appears an inflection point in the derivative of the ground-state energy with respect to α at $\alpha_c \approx 0.022$, which had been called "phase transition critical point" in previous works,[6,8,9] where the polaronic state transforms from the quasi-free to the self-trapped. When k_0 is taken as 50 and 60, the critical points are at $\alpha_c \approx 0.0175$ and 0.0135, respectively, where one can find knees in the ground-state energies, and discontinuous points in the derivatives with respect to α in Fig. 1(b) and (c). It can be found that the critical point α_c trends toward the weaker e-p coupling with the increasing cutoff wave-vector k_0. Fig. 2 exhibits the result of ground-state energies and derivatives of the acoustic polarons in QD for D = 0.03. It can be seen in Fig. 2 that the critical coupling constants are around 0.030, 0.024 and 0.020, for k_0 = 40, 50 and 60 respectively. It can also be found that the position of the *critical point* is sensitive to the cutoff wave-vector k_0 and moves also 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 k_0 is consistent with the previous papers [6,8,9].

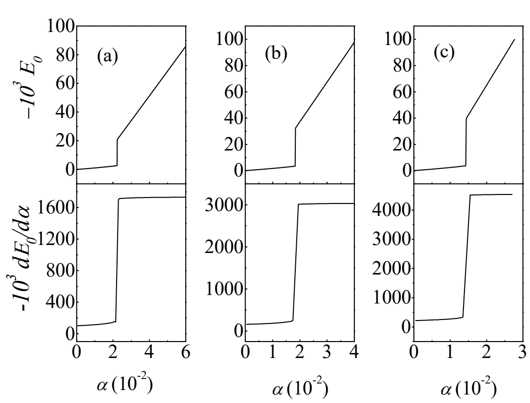

Fig. 1. Ground-state energies and their derivatives of the acoustic polarons in QD with the side-length D = 0.01 as functions of the e-p coupling constant α for (a) k_0 =40, (b) k_0 = 50 and (c) k_0 = 60, respectively.

It's worth noting that the critical values of the e-p coupling constant increase with the increasing size of the QD. For example, when the cutoff wave-vector k_0 equals to 40, the critical coupling constant, α_c, is around 0.022 for the side-length (D) is 0.01 (in Fig. 1), whereas $\alpha_c \approx 0.030$ when the D is 0.03 (in Fig. 2). The reason for this phenomenon is that the e-p coupling strength weakened with the increasing size of QD.

The $\alpha_c k_0$ had been used as a quantitative criterion for the self-trapping transition. It can be found that the $\alpha_c k_0$ for different values of cutoff wave-vectors almost tends to a given value of 0.8, when the side-length of the QD is 0.01. Similarly results can also be obtained in the QD with side-length of 0.03. The products of $\alpha_c k_0$ are close to 1.20. Therefore, $\alpha_c k_0$ can be used as a quantitative criterion for presence of the self-trapping transition of the acoustic polaron in QDs. Acoustic polaron in square QD systems can be self-trapped if αk_0 is larger than the $\alpha_c k_0$.

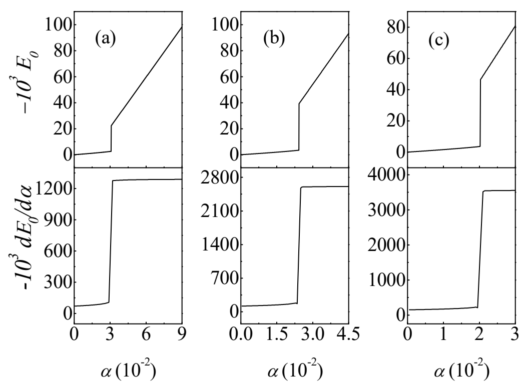

Fig. 2. Ground-state energies and their derivatives of the acoustic polarons in QD with the side-length D = 0.03 as functions of the e-p coupling constant α for (a) k_0 =40, (b) k_0 = 50 and (c) k_0 = 60, respectively.

It was indicated in our previous work that the self-trapping transition of the acoustic polaron is impossible to occur for GaN and AlN in 3D case and for GaN in 2D case.[8] In this paper, the two values of αk_0 (0.24 and 0.57 for GaN and AlN, respectively)[8] are same order of magnitude as $\alpha_c k_0$ for the side-length of the QD around 0.01, so that the acoustic poalrons in QDs of these two semiconductor materials might be self-trapped. For alkali halides, the product value of αk_0 is about 0.19-0.26.[6] One can also speculate that the αk_0 value of alkali halides (around 0.2) will large enough for the acoustic polaron to be self-trapped if the side-length of the QDs less than 0.01.

4. Conclusion

In summary, the criterion for presence of the self-trapping transition of acoustic polarons in square QD systems is determined by calculating the ground-state energies and the derivates of the acoustic polaron. Some criterion values ($\alpha_c k_0$) of the acoustic polaron in square QD systems are smaller than those in 3D systems. Therefore, the self-trapping transition of the acoustic polaron in square QD is easier to be realized than that in 3D systems. The conclusion meets the general sense that the e-p coupling effects will be substantially enhanced in confined quantum structures.

Acknowledgments

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