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A bound polaron in a spherical quantum dot

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Abstract. The binding energy of a bound polaron in a spherical quantum dot has been investigated by using the variational method. The influence of LO and SO phonons have taken into consideration. Result shows that the phonon contribution to the binding energy is dependent on the size of the quantum dot as well as the position of the impurity in the quantum dot. Numerical calculation on the ZnSe quantum dot shows that such contribution is about 5% to 20% of the total binding energy.

PACS. 71.38.+i Polarons and electron-phonon interactions – 73.20.Dx Electron states in low-dimensional structures – 71.55.Gs II-VI semiconductors

1 Introduction

In recent years, there has been great interest in investigating quantum dots (QD) both theoretically and experimentally. Due to the small structures of QD's, some physical properties such as optical and electron transport characteristics are quite different from those of the bulk materials [1,2]. The study of the impurity states in these low dimensional structures is an important aspect to which many theoretical and experimental works based. Recent investigations in the binding energy of a hydrogen-like impurity within the reduced dimensionality shows that the impurity binding energy will be enhanced with the deduction of the dimensionality [3–5].

Recently, Porras-Montenegro *et al.* [6] and Zhu *et al.* [7] made their investigation into the binding energy of the hydrogen-like impurity in a spherical QD. As expected, they found that the strong electronic confinement leads to a much higher impurity binding energy. Zhu *et al.* gave the impurity binding energy for different excited states and have considered their changes as the impurity shifts away from the center of the QD. However, in their investigation, the influence of the optical phonon on the hydrogen-like impurity binding energy is not considered. It has been showed that the electron-phonon interaction is an important factor influencing the physical properties of polar materials [8,9], and such influence could be enhanced as the confinement of electron gets stronger [10].

In the present paper, we will make a research into the hydrogen-like impurity binding energy in a spherical QD considering the influence of the longitudinal optical (LO) phonons as well as the surface optical (SO) phonons.

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2 Theory

2.1 Impurity located at the center

We consider a semiconductor sphere of radius R embedded in the surrounding medium of dielectric constant ε_d. The hydrogen-like impurity is located in $\mathbf{r}_0$ (taking the sphere center as the origin). Under the effective mass approximation, the Hamiltonian of the system can be written as [11]:

$$H = H_e + H_{ph} + H_{e-ph} \tag{1}$$

where

$$H_e = \frac{p^2}{2m} - \frac{e^2}{\varepsilon_0 |\mathbf{r} - \mathbf{r}_0|} + V(r) \tag{2}$$

with

$$V(r) = \begin{cases} \infty & r \geq R \\ 0 & r < R \end{cases}$$

is the electron Hamiltonian, and

$$H_{ph} = \sum_{l,m,k} \hbar\omega_{LO} a^{\dagger}_{lm}(k)\, a_{lm}(k) + \sum_{l,m} \hbar\omega_l b^{\dagger}_{lm} b_{lm} \tag{3}$$

is the phonon Hamiltonian, the first term is that of the longitudinal optical (LO) phonons and the second term is that of the surface optical (SO) phonons, where

$$\omega_l = \omega_{TO} \sqrt{\frac{\left(\varepsilon_0 + \dfrac{l+1}{l}\varepsilon_d\right)}{\left(\varepsilon_\infty + \dfrac{l+1}{l}\varepsilon_d\right)}} \tag{4}$$

$$N^2 = \frac{\lambda\left(k_{10}^2+\lambda^2\right)}{\pi\left\{k_{10}^2+\left[-k_{10}^2-\lambda^2+\lambda^2\cos\left(2k_{10}R\right)-k_{10}\lambda\sin\left(2k_{10}R\right)\right]e^{-2\lambda R}\right\}} \tag{11}$$

and

$$H_{e-ph} = \sum_{l,m,k} \Gamma_{lm}(k)\left[a_{lm}(k)\, j_l(kr)\, Y_{lm}(\theta,\varphi) + \text{H.c.}\right] + \sum_{l,m} \Gamma_{lm}^{s}\left[b_{lm}\left(\frac{r}{R}\right)^{l} Y_{lm}(\theta,\varphi) + \text{H.c.}\right] \tag{5}$$

is the interaction Hamiltonian between the electron and the LO and SO phonons respectively with

$$\Gamma_{lm}(k) = -\left[\frac{2\pi\hbar\omega_{LO}e^2}{R^3k^2j_{l+1}^2(kR)}\right]^{1/2}\left[\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right]^{1/2} \tag{6}$$

and

$$\Gamma_{lm}^{s} = -\frac{\sqrt{l}\varepsilon_\infty}{l\varepsilon_\infty+(l+1)\varepsilon_d}\hbar\omega_{LO}e \times\left[\frac{2\pi}{\hbar\omega_l R}\right]^{1/2}\left[\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right]^{1/2} \tag{7}$$

where $j_l(x)$ is the spherical Bessel function of order l and the $Y_{lm}(\theta,\varphi)$ is the spherical harmonic. The k's are so chosen that for each l, m

$$j_l(kR) = 0$$

so

$$k = \alpha_{n,l}/R,$$

where $\alpha_{n,l}$ is the nth zero of the spherical Bessel function of order l.

The trial wave function of the system is described by the coherent state:

$$|\Psi\rangle = \phi(r)\, U\,|0\rangle \tag{8}$$

where $|0\rangle$ is the vacuum state, and the unitary displacement transformation operator is given by

$$U = \exp\left\{\sum_{l,m,k}\left[a_{lm}(k)f_{lm}(k) + a_{lm}^{\dagger}(k)\, f_{lm}^{*}(k)\right] + \sum_{l,m}\left[b_{lm}f_{lm}^{s} + b_{lm}^{\dagger}f_{lm}^{s*}\right]\right\} \tag{9}$$

where $f_{lm}(k)$ and f_{lm}^{s} are the variational functions.

The electron trial wave function is chosen as ($\mathbf{r}_0 = 0$):

$$\phi(r) = \begin{cases} N\dfrac{\sin(k_{10}r)}{r}e^{-\lambda r} & r \le R \\ 0 & r > R \end{cases} \tag{10}$$

where λ is the variational parameter. For the ground state $k_{10} = \pi/R$ and the normalization Constance is defined in equation (11).

See equation (11) above.

λ is so chosen that the expectation value of the Hamiltonian of the system under the state$|\Psi\rangle$ reaches its minimum, *i.e.*

$$\delta E = \delta\left[\langle\Psi|\, H\,|\Psi\rangle\right] = 0 \tag{12}$$

so we obtained:

$$\begin{aligned} E = {} & \frac{\hbar^2}{2m}\left(\lambda^2+k_{10}^2\right) - \frac{4\pi e^2N^2}{\varepsilon_0}\int_0^R \frac{\sin^2(k_{10}r)}{r}e^{-2\lambda r}dr + \sum_{l,m,k}\hbar\omega_{LO}\left|f_{lm}(k)\right|^2 \\ & + \sum_{l,m,k}\Big[\Gamma_{lm}(k)\, f_{lm}(k)\,\langle\phi(r)|\, j_l(kr)\, Y_{lm}(\theta,\varphi)\,|\phi(r)\rangle \\ & + \text{H.c.}\Big] + \sum_{l,m}\hbar\omega_l\left|\mathrm{f}_{lm}^{s}\right|^2 \\ & + \sum_{l,m}\left[\Gamma_{lm}^{s}f_{lm}^{s}\,\langle\phi(r)|\left(\frac{r}{R}\right)^{l} Y_{lm}(\theta,\varphi)\,|\phi(r)\rangle + \text{H.c.}\right]. \end{aligned} \tag{13}$$

Minimizing E with respect to f_{lm}^{*} and f_{lm}^{s*} respectively leads to

$$f_{lm}(k) = -\frac{1}{\hbar\omega_{LO}}\Gamma_{lm}^{*}(k)\,\langle\phi(r)|\, j_l(kr)\, Y_{lm}^{*}(\theta,\varphi)\,|\phi(r)\rangle \tag{14}$$

and

$$f_{lm}^{s}(k) = -\frac{1}{\hbar\omega_l}\Gamma_{lm}^{s*}\,\langle\phi(r)|\left(\frac{r}{R}\right)^{l} Y_{lm}^{*}(\theta,\varphi)\,|\phi(r)\rangle\,. \tag{15}$$

At the end, we have

$$\begin{aligned} E = {} & \frac{\hbar^2}{2m}\left(\lambda^2+k_{10}^2\right) - \frac{4\pi e^2N^2}{\varepsilon_0}\int_0^R\frac{\sin^2(k_{10}r)}{r}e^{-2\lambda r}dr \\ & - \sum_{l,m,k}\frac{e^2}{\hbar\omega_{LO}}\left|\Gamma_{lm}(k)\right|^2\left|\langle\phi(r)|\, j_l(kr)\, Y_{lm}(\theta,\varphi)\,|\phi(r)\rangle\right|^2 \\ & - \sum_{l,m,k}\frac{e^2}{\hbar\omega_l}\left|\Gamma_{lm}^{s}\right|^2\left|\langle\phi(r)|\left(\frac{r}{R}\right)^{l} Y_{lm}(\theta,\varphi)\,|\phi(r)\rangle\right|^2. \end{aligned} \tag{16}$$

The bound polaron energy can be obtained from equation (17) by minimizing E according to λ. The binding energy of the bound polaron is defined at the ground-state energy of the system without the impurity present minus the impurity ground-statee energy of the system with phonon contribution [6], that is

$$E_b = \frac{\hbar^2k_{10}^2}{2m} - E. \tag{17}$$

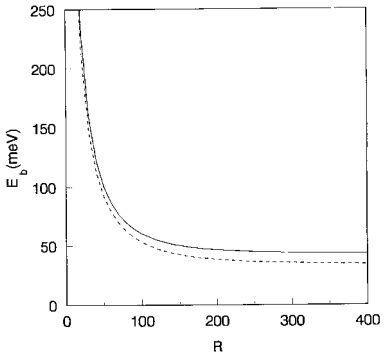

Fig. 1. The bound polaron binding energy E_b as a function of the radius of the QD R in Å. The solid line is the total binding energy with the contribution of phonons. The dash line is that without phonon contribution.

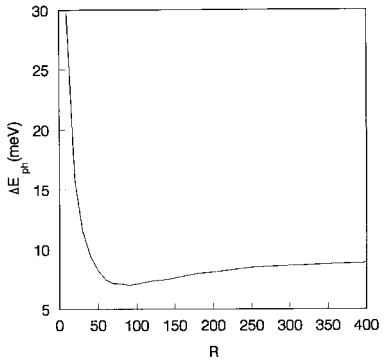

Fig. 2. The phonon contribution to the bound polaron binding energy ΔE_{ph} as a function of R. A minimum value for ΔE_{ph} can be observed at $R \approx 90$ Å.

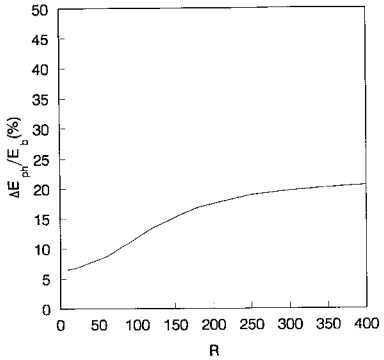

Fig. 3. The percentage of phonon contribution to the binding energy as a function of R. It increases steadily and finally comes to a certain value of around 20%.

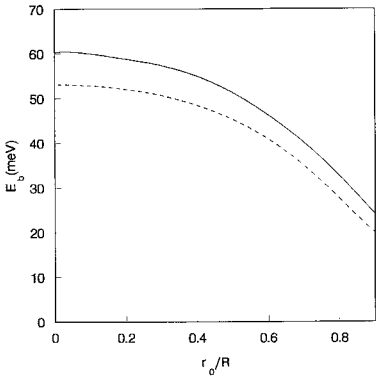

Fig. 4. The binding energy as a function of the impurity position in the QD with the radius $R = 100$ Å. The solid line is the total binding energy with the contribution of the phonons. The dash line is that without phonon contribution.

Numerical calculations are being carried out on ZnSe. The material parameters are [12,13]: $\varepsilon_0 = 8.33$, $\varepsilon_\infty = 5.9$, $m = 0.171m_0$ (m_0 is the free electron mass), $\varepsilon_d = 2.25$, $\hbar\omega_{LO} = 30.49$ meV, $\hbar\omega_{TO} = 25.65$ meV. We have calculated the impurity binding energy as a function of the radius of the QD. From Figure 1 we can observe that the bound polaron binding energy decays quickly as the radius of the QD R increases and the phonetic influence is quite important a factor influencing the binding energy, especially for larger R. This does not mean that for smaller R, under which the phonon confinement is stronger, the phonon contribution to the binding energy is smaller. In fact, the quantity of such contribution is quite large (Fig. 2). But the Coulomb impurity binding energy is so large that the percentage of the phonon contribution is relatively small (Fig. 3). Theoretical calculation shows that SO phonon does not couple with the electron wave function in a spherical QD with the impurity located at the center because the electron wave function is r dependent only. Figure 2 shows that the quantity of phonon contribution decays quickly as R increases and then comes to a minimum value when R is around 90 Å. After that, it increases monotonously and slowly as R increases. And finally comes to a certain quantity at around 20% of E_b (Fig. 3).

We have also calculated the bound polaron binding energy for GaAs QD, in which the phonon-electron coupling is rather weak. Result shows that the percentage of phonon contribution to the binding energy is quite small (at around 3 to 5%).

2.2 An off-center impurity

We now consider the case when the impurity is no longer located at the center of the QD ($r_0 \neq 0$). We revised the electron trial wave function as:

$$\phi(r) = \begin{cases} N\dfrac{\sin(k_{10}r)}{r}e^{-\lambda r'} & r \leq R \\ 0 & r > R \end{cases} \tag{18}$$

where $r' = |\mathbf{r} - \mathbf{r}_0| = \sqrt{r^2 + r_0^2 - 2rr_0\cos\theta}$, r_0 is the coordinate of the impurity in the z-axis while θ is the angle between r and z-axis. Now N, which is the normalization constant, is defined as:

$$2\pi N^2 \int_0^R \int_0^\pi \sin^2(k_{10}r)\, e^{-2\lambda r'} \sin\theta dr d\theta = 1. \tag{19}$$

The phonon terms remains unchanged but $\phi(r)$ dose not mean the same. And equation (16) now takes the form

$$E = -\frac{\hbar^2}{2m} 2\pi N^2 \int_0^R \int_0^\pi \left\{ \begin{array}{l} -2k_{10}\lambda r^2 r'^2 \cos(k_{10}r) + 2k_{10}\lambda r r_0 r'^2 \cos(k_{10}r)\cos\theta \\ + \left[\lambda r^3 + \lambda r r_0^2 - \lambda r r'^2 - \left(k_{10}^2 - \lambda^2\right) r r'^3\right] \sin(k_{10}r) \\ -\lambda\left(r^3 - r r'^2\right) \sin(k_{10}r)\cos\theta \end{array} \right\}$$
$$\times \frac{\sin(k_{10}r)}{r'^3} e^{-2\lambda r'} \sin\theta dr d\theta - \frac{2\pi e^2 N^2}{r'} e^{-2\lambda r'} \sin\theta dr d\theta$$
$$- \sum_{l,m,k} \frac{e^2}{\hbar\omega_{LO}} |\Gamma_{lm}(k)|^2 |\langle\phi(r)| j_l(kr) Y_{lm}(\theta,\varphi) |\phi(r)\rangle|^2 - \sum_{l,m} \frac{e^2}{\hbar\omega_l} |\Gamma^s_{lm}|^2 \left|\langle\phi(r)| \left(\frac{r}{R}\right)^l Y_{lm}(\theta,\varphi) |\phi(r)\rangle\right|^2 \quad (20)$$

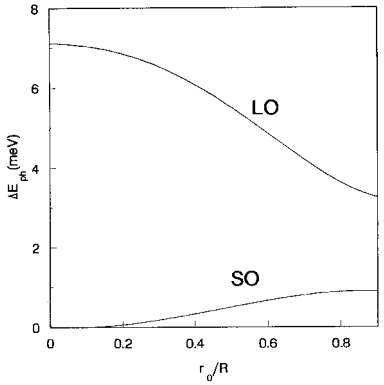

Fig. 5. The phonon contribution to the bound polaron binding energy ΔE_{ph} as a function of the impurity position in a QD with the radius $R = 100$ Å. The contributions of the LO phonon and the SO phonon are separately plotted and marked.

of equation (20).

See equation (20) above.

Minimizing E according to λ obtains the energy level of the system, while the binding energy can be calculated by using equation (17).

Numerical calculation are being carried out on ZnSe QD with $R = 100$ Å. The binding energy is plotted as a function of the impurity position (r_0/R) in Figure 4. We can observe that the impurity binding energy (both with and without phonon influence) decays as the impurity moves away from the center of the sphere. The total quantity of the phonon contribution becomes relatively smaller as the impurity approaching the boundary of the sphere. A more detail figure for the phonon contribution to the binding energy is given in Figure 5, in which the contributions of LO phonon and SO phonon are plotted separately. We can see that the contribution of LO phonon decreases while that of SO phonon increases as the impurity shifts away from the center. However, the quantity of SO phonon's contribution to the binding energy is quite small and is a relatively unimportant role when we consider the binding energy of a Coulomb impurity in a spherical quantum well.

In conclusion, we have made a research into the binding energy of an bound polaron in a spherical quantum dot, taking both the LO phonon mode and the SO phonon mode into consideration. Results show that the contribution of LO phonon to the hydrogen-like impurity binding energy may be quite important, depends on the coupling strength between electron and phonon. Such contribution is also related to the impurity position as it shifts away from the center of the sphere. SO phonon does not couple with the electron wave function when the impurity is located at the center, and its contribution to the impurity binding energy increases gradually as the impurity shifts away from the center. So, it is quite necessary to consider the influence of LO phonon mode when we consider the electronic behavior in a QD. The influence of SO phonon mode may also be obvious when asymmetry factors exist in the structures.

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