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The polaron effects and temperature dependence of the strong-coupling exciton in slab of polar crystals

Hong-Tao Yang*, Wen-Hui Ji, Huhemandula, and Wen-Tao Hu

Department of Physics, Inner Mongolia Jining Teacher's College, Wulanchabu 012000, China

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Abstract. The system, in which the excitons interact with both the weak-coupling bulk longitudinal-optical (LO) phonons and strong-coupling surface-optical (SO) phonons in a slab of polar crystal, is studied by using a linear combination operator and the Lee-Low-Pines variational method. The expression of the induced potential of the exciton is derived, and the numerical calculations for the AgBr crystal as an example are made. The results show that the induced potential of the exciton relates not only to the distance between electron and hole, but also to the thickness of slab and temperature.

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Key words: exciton, strong-coupling, induced potential

1 Introduction

The properties of the polar crystal slab, quantum well and superlattice and other low dimensional materials have aroused great interest [1-5] as the research object to the development of smaller size and dimension, and the materials to the multilayer film structure trend. In recent decades, many domestic and foreign researches on the low dimensional materials element excitation were carried out by many studies [6-12], especially the problems of exciton in a slab. In their study of the exciton in a slab, when the interaction of the exciton both with the surface-optical (SO) phonons and bulk longitudinal-optical (LO) phonons were considered, they mainly concentrated their attention on the weak and intermediate coupling case [13]. In fact, in some polar crystal, the coupling of the electrified particle with the surface or the interface optical phonons is strong, but weak with LO phonons [14]. Therefore, the research on the exciton system, in which the excitons interact with both the weak-coupling bulk LO-phonons and strong-coupling SO-phonons at finite temperature in a polar crystal slab, is more important.

*Corresponding author. *Email address:* `yanghongtao_2000@yahoo.com.cn` (H. -T. Yang)

2 Theoretical method

Consider a slab of polar crystal with thickness $2d$. In the effective-mass approximation, the Hamiltonian of the exciton-phonon system in the polar slab can be written as [15]

$$H = H_{ex} + H_{ph} + H_{e-LO} + H_{e-SO} + H_{h-LO} + H_{h-SO} \tag{1}$$

$$H_{ex} = H_e + H_h + H_{e-h} \tag{2}$$

$$H_e = \begin{cases} \frac{p_{ez}^2}{2m_e} + \frac{p_e^2}{2m_e}, & |z_e| \le d \\ \frac{p_{ez}^2}{2m_0} + \frac{p_e^2}{2m_0} + V_0, & |z_e| > d \end{cases} \tag{2a}$$

$$H_h = \begin{cases} \frac{p_{hz}^2}{2m_h} + \frac{p_h^2}{2m_h}, & |z_h| \le d \\ \frac{p_{hz}^2}{2m_0} + \frac{p_h^2}{2m_0} + V_0', & |z_h| > d \end{cases} \tag{2b}$$

$$H_{e-h} = -\frac{e^2}{\varepsilon_\infty |r_e - r_h|} \tag{2c}$$

$$H_{ph} = H_{LO} + H_{SO} \tag{3}$$

$$H_{LO} = \sum_{k,m,p} a_{k,m,p}^+ a_{k,m,p} \hbar\omega_{LO} \tag{3a}$$

$$H_{SO} = \sum_{q,p} b_{q,p}^+ b_{q,p} \hbar\omega_{SO} \tag{3b}$$

$$H_{e-SO} = \sum_q \left(\frac{\sin(2qd)}{q}\right)^{\frac{1}{2}} e^{-qd} \left[C^* e^{-iq\cdot p_e} [G_+(q,z_e) b_{q,+}^+ + G_-(q,z_e) b_{q,-}^+] + H.c.\right] \tag{4}$$

$$H_{h-SO} = -\sum_q \left(\frac{\sin(2qd)}{q}\right)^{\frac{1}{2}} e^{-qd} \left[C^* e^{-iq\cdot p_h} [G_+(q,z_h) b_{q,+}^+ + G_-(q,z_h) b_{q,-}^+] + H.c.\right] \tag{5}$$

$$H_{e-LO} = \sum_k \left[B^* e^{-ik\cdot p_e} \left[\sum_{m=1,3,5...} \frac{\cos(\frac{m\pi z_e}{2d})}{[k^2 + (\frac{m\pi}{2d})^2]^{\frac{1}{2}}} a_{k,m,p}^+ + \sum_{m=2,4,6...} \frac{\sin(\frac{m\pi z_e}{2d})}{[k^2 + (\frac{m\pi}{2d})^2]^{\frac{1}{2}}} a_{k,m,p}^+ \right] + H.c. \right] \tag{6}$$

$$H_{h-LO} = -\sum_k \left[B^* e^{-ik\cdot p_h} \left[\sum_{m=1,3,5...} \frac{\cos(\frac{m\pi z_h}{2d})}{[k^2 + (\frac{m\pi}{2d})^2]^{\frac{1}{2}}} a_{k,m,p}^+ + \sum_{m=2,4,6...} \frac{\sin(\frac{m\pi z_h}{2d})}{[k^2 + (\frac{m\pi}{2d})^2]^{\frac{1}{2}}} a_{k,m,p}^+ \right] + H.c. \right] \tag{7}$$

In calculation, we introduce the mass centre coordinate and relative coordinate of exciton, then we also introduce the Huybrechts linear combination operator for the mass center momentum and mass center coordinate. In order to simplify the calculation, we apply two unitary transformations to the Hamiltonian, finally we discuss the extremum of the