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# Effect of electric field and temperature on the binding energy of bound polaron in an anisotropic quantum dot

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**Abstract.** The ratio between the confinement lengths in the *xy*-plane and the *z* direction plays an important role in determining the properties of anisotropic quantum dot. Within a variational approach of Pekar type, we investigated theoretically the effects of electric field and temperature on the ground-state binding energies of hydrogenic impurity polarons in KBr anisotropic quantum dot. The obtained results illustrate that the binding energies increase with the electric field strength and temperature but decrease with the position of the impurity when considering different confinement lengths in the *xy*-plane and the *z* direction and present the properties of the anisotropic quantum dot.

**Keywords.** Bound polaron; electric field; temperature; quantum dot.

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## 1. Introduction

With the development of the technology of material growth in recent years, local electronic problems related to the structure of quantum dots (QDs), superlattices, heterojunctions, etc. have drawn much attention. More and more theoretical and experimental investigations focus on the local electronic systems in the external field. In addition, the influence of phonons on the local electrons has attracted increasing attention [1,2]. Kandemir and Cetin [3] have studied the ground- and first-excited state binding energies (BEs) of hydrogenic impurity magnetopolaron in a three-dimensional anisotropic QD using the variational method. Vartanian *et al* [4] have investigated the influence of electric field on the ground-state energy of hydrogenic impurity bound polaron in a cylindrical QD. The effect of electric field on the hydrogenic impurity bound polaron in a quantum well has been discussed by Chen *et al* [5] and his collaborators [6]. Considering the effects of impurities, Karabulut and Baskoutas [7] have calculated the electronic energy levels in a spherical QD subjected to an external electric field. Xiao *et al* investigated the influence of hydrogenic impurity and temperature on the coherence time of parabolic QD qubit [8]. Recently, Fotue *et al* [9] have studied the effects of temperature and electric field on the binding polaron energy level in a triangular QD. Wang *et al* [10] have calculated the influence of electric and magnetic fields on the ground-state energy of polaron confined in a cylindrical QD. However, to our knowledge, the influence of ambient temperature and electric field on the properties of polaron in anisotropic QDs is still an open question. It is well known that the magnitude of longitudinal and lateral confinement strength controls the shape of the anisotropic QDs. In the present work, we study the properties of ground-state energies of polarons in anisotropic QDs under various physical conditions, such as applied electric field, temperature, hydrogenic impurities etc. This paper is organised as follows. In §2, we derive expressions of the ground-state BE of hydrogenic impurity in terms of certain variation parameters using a variational theory of Pekar type. In §3, the numerical results of the ground-state BE in anisotropic QDs vs. the applied electric field, temperature and impurity position are presented and discussed. Finally, we give a brief conclusion in §4.

## 2. Theoretical model

An electron bounded to a hydrogenic impurity is considered to interact with the bulk longitudinal–optical (LO) phonons and is confined by a three-dimensional anisotropic harmonic potential. A uniform external electric field $\vec{F}$ is applied along the $z$ direction. The Hamiltonian of the system is given by the following equation:

$$H = H_e + H_{ph} + H_{e-ph}. \quad (1)$$

The first term $H_e$ is the electronic Hamiltonian:

$$H_e = -\frac{\hbar^2}{2m^*}\nabla^2 + \frac{1}{2}m^*\omega_\rho^2\rho^2 + \frac{1}{2}m^*\omega_z^2 z^2 - \frac{e^2}{\epsilon_0\sqrt{\rho^2 + (z - z_i)^2}} - eFz, \quad (2)$$

where $\omega_\rho$ and $\omega_z$ are the frequencies of the confining parabolic potential in the $xy$-plane and the $z$ direction, respectively. $z_i$ is the impurity position along the $z$-axis.

The second term in eq. (1) represents the LO phonon Hamiltonian:

$$H_{ph} = \sum_{\mathbf{q}} \hbar\omega_{LO} b_{\mathbf{q}}^+ b_{\mathbf{q}}, \quad (3)$$

where $b_{\mathbf{q}}^+$ ($b_{\mathbf{q}}$) denotes the creation (annihilation) operator of the bulk LO phonon with wave vector $\mathbf{q}$. The third term in eq. (1) is the electron–phonon (E–P) interaction Hamiltonian, that is

$$H_{e-ph} = \sum_{\mathbf{q}} \left(V_q e^{(i\mathbf{q}_\rho\cdot\rho + i\mathbf{q}_z z)} b_{\mathbf{q}} + \text{h.c.}\right) \quad (4)$$

with

$$V_{\mathbf{q}} = i(\hbar\omega_{LO}/\mathbf{q})\left(\hbar/2m^*\omega_{LO}\right)^{1/4}(4\pi\alpha/V)^{1/2}. \quad (5)$$

The total wave function is given by

$$|\Psi\rangle = \phi(\rho, z)\, U\, |0\rangle_{ph} \quad (6)$$

where $\phi(\rho, z)$ represents the electronic wave function and $|0\rangle_{ph}$ is the phonon vacuum state. The transformation $U$ is written as

$$U = \exp\left[\sum_{\mathbf{q}}\left(f_{\mathbf{q}} b_{\mathbf{q}}^+ - f_{\mathbf{q}}^* b_{\mathbf{q}}\right)\right], \quad (7)$$

where $f_{\mathbf{q}}(f_{\mathbf{q}}^*)$ is the variational function.

The ground-state electronic trial wave function is chosen as

$$\phi(\rho, z) = (\lambda/\pi)^{1/2}(\mu/\pi)^{1/4} e^{-\lambda\rho^2/2} e^{-\mu(z-z_i)^2/2}, \quad (8)$$

where $\lambda$ and $\mu$ are the variational parameters.

After the trial wave function is selected, we can calculate the energy expectation of the E–P system. By carrying out the theoretical calculations, we found that the energy expectation is parameterised. Thus, the size relationship between $\lambda$ and $\mu$ will affect the expression of the energy expectation. Therefore, when $\mu \geq \lambda$, one can obtain the energy expectation in the following form:

$$E(\lambda, \mu) = \frac{\hbar^2}{2m^*}\left(\lambda + \frac{\mu}{2}\right) + \frac{1}{2}m^*\omega_\rho^2\frac{1}{\lambda} + \frac{1}{2}m^*\omega_z^2\left(z_i^2 + \frac{1}{2\mu}\right) - eFz_i - \left(\frac{r_0\hbar\omega_{LO}\alpha}{\sqrt{2}} + \frac{e^2}{\epsilon_0}\right)\frac{1}{\sqrt{\pi}} \times \sqrt{\frac{\lambda\mu}{\mu - \lambda}}\left(\pi - 2\cot^{-1}\sqrt{\frac{\mu}{\lambda} - 1}\right). \quad (9)$$

Under the condition $\mu < \lambda$, we get

$$E(\lambda, \mu) = \frac{\hbar^2}{2m^*}\left(\lambda + \frac{\mu}{2}\right) + \frac{1}{2}m^*\omega_\rho^2\frac{1}{\lambda} + \frac{1}{2}m^*\omega_z^2\left(z_i^2 + \frac{1}{2\mu}\right) - eFz_i - \left(\frac{r_0\hbar\omega_{LO}\alpha}{\sqrt{2}} + \frac{e^2}{\epsilon_0}\right)\frac{2}{\sqrt{\pi}} \times \sqrt{\frac{\lambda\mu}{\lambda - \mu}}\tanh^{-1}\sqrt{1 - \frac{\mu}{\lambda}}. \quad (10)$$

In eqs (9) and (10), $r_0 = [\hbar/2m^*\omega_{LO}]^{1/2}$ is the polaron radius. For the convenience of numerical analysis, we define the effective confinement length (in units of the polaron radius) of the anisotropic QD $l_\rho = [\hbar/m^*\omega_\rho]^{1/2}$ and $l_z = [\hbar/m^*\omega_z]^{1/2}$. According to the calculation, we find that the variational parameters $\lambda$ and $\mu$ are proportional to $\omega_\rho$ and $\omega_z$, respectively. Therefore, a discussion on the relationship between $\lambda$ and $\mu$ in eqs (9) and (10) is equivalent to the discussion on the variation of $\omega_\rho$ and $\omega_z$ which is significant to the investigation of the orientated characteristics in anisotropic QD.

The ground-state energy of the E–P system can be obtained by minimising $E(\lambda, \mu)$ with respect to $\lambda$, $\mu$ and $z_i$. Another important quantity is the BE of bound polaron. Following the definition in [11], the BE of the bound polaron is

$$E_b = \hbar\omega_\rho + \frac{1}{2}\hbar\omega_z - \frac{e^2F^2}{2m^*\omega_z^2} - E_0. \quad (11)$$

At a finite temperature, according to the quantum statistics, we have

$$\bar{N} = \left[e^{(\hbar\omega_{LO}/K_BT)} - 1\right]^{-1}. \quad (12)$$

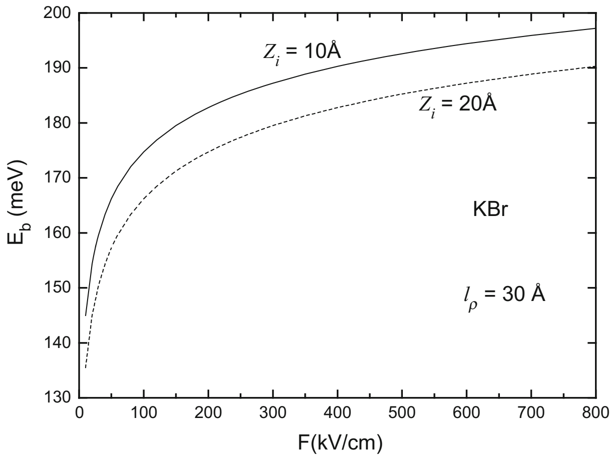


**Figure 1.** BE (in meV) of ground state $E_b$ in KBr anisotropic QD as a function of the electric field $F$ with two different $Z_i$ and $l_\rho = 30$ Å. The solid and dashed curves represent $Z_i = 10$ Å and 20 Å, respectively.

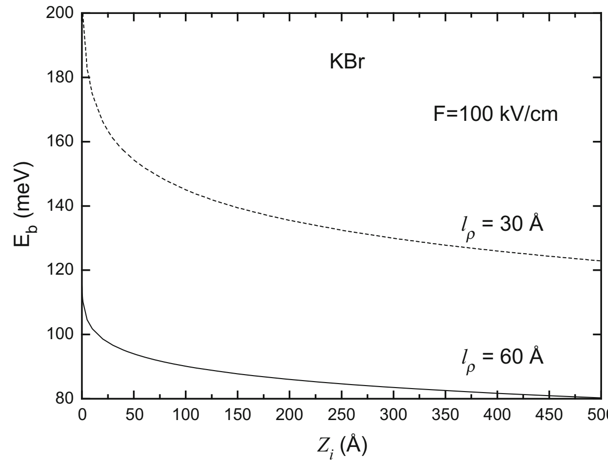


**Figure 2.** BE (in meV) of ground state $E_b$ in KBr anisotropic QD as a function of the impurity position along the $z$-axis $Z_i$ with two different $l_\rho$ and $F = 100$ kV/cm. The solid and dashed curves represent $l_\rho = 60$ Å and 30 Å, respectively.

## 3. Numerical results and discussion

We have carried out numerical calculation for a KBr semiconductor QD with a relatively high electron–phonon coupling ($\alpha = 3.05$) by using the following experimental parameters for KBr [12]: $m^* = 0.369m_0$, where $m_0$ is the free electron mass, $\epsilon_0 = 4.52$, $\epsilon_\infty = 2.39$ and $\hbar\omega_{LO} = 20.97$ meV.

The numerical results of the BE in KBr anisotropic QD for $l_\rho = 30$ Å vs. the electric field with different impurity positions ($z_i = 10$ Å and 20 Å) are shown in figure 1. As can be seen from this figure, the BE increases as the electric field strength increases for fixed confinement lengths in the $xy$-plane $l_\rho$ and impurity position $z_i$. It can be understood physically that the effect of a uniform external electric field is equivalent to changing the wave function $\phi(\rho, z)$ to $\phi(\rho, z - z_i)$. $z_i = eF/m^*\omega_z^2$ is the position of the new equilibrium point of the harmonic oscillator. Thus, for fixed $l_\rho$ and $z_i$, the increase in the electric field strength $F$ leads to an increase in $\omega_z$ and a decrease in $l_z$ simultaneously. Due to the confinement of the size of QD, an increasing BE is shown in figure 1.

In figure 2 the BE of the impurity in an anisotropic QD for two confinement lengths in the $xy$-plane ($l_\rho = 30$ Å, $l_\rho = 60$ Å) is shown as a function of the impurity position along the $z$-axis when the electric field with strength $F = 100$ kV/cm is applied. From this figure, we can find that the BE becomes extremely large when the impurity is at the centre of the QD. Under the influence of the electric field, the impurity with positive electricity deviates from the centre of the QD and therefore the BE reduces significantly at $z_i = 0{-}50$ Å, then falls gradually with an increase in $z_i$. This can be understood by the following physical philosophy. For a fixed electric field with strength $F$ and confinement lengths in the $xy$-plane $l_\rho$, the increase in $z_i$ brings a decrease of $\omega_z$, giving rise to an increase of $l_z$with respect to the expression $z_i = eF/m^*\omega_z^2$. Due to the effect of confinement of quantum size, the BE decreases as $z_i$ increases. At the same time, this figure shows that the BE becomes larger as $l_\rho$ decreases. This physical phenomenon is consistent with the result obtained by Mukhopadhyay and Chatterjee [13]. However, they neglected the $z$-direction restriction. Therefore, the influence of impurity location should be considered in the experimental work.

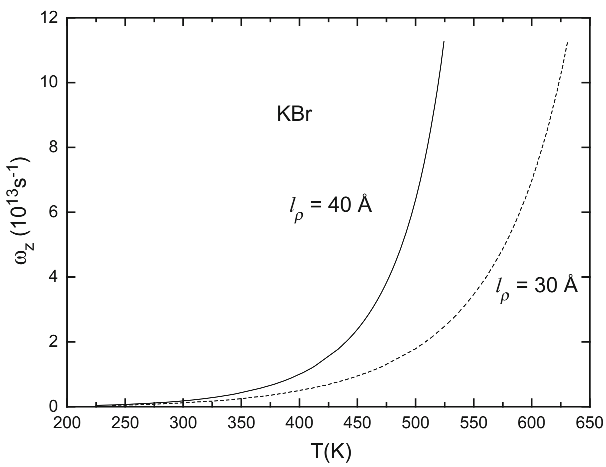


**Figure 3.** The frequencies of the confining parabolic potential in the $z$-direction $\omega_z$ in KBr anisotropic QD as a function of temperature $T$ with two different $l_\rho$. The solid and dashed curves represent $l_\rho = 40$ Å and 30 Å, respectively.

In figure 3, the frequencies of the confining parabolic potential in the $z$-direction $\omega_z$ obtained numerically are

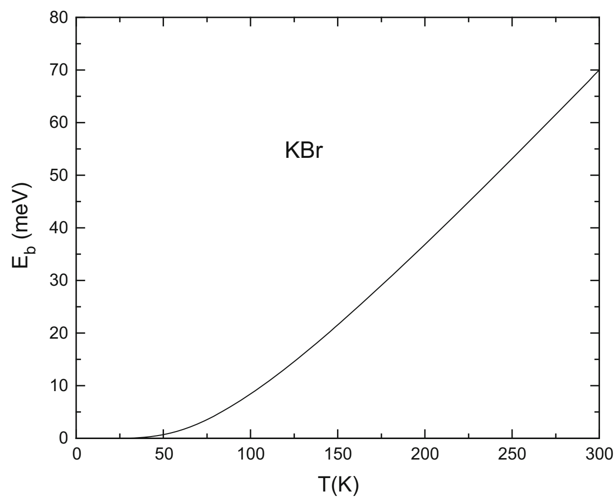


**Figure 4.** BE (in meV) of ground state $E_b$ in KBr anisotropic QD as a function of temperature $T$.

plotted with respect to the temperature $T$ for a fixed $l_\rho$ ($l_\rho = 30$ Å and 40 Å). On the one hand, one can easily observe that the frequency $\omega_z$ is almost zero at $T$ =200–300 K, then increases with increasing $T$. This variation pointed towards a relatively high electron–phonon coupling in KBr QD and few phonons are excited at low temperature. However, the effect of temperature is predominant beyond a certain temperature level. On the other hand, the frequency $\omega_z$ increases very rapidly with increasing $T$ at high temperature. Furthermore, at the same high temperature, the larger the confinement lengths in the $xy$-plane $l_\rho$, the higher the value of $\omega_z$.

Figure 4 illustrates the BE in KBr anisotropic QD against temperature $T$. From figure 4 we can see that the BE is an increasing function of $T$ for $T > 50$ K. As temperature rises, the speed and amount of electrons and phonons will increase, which results in an increase in BE.

## 4. Conclusion

We systematically studied the influence of electric field, temperature and impurity position on the BE of hydrogenic impurity polarons in anisotropic QD using the Pekar-type variational method. We derive the expression of the ground-state BE in two cases, i.e. $\mu \geq \lambda$ and $\mu < \lambda$. We have carried out numerical calculation for a KBr semiconductor QD. It has been demonstrated that the BE can be significantly reduced with impurities deviating from the centre of the QD. Moreover, the BE increases as the electric field strength increases for a QD with fixed size. The results also show that the BE is an increasing function of $T$ for $T > 50$ K. Theoretical calculations suggest that the position of impurity and the electric field strength should be considered in further theoretical or experimental work.

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