Self-trapping transition of acoustic polaron in free-standing cylindrical nanowires

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The interaction of electron and the modulated acoustic phonon in free-standing cylindrical nanowire is investigated theoretically. The interaction Hamiltonian is derived by taking the divergence of the displacement vector of the acoustic phonon. The variational computations for the ground-state energy of the acoustic polaron in cylindrical nanowires are numerically performed for different cutoff wave-vectors. The electron and the hole are confirmed to have the self-trapping transition in both the AlN and GaN cylindrical nanowire structures.

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1. Introduction

The advances in nanowire field-effect transistors research and application must be accompanied with precise modeling of device physics such as electrostatic potentials and mobility. Especially, electron mobility is important because it is a parameter which associates microscopic electron motion with macroscopic phenomena such as current-voltage characteristics [1]. 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.

The self-trapping of an electron is due to its interaction with acoustic phonons. Therefore the problems of the electron- acoustic phonon interaction (the so called acoustic polaron problems) had been maintained interest of many scientists in the past decades [2-22]. The polaron problem had also gained interest in explaining the high-T_c superconductors [23]. Recently, the polaron problem had been studied to describe impurities of lithium atoms in Bose-Einstein ultracold quantum gases condensate of sodium atoms [24]. So that it is meaningful to judge the possibility of the self-trapping of electron in nanowire systems.

Theoretical calculations for the ground-state energy of the acoustic polaron as a function of the electron- phonon (e-p) coupling strength have leaded to a discontinuous transition of polaron state from quasi-free to self-trapped [4-10]. As for the e-p coupling effect, it will be substantially enhanced in confined structures, such as nanowire systems. So the self-trapping transition of polaron would be easier to realize in confined structures.

It is determined in our previous works [14] that the self-trapping transition is expected to occur in the cylindrical quantum wire systems of alkali halides and wide-band-gap semiconductors. However, the e-p coupling Hamiltonian was derived by bulk phonon mode rather than confined phonon mode, the treatment left something to be desired [14].

Various technigues (e.g., Feynman approximation, Gaussian approximation and the approximation of Shoji and Tokuda, etc) that valid over the whole e-p coupling range and provied an upper bound to the exact acoustical polaron ground-state energy had been summarized in Ref.[10]. The Feynman path-integral approach is generally considered to be most accurate [10]. The Huybrechts variational approach has relatively simple features. It had been identified in previous work of the first author of present paper that the Huybrechts variational approach and Feynman path-integral approach are comparable in terms of accuracy [25]. So that the ground-state energy of the acoustic polaron in free-standing cylindrical nanowires will also be performed following the Huybrechts-like variational treatment in Sec. 3.

In this work, a new Hamiltonian describing the deformation potential interaction between the electron and the modulated acoustic phonon will be derived. The self-trapping transition of the acoustic polaron in free-standing cylindrical nanowires will be discussed.

2. The e-p interaction Hamiltonian

The electron and the modulated acoustic phonon interaction Hamiltonian can be obtained as following form [6]:

$$H_{int} = D\vec{\nabla}\cdot\vec{S}\,, \tag{1}$$

where D is the deformation potential constant and $\vec{S}$ the displacement vector of the acoustic phonon.

In an infinite length cylindrical nanowire in the z direction with radius R, the only longitudinal models of

confined acoustic phonons are considered. The displacements can be taken as the form [26]:

$$\vec{S}(\vec{r},t)=\sum_q C_q e^{i(m_p\theta+q_z z-\omega t)}\vec{u}_q(\vec{r}). \tag{2}$$

Where C_q is a constant, m_p is the phonon azimuthal quantum number related to rotational symmetry, q_z is a wave vector along the wire, ω is an angular frequency, and the three-dimensional vector $\vec{u}_q(\vec{r})$ represents the radial dependence of the normal mode.

The vector $\vec{u}_q(\vec{r})$ must satisfy the following normalization integral [26]

$$\int_0^R \rho(r)u_q^*(r)\cdot u_{q'}(r)r\,\mathrm{d}\,r=\frac{\delta_{q,q'}}{2\pi L_z} \tag{3}$$

Where L_z and R denote the length and radius of the nanowire, respectively. The $\rho(r)$ is the position-dependent mass density of the nanowire.

In a free-standing nanowire, general solution of the vector $\vec{u}_q(\vec{r})$ in the cylindrical coordinate is given by [1]

$$u_q(r)=\begin{pmatrix} A_1 q_l J'_{m_p}(q_l r) \\ iA_1 m_p J_{m_p}(q_l r)/r \\ iA_1 q_z J_{m_p}(q_l r)\end{pmatrix}. \tag{4}$$

Where J_{m_p} and J'_{m_p} are Bessel function of the first kind with order m_p and its first derivative.

Consider the isotropic system, $m_p=0$, $q_z=q_l$. By using the Eq.(4), the interaction Hamiltonian becomes

$$H_{int}=-\frac{2D_{ac}}{\sqrt{N}}\sum_q a_q A_1 q^2 J_0(qr)+h.c. \tag{5}$$

Here, *N* is number of the unit cell. The linear dispersion, $\omega = cq$, presents the relation of the acoustic phonon frequency with a finite wave-vector *q*, *c* is the sound velocity.

The e-p interaction Hamiltonian in Eq.(5) can be written as the following

$$H_{int}=\sum_q (G_q a_q+G_q^\dagger a_q^\dagger). \tag{6}$$

where the e-p coupling function is given by

$$G_q=-\frac{2D}{\sqrt{N}}A_1 q^2 J_0(qr). \tag{7}$$

Consider the electron in the nanowire is confined in radial plane and free in axial direction. The electron and the modulated acoustic phonon interaction Hamiltonian in the free-standing cylindrical nanowire is then written as

$$H=\frac{p^2}{2m}+\sum_q \hbar\omega a_q^\dagger a_q+\sum_q (G_q a_q+G_q^* a_q^\dagger). \tag{8}$$

where $p^2/2m$ denotes the kinetic energy of the electron. The acoustic phonon contribution is given by $\sum_q \hbar\omega a_q^\dagger a_q$.

3. Variational treatment

Now we start from the Hamiltonian of (8) to calculate the ground-state energy of the acoustic polaron in cylindrical nanowires, by using a Huybrechts-like variational approach [27]

Carry out a unitary transformation firstly

$$U_1=\exp\left(-ia\sum_q \vec{q}\cdot\vec{z}a_q^\dagger a_q\right) \tag{9}$$

where *a* is a variational parameter , which will take the value of 0 in the strong coupling limit and 1 in the weak coupling case. Doing so, the Hamiltonian turns into

$$H_1=\frac{1}{2m}\left(\vec{p}-a\sum_q \hbar q a_q^\dagger a_q\right)^2+\sum_q \hbar\omega a_q^\dagger a_q.$$
$$+\sum_q\left[G_q a_q\exp\left(i(1-a)\vec{q}\cdot\vec{z}\right)+h.c.\right] \tag{10}$$

Then introducing the linear combination operators of the position and momentum of the electron by the following relations

$$p_z=\left(\frac{m\hbar\lambda}{2}\right)^{1/2}\left(b_z^\dagger+b_z\right) \tag{11a}$$

and

$$z=i\left(\frac{\hbar}{2m\lambda}\right)^{1/2}\left(b_z-b_z^\dagger\right) \tag{11b}$$

where $b_z^\dagger$ and b_z present creation and annihilation operator, respectively. λ is another variational parameter.

Inserting (11a) and (11b) into (10) and performing the second unitary transformation

$$U_2=\exp\sum_q\left(f_q a_q^\dagger-f_q^* a_q\right), \tag{12}$$

the Hamiltonian finally becomes as the following form

$$H_2=\frac{\hbar\lambda}{2}\left(b_z^\dagger b_z+1\right)+\sum_q\left(\hbar\omega_q+a^2\frac{\hbar^2q^2}{2m}\right)$$
$$\left(a_q^\dagger a_q+f_q^* a_q+f_q a_q^\dagger+|f_q|^2\right)$$
$$+\sum_q\left\{\left(G_q^* a_q^\dagger+G_q^* f_q^*\right)\exp\left[-\frac{\hbar(1-a)^2q^2}{4m\lambda}\right]\right.$$
$$\exp\left[-(1-a)\left(\frac{\hbar}{2m\lambda}\right)^{1/2}q_z b_z^\dagger\right]$$
$$\left.\cdot\exp\left[(1-a)\left(\frac{\hbar}{2m\lambda}\right)^{1/2}q_z b_z\right]+h.c.\right\}$$
$$+\frac{a^2}{2m}\left(\sum_q \hbar q|f_q|^2\right)^2-2a\sum_{qz}\frac{\hbar q_z P_z}{2m}|f_q|^2. \tag{13}$$

The multi-phonon processes contribute less to the polaronic energy in above, which have been omitted.

The displacement amplitude in the second unitary transformation is determined as

$$f_q = -\frac{G_q^* \exp\left[-\hbar(1-a)^2 q^2 / 4m\lambda\right]}{\hbar\omega + a^2\hbar^2 q^2 / 2m} \qquad (14)$$

by the condition of diagonalization of the vital important part of H_2.

The ground-state energy can be calculated by averaging Hamiltonian of Eq.(13) on the zero-phonon state $|0\rangle$ of acoustic polaron, for which one have

$$b_z|0\rangle = a_q|0\rangle = 0.$$

By using the standard treatments, the variational energy of the polaronic ground-state can be obtained as following

$$E_0 = \frac{\lambda}{4}(1-a)^2$$

$$-16\alpha\int_0^R\int_0^{q_0} q^2 J_0^2(qr)\frac{\exp\left[-(1-a)^2 q^2 / 2\lambda\right]}{\pi r J_1^2(qr)\left(1+a^2 q/2\right)}dqdr \qquad (15)$$

The α in above equation is e-p coupling constant and given by

$$\alpha = \frac{D^2 m^2}{8\pi\rho\hbar^3 c}. \qquad (16)$$

Here ρ is the mass density of the crystal.

4. Numerical results and discussions

The theoretical computations for the ground-state energy of the acoustic polaron, as functions of α for three cutoff wave-vector q_0 of 40, 60 and 80, in free-standing cylindrical nanowires with the radius R of 0.4 and 0.6, are numerically performed by using Eq.(15). To compare with the earlier results, we have also expressed the energy in units of mc^2 and the phonon vector in units of $mc/\hbar$ in the calculations.

As be seen in Fig. 1(a) (q_0 = 40) a knee in the ground state energy curve with respect to α at $\alpha_c \approx 0.00052$, which is called the "phase transition" critical point, where the polaron state transforms from the quasi-free to the self-trapped [3,4,10,11,14]. In terms of q_0 = 60 and 80, one can find the critical points are at $\alpha_c \approx 0.0004$ and 0.0003 in Fig. 1(b) and (c). The critical points can be found more clearly in the derivatives of the acoustic polaron for their discontinuous behaviors. It is obviously that the critical point α_c shifts toward the weaker e-p coupling with increasing the cutoff wave-vector q_0. The character of the critical coupling constant varying with the cutoff wave-vector q_0 is corresponding to the previous papers [10,14]. Fig. 2 exhibits the results of ground-state energies and derivatives of the acoustic polarons in cylindrical nanowire for R = 0.6. One can find in Fig. 2 that the critical coupling constants are around 0.00105, 0.00072 and 0.00054, for q_0 = 40, 60 and 80, respectively. It is also found that the position of the critical point is sensitive to the cutoff wave-vector q_0 and shifts 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 q_0 is consistent with the previous studies [10,14].

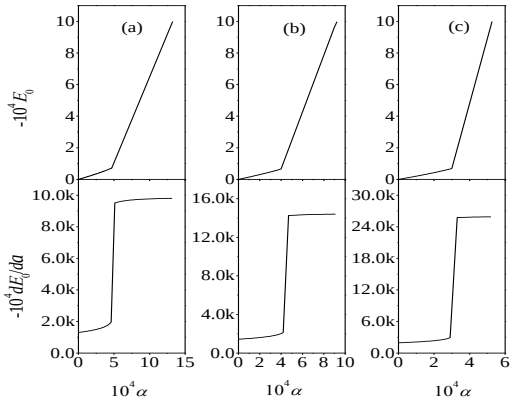

Fig. 1. Ground-state energies and their derivatives of the acoustic polarons in cylindrical nanowire with the radius R = 0.4, as functions of the e-p coupling constant α for (a) q_0= 40, (b) q_0= 60 and (c) q_0= 80, respectively.

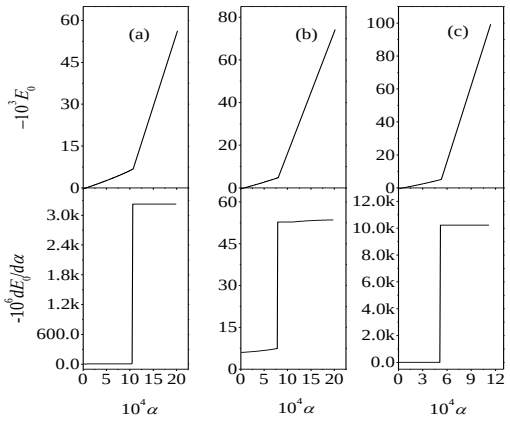

Fig. 2. Ground-state energies and their derivatives of the acoustic polarons in cylindrical nanowire with the radius R = 0.6, as functions of the e-p coupling constant α for (a) q_0= 40, (b) q_0 = 60 and (c) q_0 = 80, respectively.

As be seen in the above figures the critical values of the e-p coupling constant increase with the increasing radius of the cylindrical nanowire. For example, when the cutoff wave-vector q_0 equals to 40, the critical coupling constant, α_c, is around 0.00052 for the radius is 0.4 (Fig. 1), whereas $\alpha_c \approx 0.00105$, when the radius is 0.6 (Fig. 2). Which we thought the e-p coupling strength weakened with the increasing radius of cylindrical nanowire.

Additionally, we also checked the products of α_c by q_0 of the acoustic polarons in cylindrical nanowires with different radius. The $\alpha_c q_0$ had been used as a criterion for the self-trapping transition qualitatively. It is obviously that the $\alpha_c q_0$ for different values of cutoff wave-vectors

almost tend to a given value of 0.024, when the radius of the cylindrical nanowire is 0.4. Similarly result had also been obtained in the cylindrical nanowires with radius of 0.6. Where the products of $\alpha_c q_0$ are all close to 0.04. Therefore, $\alpha_c q_0$ can also be used as a qualitative criterion for the presence of the self-trapping transition of the acoustic polaron in cylindrical nanowires. Acoustic polaron in cylindrical nanowire systems can be self-trapped if αq_0 (determined by the material parameters) is larger than the $\alpha_c q_0$ [14].

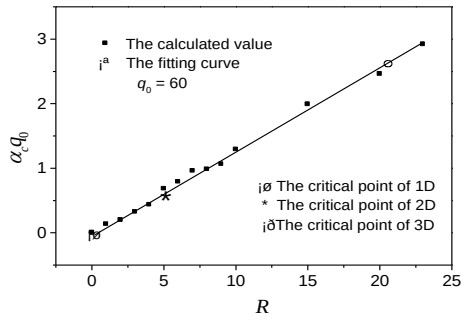

Fig. 3. The products of α_c by q_0 of the acoustic polarons as the function of R in cylindrical nanowires.

Now we use the criterion of the $\alpha_c q_0$ to judge the possibility of self-trapping transition for the acoustic polaron in real cylindrical nanowire materials. First we consider the semiconductors of GaN and AlN. In our previous work, it was indicated that the self-trapping transition of the acoustic polaron is impossible to occur for these two materials in 3D case and for GaN in 2D case [25]. In present work, the two values of αq_0 (0.24 and 0.57 for GaN and AlN, respectively) are all larger than the $\alpha_c q_0$, so that the acoustic poalrons in free-standing cylindrical nanowire of these two semiconductor materials can be self-trapped.

Fig. 3 exhibits the relation of $\alpha_c q_0$ and the cylindrical nanowire radius owing to the e-p coupling strength varies with it's confined dgree. One can find the criterion ($\alpha_c q_0$) for the self-trapping transition of the acoustic polaron will reach to 0.6 (self-trapping criterion of the 2D acoustic polaron in Ref. 27) in case of cylindrical nanowire with a radius of 5.2. The e-p coupling weakend with the decreasing confined degree is verified again. The increasing $\alpha_c q_0$ will reach the self-trapping criterion of 3D acoustic polaron, i.e. 2.6 [25], when the radius of the wire increases to 20.6. Where the confined effect has vanished. It can be taken as a result that the 20.6 times of $\hbar/mc$ (has an order of 100 Å in this paper) is greatly exceeding the general radius size of nanowires.

5. Conclusion

Considering the trapped electron influences luminescence properties of photoelectric material. The self-trapping transition of acoustic polaron in free-standing cylindrical nanowires was reconsidered by using a new Hamiltonian of deformation potential interaction between the electron and the modulated acoustic phonon. It can be concluded that the electrons and holes in both GaN and AlN cylindrical nanowires with a general radius are expected to have the self-trapping transition.

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