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强耦合表面激子内部激发态的性质

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摘要: 采用线性组合算符和幺正变换方法, 研究极性晶体中强耦合表面激子内部激发态的性质。计算了表面激子的激发态能量、激发能量和平均声子数。

关 键 词: 表面激子; 内部激发态; 平均声子数
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1 引 言

激子在晶体表面层中的性质对晶体性质的影响十分显著。最近十几年, 国内外对表面极化子和表面激子的研究十分活跃。许多学者从理论上采用许多方法研究了激子的性质[1]。Sumi 等[2]研究了通过短程势和声子相互作用的激子的自陷。用变分方法 Chen 等[3]计算了强束缚激子-声子系统的基态能量。我们[4]用微扰法讨论了电子在反冲效应中发射和吸收不同波矢的声子之间相互作用对激子的有效势, 自陷能和自陷条件的影响。Luban 等[5]用最近邻紧束缚近似计算了有效一维电子的最低束缚态能量, 得到了激子的结合能, 所得结果与实验和其他理论计算结果完全一致。郭等[6]利用密度矩阵算符理论研究激子效应对双曲型量子线中非线性光学吸收率的影响。Xie[7]用少体物理方法研究在量子点中的带负电激子的第二束缚态的性质。上述各种理论方法各有特性。

对激子性质的研究, 强耦合的情形研究得较少, 研究激子激发态能量和平均声子数的更少。最近本文作者[8]采用 Huybrechts 的线性组合算符方法研究了弱耦合表面磁极化子的内部激发态的性质。采用线性组合算符和幺正变换的方法研究极性晶体中强耦合表面激子的内部激发态性质, 计算了强耦合表面激子的激发态能量、激发能量和平均声子数。

2 哈密顿量

理论证明[9]在与表面的距离小于极化子半径的范围内, 可以把表面层看成一个纯粹的二维晶体, 在这个范围内, 晶体内部的体光学声子对带电粒子没有作用。因此, 表面层附近的电子只与表面光学声子相互作用, 极性晶体中表面激子-声子系的哈密顿量为

$$H = -\frac{\hbar^2}{2M}\nabla_R^2 - \frac{\hbar^2}{2}\nabla^2 - \frac{e^2}{\varepsilon^*} + \sum_q a_q^+ a_q \omega_s + \sum_q \left(\frac{C_q}{\sqrt{q}} a_q e^{iq\cdot R} + \text{h.c}\right) \tag{1a}$$

$$C_q = 2\pi ie\left(\frac{\hbar\omega_s}{4\pi A}\right) \tag{1b}$$

$$\frac{1}{\varepsilon^*} = \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0} \tag{1c}$$

$$q = e^{i\alpha_1 q} - e^{-i\alpha_2 q} \tag{1d}$$

$$\alpha_1 = \frac{m_e}{M}, \quad \alpha_2 = \frac{m_h}{M},$$

$$M = m_e + m_h, \quad \mu = \frac{m_e m_h}{m_e + m_h} \tag{1f}$$

诸式中各量的物理意义与文献[10]相同。

对表面激子的质心坐标 R 和质心动量 P 引进线性组合算符:

$$P_j = \left(\frac{M\omega_s}{2\hbar}\right)^{\frac{1}{2}} (b_j + b_j^+)$$
$$R_j = i\left(\frac{\hbar}{2M\omega_s}\right)^{\frac{1}{2}} (b_j - b_j^+) \qquad j = x, y \tag{2}$$

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其中　是变分参量, 将(2)式代入(1a)并同时作幺正变换

$$U = \exp\left[\sum_q (a_q^+ f_q - a_q f_q^*) \right] \tag{3a}$$

$$f_q = - \frac{C_q^* \ {}_q^* \exp\left(- \frac{q^2}{4M} \right)}{{}_S \sqrt{q}} \tag{3b}$$

其中$f_q(f_q^*)$是变分参量。强耦合表面激子–声子系的哈密顿量为

$$\begin{aligned}
\mathcal{H} &= U^{-1} H U \\
&= - \frac{{}^2}{2} \ {}^2 - \frac{e^2}{{}^*} + \frac{}{2} \left(\sum_j b_j^+ b_j + 1 \right) + \\
&\quad \frac{}{4} \sum_j (b_j b_j + b_j^+ b_j^+) + \\
&\quad \sum_q {}_S (a_q^+ + f_q^*) (a_q + f_q) + \\
&\quad \sum_q \left\{ \frac{C_q^*}{\sqrt{q}} \ {}_q^* (a_q^+ + f_q^*) \exp\left(- \frac{q^2}{4M} \right) \right. \\
&\quad \exp\left[- \left(\frac{}{2M} \right) \sum_j q_j b_j^+ \right] \\
&\quad \left. \exp\left[\left(\frac{}{2M} \right) \sum_j q_j b_j \right] + h \quad c \right\} - \\
&\quad \frac{{}^2}{2} \sum_{q \ q} (\quad f_q \quad f_q a_q^+ a_q^+ + \\
&\quad f_q^* \quad f_q^* a_q \ a_q) + \\
&\quad \frac{{}^2}{} \sum_q \quad f_q \quad f_q^* a_q^+ a_q + \\
&\quad \frac{{}^2}{2} \sum_q \ | \quad f_q |^2 - \\
&\quad \frac{{}^2}{2} \sum_q (a_q^+ \quad f_q - a_q \quad f_q^*) \quad - \\
&\quad \frac{{}^2}{2} \sum_q (a_q^+ \quad {}^2 f_q - a_q \quad {}^2 f_q^*)
\end{aligned} \tag{4}$$

令系统的基态波函数为

$$| \ {}_0 = | \ (\ ) \ | 0 \ {}_a | 0 \ {}_b ,$$

其中$| 0 \ {}_a$表示零声子态, $| 0 \ {}_b$表示 b 算符的真空态, 而 $b_j | 0 \ {}_b = a_q | 0 \ {}_a = 0$, $| \ (\ )$ 为描述表面激子内部运动的波函数。令$| \ {}_1 = | \ (\ ) \ | 0 \ {}_a | 1 \ {}_b$为表面激子的第一内部激发态, 且$| 1 \ {}_b = b_j^+ | 0 \ {}_b$, (4)式对$| \ {}_0$ 的久期值 $E_0(\ )$对　的变分极值给出表现激子的基态能量的上限。

$$E_0(\ ) = \quad {}_0 | \ \mathcal{H} | \ {}_0 = \quad (\ ) | \ F_0(\ ) | \ (\ ) \tag{5}$$

$$\begin{aligned}
F_0(\ ) &= \ {}_b 0 | \ {}_a 0 | \ \mathcal{H} | \ 0 \ {}_a | \ 0 \ {}_b \\
&= \frac{P^2}{2} - \frac{e^2}{{}^*} + \frac{1}{2} \quad - \\
&\quad \sum_q \frac{| \ C_q |^2 | \ {}_q |^2 \ {}^{-\frac{q^2}{2M}}}{{}_S q} + \\
&\quad \frac{{}^2}{2} \sum_q \frac{| \ C_q |^2 | \quad {}_q |^2 \ {}^{-\frac{q^2}{2M}}}{{}^2 \ {}_S^2 q}
\end{aligned} \tag{6}$$

将(6)式最后两项求和变积分, 经过计算可得

$$\begin{aligned}
F_0(\ ) &= \frac{P^2}{2} - \frac{e^2}{{}^*} + \frac{}{2} - \\
&\quad {}_S \ {}_S \left(\frac{}{{}_S} \right) \left[1 - \frac{2}{} (\ ) \right] + \\
&\quad \sqrt{} \ {}_S \ {}_S \left(\frac{}{{}_S} \right) \left[\frac{1}{2} + \frac{1}{} \left(1 + \frac{d}{} \right) \right. \\
&\quad \left. (\ ) \right]
\end{aligned} \tag{7a}$$

其中

$$(\ ) = \int_0^{\overline{2}} e^{ - \frac{}{4} u_s^2 \ {}^2 \cos^2 } d \tag{7b}$$

$$u_s = \left(\frac{2M \ {}_S}{} \right) \tag{7c}$$

$$= \frac{{}^2_1 + \quad {}^2_2}{2 \ {}_1 \ {}_2} \tag{7d}$$

对于 Wannier 激子 $u_s \quad 1$, $F_0(\ )$ 可以近似写成

$$F_0(\ ) = \frac{P^2}{2} - \frac{e^2}{{}^*} + \frac{1}{2} \quad - \quad {}_S \ {}_S \left(\frac{}{{}_S} \right) + \frac{\sqrt{}}{2} \ {}_S \ {}_S \left(\frac{}{{}_S} \right) \tag{8}$$

$F_0(\ )$对　的变分极值条件为$\frac{F_0(\ )}{} = 0$, 由此得

$$\frac{{}_S}{\sqrt{}_S} + \frac{2}{3} \sqrt{} - \frac{2}{3} \ {}_S \sqrt{}_S = 0 \tag{9a}$$

(9a) 式的解为

$$\sqrt{} = - \frac{\sqrt{}_S}{3 \sqrt{} \ {}_S} + \sqrt{\frac{2 \ {}_S}{3}} \left(1 + \frac{1}{6 \ {}^2_S} \right) \tag{9b}$$

对于强耦合$\frac{1}{6 \ {}^2_S} \quad 1$, 可以将(9b)式按小量展开

$$\sqrt{} = \sqrt{\frac{2 \ {}_S}{3}} \left(1 - \frac{1}{\sqrt{6} \ {}_S} + \frac{1}{12 \ {}^2_S} + \right) \tag{9c}$$

对于强耦合表面激子的第一内部激发态有

$$E_1(\ ) = \quad {}_1 | \ \mathcal{H} \quad {}_1 = \quad (\ ) | \ F_1(\ ) | \ (\ ) \tag{10a}$$

$$\begin{aligned}
F_1(\ ) &= \ {}_b 1 | \ {}_a 0 | \ \mathcal{H} | \ 0 \ {}_a | \ 1 \ {}_b = \\
&\quad \frac{P^2}{2} - \frac{e^2}{{}^*} + \frac{3}{2} \quad -
\end{aligned}$$

$$\frac{|C_q|^2|\ _q|^2}{{}_s q}e^{-\frac{q^2}{2M}}\left(1-\frac{q^2}{2M}\right)+\frac{2}{2}\ _q\frac{|C_q|^2|\ _q|^2}{{}^2_s q}e^{-\frac{q^2}{2M}} \quad (10b)$$

将(10b)式最后两项求和变积分, 经过计算可得

$$F_1(\ )=\frac{P^2}{2}-\frac{e^2}{*}+\frac{3}{2}\ -\ {}_s\ {}_s\left(\frac{}{{}_s}\right)\left[\frac{1}{2}-\frac{1}{}\left(3+\frac{d}{}\right)(\ )\right]+\sqrt{}\ {}_s\ {}_s\left(\frac{}{{}_s}\right)\left[\frac{1}{2}+\frac{1}{}\left(1+\frac{d}{d}\right)(\ )\right] \quad (10c)$$

强耦合表面激子第一内部激发态能量 $F_1(\ )$ 与表面激子的基态能量 $F_0(\ )$ 之差为

$$F(\ )=F_1(\ )-F_0(\ )=+\ {}_s\ {}_s\left(\frac{}{{}_s}\right)\left[\frac{1}{2}+\frac{1}{}(3+\frac{d}{d})(\ )\right] \quad (11)$$

表面激子的平均声子数为

$$\overline{N}=\ {}_b0|\ {}_a0|\ U^{-1}NU|\ 0\ {}_a|\ 0\ {}_b=\ {}_q|f_g|^2 \quad (12a)$$

将(3b)式代入变求和为积分可得

$$\overline{N}=\ {}_s\left(\frac{}{{}_s}\right)\ [1-\frac{2}{}(\ )] \quad (12b)$$

3 结果和讨论

由(7a)式可以看出, 其表达式很复杂, (7a)式对 变分, 无法精确求出变分参量 , 仅对于强耦合的 Wannier 激子, 才可以近似求出变分参量 的表达式(9c)。

对于 Wannier 激子, u_s 1, (10c)式, (11)式和(12b)式近似表示为

$$F_1(\ )=\frac{P^2}{2}-\frac{e^2}{*}+\frac{3}{2}\ -\frac{\sqrt{}}{2}\ {}_s\ {}_s\left(\frac{}{{}_s}\right)^{\ }+\frac{\sqrt{P}}{2}\mathrm{A}\ {}_{Xs}\left(\frac{K}{X_s}\right)^{\$}{}_B \quad (13)$$

$$\$F(K)=\ K+\frac{\sqrt{P}}{2}\mathrm{A}\ {}_{Xs}\left(\frac{K}{X_s}\right)^{\ } \quad (14)$$

$$\overline{N}=\ A_s\left(\frac{PK}{X_s}\right)^{\$} \quad (15)$$

将(9c)式代入(8)式, (13)式, (14)式和(15)式, 可得

$$H^0_{\mathrm{eff}}=\frac{P^2}{2\mathrm{L}}-\frac{e^2}{{}^*_{\mathrm{E}]\ Q}}-\frac{4}{3}\left(\frac{\mathrm{P}}{6\mathrm{B}}\right)^{\ }\mathrm{A}_s\ {}_{Xs}+\frac{X_s}{3\mathrm{B}}-\frac{X_s}{\sqrt{6\mathrm{PB}}3\mathrm{B}}\frac{1}{\mathrm{A}_s}+\ , \quad (16)$$

$$H^1_{\mathrm{eff}}=\frac{P^2}{2\mathrm{L}}-\frac{e^2}{{}^*_{\mathrm{E}]\ Q}}-\frac{1}{3}\left(\frac{\mathrm{P}}{6\mathrm{B}}\right)^{\ }\mathrm{A}_s\ {}_{Xs}+\frac{5\ X_s}{6\mathrm{B}}-\frac{19}{12}\frac{X_s}{\sqrt{6\mathrm{PBB}}}\frac{1}{\mathrm{A}_s}+\ , \quad (17)$$

$$\$H_{\mathrm{eff}}=\left(\frac{P}{6\mathrm{B}}\right)^{\ }\mathrm{A}_s\ {}_{Xs}+\frac{X_s}{2\mathrm{B}}-\frac{5}{4}\frac{X_s}{\sqrt{6\mathrm{PBB}}}\frac{1}{\mathrm{A}_s}+\ , \quad (18)$$

$$\overline{N}=\left(\frac{2\mathrm{P}}{3\mathrm{B}}\right)^{\ }\mathrm{A}_s-\frac{1}{3\mathrm{B}}+\frac{1}{\sqrt{6\mathrm{PB}}6\mathrm{B}}\frac{1}{\mathrm{A}_s}+\ , \quad (19)$$

分别为强耦合表面激子的基态的有效哈密顿量、强耦合表面激子的第一内部激发态的有效哈密顿量、表面激子的激发能量和表面激子的平均声子数。在(16)式和(17)式中第一项为表面激子内部运动的动能, 第二项为表面激子内部电子-空穴间的库仑势。第三项, 第四项和第五项是电子、空穴与表面光学声子相互作用引起的表面激子的自能, 强耦合表面激子的自能表示为耦合参量 A_s 的降幂级数, 其首项为 A_s 的一次项。

强耦合表面激子的激发能量 $\$H_{\mathrm{eff}}$ 和平均声子数 $\overline{N}$ 也表示为耦合参量 A_s 的降幂级数, 其首项为 A_s 的一次项。

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Properties of Internal Excited State of the Strong Coupling Surface Exciton

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Abstract: The properties of the exciton in the surface layer of crystals influence the properties of crystals very remarkably. In recent years, a lot of authors studied the surface polaron and the surface exciton. The properties of the exciton have been studied by many theoretical method by many investigators. Sumi *et al.* studied self-trapping of excitons (or electrons) interacting with phonons via short-range potential and found that the self-trapping depends strongly on the degree of lattice freedom. Chen *et al.* calculated the ground state energy of the strongly bound exciton-phonon system by using a concise variational approach. The influence of the interaction between phonons of different wave vectors in the recoil process on the effective potential between electron and hole, the self-trapping energy, and the self-trapping condition of the exciton in polar crystals has been discussed by using a perturbation method by present authors. Using the nearest-neighbor tight-binding approximation Luban *et al.* calculated the lowest bound-state energy of the effective 1D electron Hamiltonian and the exciton binding energy is obtained. The results for the exciton binding energy are in very good agreement both with experiment and the results of other theoretical calculations. Kasapoglu *et al.* calculated the binding energy of the exciton in the symmetric and asymmetric quantum wells by using a variational approach. The third-order nonlinear optical absorptions in hyperbolic quantum wires are studied by Guo *et al.*, with most emphasis devoted to the influence of excitons on the third-order nonlinear optical absorptions. The analytic form for the third-order nonlinear optical absorption coefficient of this system is derived by means of density matrix treatment. A variational calculation of the ground-state energy of neutral excitons and of positively and negatively charged excitons (trions) confined in a single-quantum well is presented by Riva *et al.* They studied the dependence of the correlation energy and of the binding energy on the well width and on the hole mass. By using the method of few-body physics, the binding energy spectra of the second bound state of a negatively charged exciton X in a GaAs quantum dot with a parabolic confinement have been calculated as a function of the electron-hole mass ratio and of the dot radius by Xie.

The properties of the exciton have been investigated by many methods. Many of these mainly concentrated attention on the weak-and intermediate-coupling cases and on the ground state energy. However, the exciton in strong-coupling polar crystals and the excited state energy of the exciton has not been studied so far. Recently we study the internal excited state of the weak-coupling surface magnetopolaron by means of Huybrechts. s linear combination op-

erator method. In this paper, the properties of internal excited state of the strong-coupling surface exciton in polar crystals are investigated by using the linear combination operator and the unitary transformation method and the excited state energy, the excitation energy and the mean number of phonon of the strong-coupling surface exciton are calculated. The results show that the self-energy of ground state and excited state, the excitation energy and the mean number of phonon of the strong-coupling surface exciton could be written as a series in A_s^{-1}, the first term being proportion to, the coupling constant A_s for Wannier surface exciton.

Key words: surface exciton; internal excited state; mean number of phonon

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