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Properties of the surface magnetopolaron in polar crystals

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Abstract. There is weak bulk but strong surface coupling between the electron and phonons for polar crystals in a magnetic field. In this paper, the influences of the electron interaction with both the weak-coupling bulk longitudinal optical phonons and the strong-coupling surface optical phonons on the properties of the surface polaron in a magnetic field are studied. The effective Hamiltonian of the surface polaron is derived by using a linear-combination operator method. Numerical calculations on the AgCl crystal, as an example, are performed, and some properties of the vibration frequency and the effective interaction potential of the surface polaron in a magnetic field are discussed.

1. Introduction

With the development of magneto-optical technology, the properties of the polaron in polar crystals in a magnetic field of arbitrary strength have been of considerable interest [1–4]. In the early 1960s, Larsen [5, 6] investigated the energy level of the polaron in magnetic field and the cyclotron-resonance problem of the piezopolaron. Then he [7] studied the cyclotron resonance of a two-dimensional (2D) polaron using the Rayleigh–Schrödinger perturbation theory (RSPT). Recently, he [8] proposed a novel fourth-order perturbation method to investigate the properties of 2D polarons. Special attention is focused on the cyclotron-resonance frequency and the cyclotron-resonance mass of an electron in 2D systems because they can be obtained from the position of certain peaks in the magneto-optical absorption spectrum. Wu *et al* [9] discussed the magneto-optical absorption of a 2D polaron in detail using the memory-function approach. Considering both the electron–bulk-longitudinal–optical (LO)-phonon and electron–surface-optical (SO)-phonon interactions, Gu and co-workers [10] have generalized this method to treat the magnetopolaron in a semiconductor quantum well. Later, Osorio *et al* [11] reported for the first time a theoretical calculation for the resonant donor-impurity magnetopolaron in GaAs–Ga_{1-x}Al_xAs quantum well structures. Employing Haga's perturbation method, Ze *et al* [12] derived an effective Hamiltonian for the interface magnetopolaron in polar crystals at zero temperature, in which the interactions of both bulk LO phonons and interface phonons have been taken into account. Wei and co-workers [13, 14] studied the induced potential and the self-energy of an interface magnetopolaron interacting with bulk LO phonons as well as interface-optical phonons using the Green-function method.

For the bulk polaron, the weak- and intermediate-coupling theories are applicable for the electron–bulk-LO-phonon coupling constant $\alpha < 6$ [15], whereas for the surface polaron this confinement is about 2.5 [16]. Hence, when the electron–SO-phonon coupling constant satisfied $\alpha > 2.5$, the strong-coupling theory must be applied. There is weak coupling between the electron and the bulk LO phonon but strong coupling between the electron and the SO phonon for many polar crystals. So far, research into this has been very scarce. The properties of the surface or interface polaron in corresponding polar crystals have been discussed by the method of a linear-combination operator and a simple unitary transformation by the present authors [17–19].

Huybrechts [20] proposed a linear-combination operator method, by which a strong-coupling polaron was investigated. Later, many workers [21, 22] studied many aspects of the strong-coupling polaron by this method.

The ground-state energy and the cyclotron-resonance frequency of the surface polaron in a magnetic field have been calculated by many methods. Many of these mainly concentrated attention on the weak- and intermediate-coupling cases. However, the surface magnetopolaron in strong-coupling polar crystals has not been investigated so far.

The purpose of this present paper is to explore the effect of the magnetic field on the properties of surface polarons. With both weak coupling between the electron and bulk LO phonon and strong coupling between the electron and SO phonon included, we obtain an expression for the effective Hamiltonian, the effective interaction potential and the cyclotron-resonance frequency of the surface polaron as a function of the magnetic field strength by using the linear-combination operator method. Numerical calculations, taking a AgCl crystal as an example, are performed and the properties of these quantities for the surface polaron in polar crystals in a magnetic field are discussed.

2. The Hamiltonian

A surface between a AgCl crystal and a vacuum is perpendicular to the z axis; the semi-infinite space $z > 0$ is occupied by the AgCl crystal, whereas the space $z < 0$ is the vacuum. A slow electron is placed inside the AgCl crystal at a distance $z (> 0)$ from the surface. On the assumption that an external magnetic field $\mathbf{B} = (0, 0, B)$ (applied normal to the surfaces) exists, the Hamiltonian of the electron, interacting with both the bulk LO phonon and the SO phonon, can be written as

$$\begin{aligned}
 H = & \frac{P_z^2}{2m} + \frac{e^2(\varepsilon_\infty - 1)}{4z\varepsilon_\infty(\varepsilon_\infty + 1)} + \frac{1}{2m} \left(P_x - \frac{\beta^2}{4}y \right)^2 + \frac{1}{2m} \left(P_y + \frac{\beta^2}{4}x \right)^2 \\
 & + \sum_w \hbar\omega_l a_w^\dagger a_w + \sum_Q \hbar\omega_s b_Q^\dagger b_Q \\
 & + \sum_w \frac{1}{w} \sin(w_z z) [V_w^* \exp(-i\mathbf{w}_\parallel \cdot \boldsymbol{\rho}) a_w^\dagger + \text{HC}] \\
 & + \sum_Q \frac{1}{\sqrt{Q}} \exp(-Qz) [C^* \exp(-i\mathbf{Q} \cdot \boldsymbol{\rho}) b_Q^\dagger + \text{HC}]
 \end{aligned} \tag{1a}$$

$$V_w^* = i \left(\frac{4\pi e^2 \hbar \omega_l}{\varepsilon V} \right)^{1/2} \tag{1b}$$

$$C^* = i \left(\frac{\pi e^2 \hbar \omega_s}{\varepsilon^* S} \right)^{1/2} \tag{1c}$$

$$\frac{1}{\varepsilon} = \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0} \quad (1d)$$

$$\frac{1}{\varepsilon^*} = \frac{\varepsilon_0 - 1}{\varepsilon_0 + 1} - \frac{\varepsilon_\infty - 1}{\varepsilon_\infty + 1} \quad (1e)$$

$$\omega_s^2 = \frac{1}{2}(\omega_T^2 + \omega_L^2) \quad (1f)$$

$$\beta^2 = \frac{2eB}{c} \quad (1g)$$

where $\mathbf{P}(P_x, P_y, P_z)$ is the electron momentum and m is the band mass of the electron. S and V are the surface area and the volume, respectively, of the AgCl crystal. $\varepsilon_0(\varepsilon_\infty)$ is the static (high-frequency) dielectric constant. ρ is the position vector in the x - y plane of the electron. \mathbf{K} and \mathbf{Q} are the 2D wavevectors of bulk LO and SO phonons, respectively. a_w^+ and a_w are the creation and annihilation operators, respectively, of a bulk LO phonon with a three-dimensional wavevector \mathbf{w} , and b_Q^+ and b_Q are the corresponding operators for the SO phonon with a two-dimensional wavevector \mathbf{Q} . ω_L , ω_S and ω_T are the frequencies of the bulk LO, SO and bulk transverse optical phonons.

The Hamiltonian can formally be divided into two parts:

$$H = H_{\parallel} + H_Z \quad (2a)$$

where

$$H_Z = \frac{P_z^2}{2m} + \frac{e^2(\varepsilon_\infty - 1)}{4Z\varepsilon_\infty(\varepsilon_\infty + 1)} \quad (2b)$$

and the rest is called H_{\parallel} . On the assumption that the motion in the z direction is slow, therefore, when determining the motion state in the x - y plane, quantities such as the momentum and position in the z direction may be regarded as parameters. This procedure is exactly analogous to the quasi-adiabatic approximation [23–25]. For motion parallel to the x - y plane, we introduce the unitary transformations

$$U_1 = \exp\left(-iA_1 \sum_w a_w^+ a_w \mathbf{w}_{\parallel} \cdot \rho - iA_2 \sum_Q b_Q^+ b_Q \mathbf{Q} \cdot \rho\right) \quad (3a)$$

where $A_i (i = 1, 2)$ is a parameter characterizing the coupling strength. In the unitary transformation U_1 , where $A_1 = 1$ corresponds to the weak coupling between the electron and the bulk LO phonon, and $A_2 = 0$ corresponds to the strong coupling between the electron and the SO phonon, we can easily obtain

$$U_1 = \exp\left(-i \sum_w a_w^+ a_w \mathbf{w}_{\parallel} \cdot \rho\right). \quad (3b)$$

Carrying out the unitary transformation with (3b), the Hamiltonian (1a) is transformed to H_1 :

$$\begin{aligned} H_1 = U_1^{-1} H U_1 = & \frac{1}{2m} \left(P_x - \sum_w a_w^+ a_w \hbar w_x - \frac{\beta^2}{4} y \right)^2 + \frac{1}{2m} \left(P_y - \sum_w a_w^+ a_w \hbar w_y + \frac{\beta^2}{4} x \right)^2 \\ & + \sum_w a_w^+ a_w \hbar \omega_l + \sum_Q b_Q^+ b_Q \hbar \omega_s + \sum_w \frac{1}{w} \sin(w_z z) (V_w^* a_w^+ + \text{HC}) \\ & + \sum_Q \frac{1}{Q} \exp(-Qz) [C^* \exp(-i\mathbf{Q} \cdot \rho) b_Q^+ + \text{HC}]. \end{aligned} \quad (4)$$

Following Huybrechts [20] we also introduce the linear combination of the creation and annihilation operators b^+ and b to represent the momentum and position of the electron:

$$P_j = \left(\frac{m\hbar\lambda}{2} \right)^{1/2} (b_j + b_j^+) \quad (5a)$$

$$\rho_j = i \left(\frac{\hbar}{2m\lambda} \right)^{1/2} (b_j - b_j^+) \quad (5b)$$

where the suffix j refers to the x and y directions, λ is a variational parameter and b_j^+ and b_j are Bose operators satisfying the Bose commutative relation. Substituting (5) into (4), we have

$$H_1 = H_2 + H_3 \quad (6a)$$

$$\begin{aligned} H_2 = & \frac{\hbar\lambda}{4} ((b_x + b_x^+)^2 + (b_y + b_y^+)^2) - \frac{\beta^4\hbar}{64m^2\lambda} ((b_x - b_x^+)^2 + (b_y - b_y^+)^2) \\ & + \sum_w \left(\hbar\omega_l + \frac{\hbar^2 w_{\parallel}^2}{2m} \right) a_w^+ a_w + \sum_Q \hbar\omega_s b_Q^+ b_Q + \sum_w \frac{1}{w} \sin(w_z z) (V_w^* a_w^+ + \text{HC}) \\ & + \sum_Q \left\{ \frac{C^*}{\sqrt{Q}} \exp(-Qz) b_Q^+ \exp\left(-\frac{\hbar Q^2}{4m\lambda}\right) \exp\left[-\left(\frac{\hbar}{2m\lambda}\right)^{1/2} \sum_j Q_j b_j^+\right] \right. \\ & \times \exp\left[\left(\frac{\hbar}{2m\lambda}\right)^{1/2} \sum_j Q_j b_j\right] + \text{HC} \left. \right\} \\ & + \frac{1}{m} \left[-\left(\frac{m\hbar\lambda}{2}\right)^{1/2} \left((b_x + b_x^+) \sum_w a_w^+ a_w \hbar w_x + (b_y + b_y^+) \sum_w a_w^+ a_w \hbar w_y \right) \right. \\ & - i \frac{\hbar\beta^2}{4} ((b_x + b_x^+)(b_y - b_y^+) - (b_y + b_y^+)(b_x - b_x^+)) + i \frac{\beta^2}{4} \left(\frac{\hbar}{2m\lambda}\right)^{1/2} \\ & \left. \times \left((b_y - b_y^+) \sum_w a_w^+ a_w \hbar w_x - (b_x - b_x^+) \sum_w a_w^+ a_w \hbar w_y \right) \right] \quad (6b) \end{aligned}$$

$$H_3 = \frac{1}{2m} \sum_{w \neq w'} a_w^+ a_w^+ a_w a_w \hbar^2 w_x w'_x + \frac{1}{2m} \sum_{w \neq w'} a_w^+ a_w^+ a_w a_w \hbar^2 w_y w'_y. \quad (6c)$$

H_3 is a term describing the interaction between phonons of different wavevectors in the recoil process and we shall neglect the recoil energy H_3 .

Carrying out a second unitary transformation,

$$\mathcal{H}_{\parallel} = U_2^{-1} H_2 U_2 \quad (7a)$$

where

$$U_2 = \exp \left(\sum_w (a_w^+ f_w - a_w f_w^*) + \sum_Q (b_Q^+ g_Q - b_Q g_Q) \right). \quad (7b)$$

$f_w (f_w^*)$ and $g_Q (g_Q^*)$ are variational parameters; then the transformed Hamiltonian can be rewritten as

$$\begin{aligned} \mathcal{H}_{\parallel} = & \frac{\hbar\lambda}{4} ((b_x + b_x^+)^2 + (b_y + b_y^+)^2) - \frac{\beta^4\hbar}{64m^2\lambda} ((b_x - b_x^+)^2 + (b_y - b_y^+)^2) \\ & + \sum_w \left(\hbar\omega_l + \frac{\hbar^2 w_{\parallel}^2}{2m} \right) (a_w^+ + f_w^*) (a_w + f_w) + \sum_Q \hbar\omega_s (b_Q^+ + g_Q^*) (b_Q + g_Q) \end{aligned}$$

$$\begin{aligned}
& + \sum_w \frac{1}{w} \sin(w_z z) (V_w^* (a_w^+ + f_w^*) + \text{HC}) \\
& + \sum_Q \left\{ \frac{C^*}{\sqrt{Q}} \exp(-Qz) (b_Q^+ + g_Q^*) \exp\left(-\frac{\hbar Q^2}{4m\lambda}\right) \right. \\
& \times \exp\left[-\left(\frac{\hbar}{2m\lambda}\right)^{1/2} \sum_j Q_j b_j^+\right] \exp\left[\left(\frac{\hbar}{2m\lambda}\right)^{1/2} \sum_j Q_j b_j\right] + \text{HC} \left. \right\} \\
& + \frac{1}{m} \left[-\left(\frac{m\hbar\lambda}{2}\right)^{1/2} \left((b_x + b_x^+) \sum_w (a_w^+ + f_w^*) (a_w + f_w) \hbar w_x \right. \right. \\
& \left. \left. + (b_y + b_y^+) \sum_w (a_w^+ + f_w^*) (a_w + f_w) \hbar w_y \right) \right. \\
& \left. - i \frac{\hbar\beta^2}{8} ((b_x + b_x^+)(b_y - b_y^+) - (b_y + b_y^+)(b_x - b_x^+)) \right. \\
& \left. + i \frac{\beta^2}{4} \left(\frac{\hbar}{2m\lambda}\right)^{1/2} \left((b_y - b_y^+) \sum_w (a_w^+ + f_w^*) (a_w + f_w) \hbar w_x \right. \right. \\
& \left. \left. - (b_x - b_x^+) \sum_w (a_w^+ + f_w^*) (a_w + f_w) \hbar w_y \right) \right]. \tag{8}
\end{aligned}$$

The ground-state wavefunction of the system is $\phi = \varphi(\rho)|0\rangle$ where $\varphi(\rho)$ is the normalized surface polaron wavefunction. $|0\rangle$ is the zero-phonon state, which satisfied

$$a_w|0\rangle = b_Q|0\rangle = b_j|0\rangle = 0. \tag{9}$$

Then the effective Hamiltonian of the system can be obtained as

$$H_{eff} = H_z + H_{||eff} \tag{10a}$$

$$\begin{aligned}
H_{||eff} = \min[F(\lambda, f_w, g_Q)] = \langle 0|\mathcal{H}_{||}|0\rangle &= \frac{\hbar\lambda}{2} + \frac{\beta^4\hbar}{32m^2\lambda} + \sum_w \left(\hbar\omega_l + \frac{\hbar^2 w_{||}^2}{2m} \right) |f_w|^2 \\
& + \sum_Q \hbar\omega_s |g_Q|^2 + \sum_w \frac{1}{w} \sin(w_z z) (V_w^* f_w^* + \text{HC}) \\
& + \sum_Q \left[\frac{C^*}{\sqrt{Q}} \exp(-Qz) g_Q^* \exp\left(-\frac{\hbar Q^2}{4m\lambda}\right) + \text{HC} \right]. \tag{10b}
\end{aligned}$$

Using the variational method, we get

$$f_w = -\frac{V_w^* \sin(w_z z)}{w(\hbar\omega_l + \hbar^2 w_{||}^2/2m)} \tag{11a}$$

$$g_Q = -\frac{C^* \exp(-Qz)}{\sqrt{Q}\hbar\omega_s} \exp\left(-\frac{\hbar Q^2}{4m\lambda}\right). \tag{11b}$$

Substituting (11) into (10), we have

$$\begin{aligned}
F(\lambda) = \frac{\hbar\lambda}{2} + \frac{\hbar\omega_c^2}{8\lambda} - \alpha_l \hbar\omega_l \left(\frac{\pi}{2} - \eta(z) \right) \\
- \frac{\sqrt{\pi}}{2} \alpha_s \hbar\omega_s \left(\frac{\lambda}{\omega_s} \right)^{1/2} \exp\left(\frac{\lambda}{\omega_l} u_l^2 z^2\right) \text{erfc} \left[\left(\frac{\lambda}{\omega_l} \right)^{1/2} u_l z \right] \tag{12a}
\end{aligned}$$

where

$$\begin{aligned}\alpha_l &= \frac{me^2}{\varepsilon\hbar u_l} & \alpha_s &= \frac{me^2}{\varepsilon^*\hbar u_s} \\ \hbar\omega_l &= \frac{\hbar^2 u_l^2}{2m} & \hbar\omega_s &= \frac{\hbar^2 u_s^2}{2m} \\ \eta(z) &= \int_0^\infty \frac{\exp(-2u_l z x)}{1+x^2} dx & \omega_c &= \frac{eB}{mc}.\end{aligned}\quad (12b)$$

Performing the variation of $F(\lambda)$ with respect to λ , we obtain

$$\lambda = \left\{ \frac{\omega_c^2}{4} + \frac{\sqrt{\pi}}{2} \alpha_s \sqrt{\omega_s} \lambda^{3/2} \exp\left(\frac{\lambda}{\omega_l} u_l^2 z^2\right) \operatorname{erfc}\left[\left(\frac{\lambda}{\omega_l}\right)^{1/2} u_l z\right] - 2\alpha_s u_l z \left(\frac{\omega_s}{\omega_l}\right)^{1/2} \lambda^2 \int_0^\infty x \exp\left[-x^2 - 2\left(\frac{\lambda}{\omega_l}\right)^{1/2} u_l z x\right] dx \right\}^{1/2}. \quad (13)$$

From (13), one can determine the frequency λ at different coordinates z . Finally, the effective Hamiltonian can be expressed as

$$H_{eff} = \frac{P_z^2}{2m} + \frac{e^2(\varepsilon_\infty - 1)}{4z\varepsilon_\infty(\varepsilon_\infty + 1)} + V_i^l V_i^s + \frac{\hbar\lambda}{2} + \frac{\hbar\omega_c^2}{8\lambda} \quad (14a)$$

where

$$V_i^l = -\alpha_l \hbar \omega_l \left(\frac{\pi}{2} - \int_0^\infty \frac{\exp(-2u_l z x)}{1+x^2} dx \right) \quad (14b)$$

$$V_i^s = -\frac{\sqrt{\pi}}{2} \alpha_s \hbar \omega_s \left(\frac{\lambda}{\omega_s} \right)^{1/2} \exp\left(\frac{\lambda}{\omega_l} u_l^2 z^2\right) \operatorname{erfc}\left[\left(\frac{\lambda}{\omega_l}\right)^{1/2} u_l z\right] \quad (14c)$$

$$V_{eff} = \frac{e^2(\varepsilon_\infty - 1)}{4z\varepsilon_\infty(\varepsilon_\infty + 1)} + V_i^l V_i^s \quad (14d)$$

are the induced potential and the effective interaction potential, respectively.

In the following, the effective Hamiltonian H_{eff} of the electron–phonon coupling system will be considered in two different limiting cases.

(1) The electron is very near the surface, i.e. $z \ll u_l^{-1}$ or u_s^{-1} . In this case, we have

$$F(\lambda) = \frac{\hbar\lambda}{2} + \frac{\hbar\omega_c^2}{8\lambda} - \frac{\sqrt{\pi}}{2} \alpha_s \hbar \omega_s \left(\frac{\lambda}{\omega_s} \right)^{3/2}. \quad (15)$$

The variation in $F(\lambda)$ with respect to λ yields

$$x^4 - \frac{1}{2} \alpha_s (\pi \omega_s)^{1/2} x^3 - \frac{1}{4} \omega_c^2 = 0 \quad (16)$$

where $\lambda = x^2$. Solving the quartic equation (16), we get

$$\lambda = \lambda_0 \quad (17)$$

and $F(\lambda_0)$ is the minimal value. Finally, the effective Hamiltonian of the surface polaron can be expressed as

$$H_{eff} = \frac{P_z^2}{2m} + \frac{e^2(\varepsilon_\infty - 1)}{4z\varepsilon_\infty(\varepsilon_\infty + 1)} + \frac{\hbar\lambda_0}{2} + \frac{\hbar\omega_c^2}{8\lambda_0} - \frac{\sqrt{\pi}}{2} \alpha_s \hbar \omega_s \left(\frac{\lambda_0}{\omega_s} \right)^{1/2}. \quad (18)$$

From (18), one can see that the effective Hamiltonian of the surface polaron is independent of the interaction between the electron and the bulk LO phonon, whereas it is only dependent on the interaction between the electron and the SO phonon. The self-trapping energy is

$$E_{tr} = \frac{\sqrt{\pi}}{2} \alpha_s \hbar \omega_s \left(\frac{\lambda_0}{\omega_s} \right)^{1/2} - \frac{\hbar \lambda_0}{2} - \frac{\hbar \omega_c^2}{8 \lambda_0}. \quad (19)$$

In (19), the first two terms are the self-trapping energy induced by the polarization of SO vibration. The third term represents the self-trapping energy induced by coupling between the surface polaron and magnetic field.

(2) The electron is very deep in the bulk, i.e. $z \gg u_l^{-1}$ or u_s^{-1} . In this case, we have

$$F(\lambda) = \frac{\hbar \lambda}{2} + \frac{\hbar \omega_c^2}{8 \lambda} - \frac{\pi}{2} \alpha_l \hbar \omega_l. \quad (20a)$$

The variation in $F(\lambda)$ with respect to λ yields

$$\lambda = \frac{\omega_c}{2}. \quad (20b)$$

The effective Hamiltonian of the surface polaron can be written as

$$H_{eff} = \frac{P_z^2}{2m} + \frac{e^2(\varepsilon_0 + 1)}{4z\varepsilon_0(\varepsilon_0 + 1)} + \frac{1}{2} \hbar \omega_c - \frac{\pi}{2} \alpha_l \hbar \omega_l. \quad (21)$$

The effective Hamiltonian of the surface polaron is only dependent on the interaction between the electron and the bulk LO phonon. The self-trapping energy is

$$E_{tr} = \frac{1}{2} \hbar \omega_c + \frac{\pi}{2} \alpha_l \hbar \omega_l. \quad (22)$$

In (22), the first term is the Landau ground-state energy. The second term represents the self-trapping energy originating from the interaction between the electron and the bulk LO phonons.

This shows that, when the distance between the electron and the surface is much smaller than the radius of the bulk polaron, the effect of the bulk phonons can be neglected and so can the effect of the surface phonons when the corresponding distance is much larger than the corresponding radius.

In general, as the distance between the electron and the surface is the same order of magnitude as the radius of the bulk polaron, the effects of both the bulk LO and the SO phonons must be taken into account. In this case the electron moves in a non-local potential as (14a).

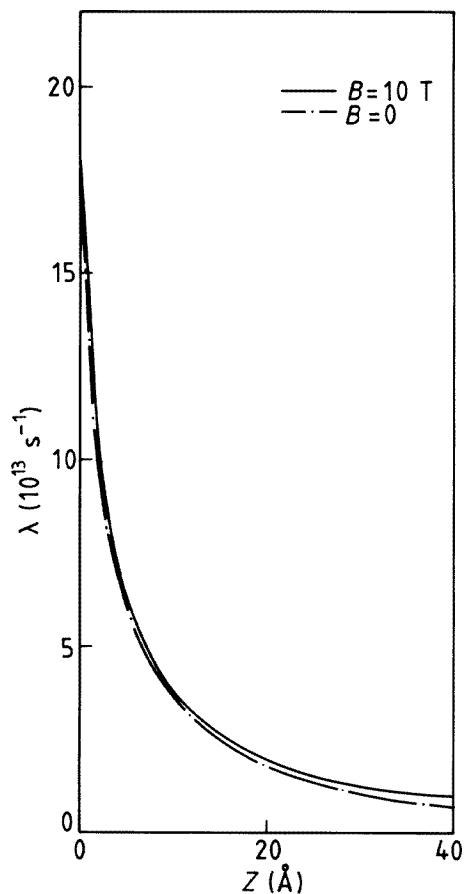
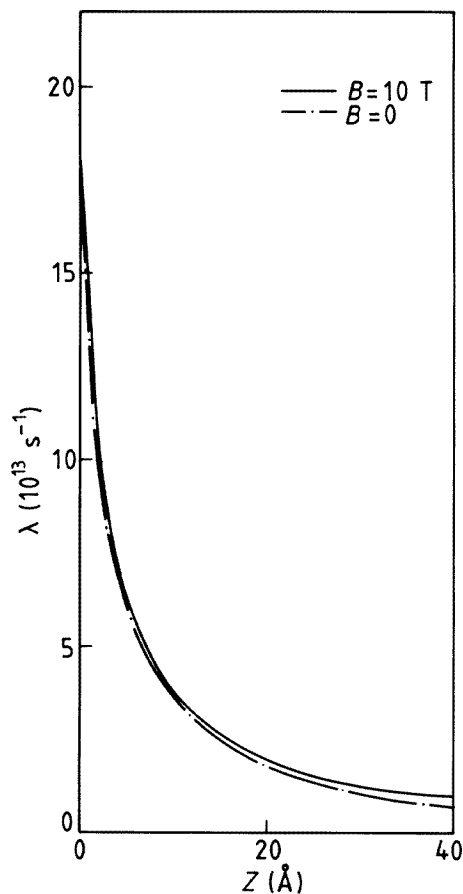
3. Results and discussion

In this section, taking the polaron in the surface of a AgCl crystal as an example, we perform a numerical evaluation. In table 1, the data for a AgCl crystal are given. Figure 1 shows the variation in the frequency λ of the surface polaron in a AgCl crystal with the coordinate z at different magnetic fields B . The solid curve denotes the case $B = 10$ T, and the broken curve represents the case $B = 0$. From the figure, one can see that the frequency λ will decrease with increasing z . At the same position (same value of z), the higher magnetic field, the higher is the value of λ .

In (14a), the first term is the kinetic energy of the electron in the direction perpendicular to the surface of the crystal. The second term represents the energy of the image potential. The third and fourth terms stand for the induced potential resulting from the electron–bulk-LO-phonon interaction and the electron–SO-phonon interaction. This indicates that only

Table 1. The data for a AgCl crystal. All the parameters are taken from [26].

Material	ϵ_0	ϵ_∞	$\hbar\omega_l$ (meV)	$\hbar\omega_s$ (meV)	α_l	α_s
AgCl	9.5	3.97	23.0	21.6	1.97	2.89

**Figure 1.** The relation between the vibrational frequency λ and the coordinate z in a AgCl crystal at different magnetic fields B .**Figure 2.** The relation between the effective interaction potential V_{eff} and the coordinate z in a AgCl crystal at different magnetic fields B .

the electron–SO-phonon interaction is dependent on the magnetic field, whereas the image potential and the electron–bulk-LO-phonon interaction are independent of the magnetic field. Figure 2 shows the relationship between the effective interaction potential V_{eff} in a AgCl crystal with the coordinate z at different magnetic fields B . The solid curve denotes the case $B = 0$, and the broken curve represents the case $B = 10$ T. As $z \rightarrow 0$, the first term of (14d) is dominant, and the surface polaron will be repulsed away from the surface (see figure 2). Thus the surface polaron cannot get infinitely near the surface; there is no surface polaron in the range near the surface ($V_{eff} > 0$). Because of the similarity to the case of excitons we call the thin layer the surface-polaron-free surface layer (SPFSL) or the ‘dead

layer' of surface polarons. Solving the equation

$$V_{eff}(z) = 0 \quad (23)$$

the root is the depth of SPFSL, which we denote as d (for the AgCl crystal in magnetic field, $d = 6.38 \text{ \AA}$). From figure 2, one can see that the effective interaction potential V_{eff} of the surface polaron for a AgCl crystal in a magnetic field will increase with increasing coordinate z at the same magnetic field B . From figure 2, we also see that the effective interaction potential V_{eff} will increase with increase in magnetic field B .

From equations (14), one can see that, for a system having a surface, the properties of system depend not only on the electron–SO-phonon coupling constant α_s , the electron–bulk-LO phonon coupling constant α_l and the magnetic field B but also on the distance z between the electron and the surface. When the electron is very near the surface, i.e. $z \ll u_l^{-1}$ or u_s^{-1} , the frequency λ (17) and self-trapping energy E_{tr} (19) of the surface magnetopolaron are only dependent on the magnetic field B and coupling constants α_s , whereas it is independent of the distance z and coupling constant α_l . The effective Hamiltonian H_{eff} (18) of the surface polaron is dependent on the magnetic field B , the coupling constant α_s and the distance z , whereas it is independent of only the coupling constant α_l . When the electron is very deep in the bulk, i.e. $z \gg u_l^{-1}$ or u_s^{-1} , the frequency λ (20b) and self-trapping E_{tr} (22) of the surface magnetopolaron are dependent only on the magnetic field B and the coupling constant α_l , whereas they are independent of the distance z and coupling constant α_s . The effective Hamiltonian H_{eff} (21) of the surface magnetopolaron is dependent on the magnetic field B , the coupling constant α_l and the distance z , whereas it is independent of only the coupling constant α_s .

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