The ground state energy of an exterior surface polaron under the effect of an external magnetic field

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الملخص

تم دراسة طاقة الوضع الأرضي لإلكترون مقترن بالبولارن السطحي تحت تأثير مجـال مغناطيسي خارجي. الطريقة المستخدمة هي طرقة التغيير والتي تصلح لكل قيم ثابـت الإقتـران بين الإلكترون والبولارون. لقد لوحظ أن المجال المغناطيسي يعزز أهمية إقتران الفونونات مـع الإلكترون بصورة واضحة.

ABSTRACT

Under the effect of an external magnetic field the ground state energy of an extrinsic electron interacting with the surface modes of a semi-infinite medium is calculated using a variational approach. The approach is to be valid for all values of the electron-phonon coupling. It is observed that the magnetic field enhances the effective electron-phonon coupling rather prominently.

Keywords: phonon, polaron, surface polaron, magnetopolaron, surface exitations.

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INTRODUCTION:

The interaction of an electron with the surface elementary excitations on a semi-infinite medium has received much attention in the past decades [1-]. The problem is interesting from a technological viewpoint in the context of surface spectroscopy and the study of the optical properties of polar thin films and interfaces.

Evans and Mills [1] used the Lee-Low-Pines theory to study the binding of electrons to the crystal surface. They considered the cases where the electron is outside and inside the crystal. Tokuda [2], and Bodas and Hipolito [3] considered only the case where the electron lies outside the crystal. They observed a phase-transition-like behavior from the quasi-free to the self-trapping electron state as the electron-phonon coupling constant exceeds a certain critical value. The effect of the magnetic field on the problem is investigated by Bhattacharya et al [4] using a canonical transformations method. Using a variational approach, Ninno and Iadonisi [5], calculated the ground state energy and the wave function of an electron near the surface of a polar crystal. Saqqa et al [6] and Xiukun [7] studied the effect of the magnetic field on an electron near the surface of a crystal using the strong-coupling theory. The effect of both the magnetic field and the temperature is addressed by Eerdunchaolu et al [8].

The common conclusion reached by the previous mentioned works is that for a sufficiently large coupling constant the electron goes into a bound state in which it is localized in the close vicinity of the exterior face of the material by the strong interaction with the surface oscillation modes. It has been observed that certain polaron quantities such as the ground state energy, the mean number of phonons around the electron, or the degree of localization are all enhanced by coupling strength. A further important finding is that the effective potential deviates considerably from the classical Coulomb profile (and in particular, at a distances close to the surface, the electron-phonon coupling imposes a rounding off of the divergence encountered in the classical picture. The application of an external magnetic field in the problem brought about an additional contribution to the localization of the electron so that the electron interacts with the phonons in a more efficient manner. This leads to an enhancement in the binding and an increase in the degree of confinement of the electron toward the surface .

In the following it is referred to the surface polaron problem considering the case where the electron is outside the medium and study the effect of an external magnetic filed using the variational method of Devreese et al [9].

The procedure is a combination between the adiabatic approximation and the first order perturbation method by adopting a variational trial function by which it is possible to extrapolate from the strong coupling regime toward the weak coupling one.

The model adopted in this work consists of an ionic or polaro material filling the half space and an electron localized near, but completely external to, the material surface. The exterior electron has an electric field which influences and polarizes the surface modes. These modes, when polarized, create electric fields which in turn act back upon the electron. The electron is therefore attracted to the surface by its image potential and in the mean time is repelled away by the repulsive barrier resulting from the large difference between the bottom of the conduction band and the vacuum level of the material. It should be noted that the interaction of the electron with the bulk modes are ignored since the electron is outside the material.

Theory:

Using the symmetric gauge for the vector potential, the Hamiltonian describing an electron with position coupled to the surface optical (SO) phonons and acted upon by a uniform magnetic field perpendicular to the surface can be written as

$$H = H_0 + \sum_{\kappa} a_{\kappa}^{\dagger}\, a_{\kappa} + \sum_{\kappa} \Gamma_{\kappa} \left(a_{\kappa} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{\rho}} + a_{Q}^{\dagger} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{\rho}} \right) \qquad (1)$$

$$H_0 = p_x^2 + p_y^2 + \tfrac{1}{4}(\Omega/2)^2 \left(x^2 + y^2 \right) + (\Omega/2) l_z \qquad (2)$$

where the operators $a_{\kappa}^{\dagger}$ and are the creation and annihilation operators of a phonon of wave vector $\boldsymbol{\kappa}$,, respectively andΩ is the dimensionless cyclotron frequency. The interaction amplitude is related to the electron-SO-phonons coupling constant α and the phonon wave vector $\boldsymbol{\kappa}$ through the relation [1]

$$\Gamma_{\kappa} = \sqrt{\frac{2\pi\alpha}{S\kappa}}\, e^{-\kappa z} \qquad (3)$$

where S is the normalization area. L_z in equation (2) is the z-component of the angular momentum. It should be noted that all physical quantities and

operators will be given in dimensionless form where energies are scaled by the SO-phonon $\hbar\omega$ and lengths by the polaron radius $\sqrt{\hbar/2m\omega}$

The variational procedure followed here assumes the electron and the lattice variables are totally separable with the wave function given by

$$\Psi = \Phi_e \, \Phi_{ph} \qquad (4)$$

With Φ_e and Φ_{ph} represent, respectively the electron part and the phonon part of the wave function. For the strong-coupling approximation the phonon part of the wave function is given as

$$\phi_{ph} = e^S \left| 0 \right\rangle \qquad (5)$$

where is the phonon vacuum. The exponential operator with

$$S = \sum_{\kappa} F_{\kappa} \left(a_{\kappa} - a_{\kappa}^{\dagger} \right) \qquad (6)$$

is the canonical coherent state transformation which, in the semi-classical, leads to the optimal surface polarization centered on the mean charge density induced, by electron, on the surface of the material. The amplitude F_κ depends implicitly on the electron wavefunction and must be treated as a variational parameter to be determined by the requirement that the energy of the system be minimized. Optimization of the transformed Hamiltonian

$$H' = e^{-S} H e^{S} = H_0 + \sum_{\kappa} a_{\kappa}^{\dagger} a_{\kappa} + \sum_{\kappa} F_{\kappa}^2 - \sum_{\kappa} F_{\kappa} \left(a_{\kappa} + a_{\kappa}^{\dagger} \right) + \sum_{\kappa} \Gamma_{\kappa} \left(a_{\kappa} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{\rho}} + a_{\kappa}^{\dagger} e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{\rho}} \right) - \sum_{\kappa} \Gamma_{\kappa} F_{\kappa} \left(e^{i\boldsymbol{\kappa}\cdot\boldsymbol{\rho}} + e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{\rho}} \right) \qquad (7)$$

With respect to the ground state we obtain

$$F_{\kappa} = \left\langle \phi_e \left| \Gamma_{\kappa} e^{\pm i\boldsymbol{\kappa}\cdot\boldsymbol{\rho}} \right| \phi_e \right\rangle \qquad (8)$$

And the ground state energy in the strong coupling regime is given by

$$E_{sc} = e_o - e_p = \left\langle \phi_e \left| H_o \right| \phi_e \right\rangle - \sum_{\kappa} F_{\kappa}^2 \qquad (9)$$

To extend the formulation to the weak coupling case we include a first order correction to the trial state $\Phi_e \left| 0 \right\rangle$ with the last term in equation (7) being a perturbation. We then have

$$\delta\Psi = \sum_{\kappa} \sum_{j} \frac{\left| j \right\rangle \left\langle j \right| \eta_{\kappa}^{*} a_{\kappa}^{\dagger} \left| \phi_e \right\rangle \left| 0 \right\rangle}{\varepsilon_o - \varepsilon_j - 1} \qquad (10)$$

Where

$$\eta_\lambda = \Gamma_\kappa e^{i\boldsymbol{\kappa}\cdot\boldsymbol{\rho}} - F_\kappa \qquad (11)$$

The summation over the intermediate states can be projected out simply by replacing the energy dominator by an average quantity which in the calculation will be determined variationally. Using completeness we write

$$\delta\Psi = \sum_\kappa \Gamma_\kappa g_\kappa \eta_\kappa^* a_\kappa^\dagger \left|\phi_e\right\rangle \left|0\right\rangle \qquad (12)$$

Where g_κ is another variational parameter. The trial wavefunction of the Hamiltonian H' is then extended to

$$\Psi' = n\phi_e \left|0\right\rangle + \delta\Psi \qquad (13)$$

Where n is a normalization constant. The optimal fit to g_κ is achieved by minimizing $\left\langle \Psi' \left| H' \right| \Psi' \right\rangle$ subject to the constraint

$$\left\langle \Psi' \middle| \Psi' \right\rangle = n^2 \left(1 + \sum_\kappa \Gamma_\kappa^2 \left(g_\kappa / n \right)^2 h_\kappa \right) = 1 \qquad (14)$$

In which

$$h_\kappa = \left\langle \phi_e \left| \eta_\kappa \eta_\kappa^* \right| \phi_e \right\rangle \qquad (15)$$

For the energy we then have

$$E_g = E_{sc} + \lambda \qquad (16)$$

Where λ is a Lagrange multiplier depending on α and Ω through the equation

$$\lambda = \sum_\kappa \Gamma_\kappa^2 \left(g_\kappa / n \right) h_\kappa \qquad (17)$$

where

$$g_\kappa / n = -h_\kappa / \left[e_\kappa - f_\kappa + \left(1 - \lambda - e_o - e_p \right) h_\kappa \right] \qquad (18)$$

With

$$e_\kappa = \left\langle \phi_e \left| \eta_\kappa H_o \eta_\kappa^* \right| \phi_e \right\rangle \qquad (19)$$

And

$$f_\kappa = \sum_{\kappa'} \Gamma_{\kappa'}^2 F\kappa' \left\langle \phi_e \left| \eta_\kappa \left(e^{i\boldsymbol{\kappa}\cdot\boldsymbol{\rho}} + e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{\rho}} \right) \eta_{\kappa'}^* \right| \phi_e \right\rangle \qquad (20)$$

Selecting a Gaussian spread (with variance σ^2) in the transverse direction and describing the localization in the remaining direction by

$$\phi_z = \left(\beta^2/2\right)^{1/2} z\, e^{-\beta z/2} \qquad (21)$$

with β is to be determined variationaly, we obtain

$$e_o = \sigma^{-2} + \tfrac{1}{4}\beta^2 + \left(\tfrac{1}{4}\Omega\sigma\right)^2 \qquad (22)$$

$$e_p = \alpha\int_0^\infty d\kappa\, F_\kappa^2 \qquad (23)$$

$$F_\kappa = S_\kappa(\sigma)\, R_\kappa(\beta) = e^{-\left(\frac{1}{4}\sigma^2\kappa^2\right)}\left(1+\frac{\kappa}{\beta}\right)^{-3} \qquad (24)$$

$$h_\kappa = R_{2\kappa}(\beta) - S_\kappa^2(\sigma)\, R_\kappa^2(\beta) \qquad (25)$$

$$\begin{aligned} e_\kappa &= R_{2\kappa}(\beta)\left[e_o + 2\kappa^2 + \kappa\beta\right] \\ &\quad + S_\kappa^2(\sigma)\, R_\kappa^2(\beta)\left[e_o - 2\sigma^{-2} - \tfrac{1}{2}(\kappa+\beta)^2\right] \end{aligned} \qquad (26)$$

$$\begin{aligned} f_\kappa &= 2\alpha\int_0^\infty d\kappa' S_{\kappa'}^2 R_{\kappa'}\left[R_{2\kappa+\kappa'} + S_\kappa^2 R_\kappa^2 R_{\kappa'}\right] \\ &\quad - 4\alpha S_\kappa^2 R_\kappa \int_0^\infty d\kappa' S_{\kappa'}^2 R_{\kappa'} R_{\kappa+\kappa'} I_o\left(\kappa\kappa'\sigma^2/2\right) \end{aligned} \qquad (27)$$

In which Io is the modified Bessel function of order zero.

RESULTS AND DISCUSSION:

It is clear from equation (16) that the energy differs from that of the strong coupling regime, given by equation (9), by the additive term λ through which the adiabatic theory goes over to the weak coupling regime. For large values of the coupling constant α, $S_\kappa(\sigma)$ and $R_\kappa(\beta)$ defined by equation (24) both approach unity and hence $\lambda \to 0$ Consequently the strong coupling limit is readily obtained. For small α however the role of λ becomes very prominent and the polaron binding is dominantly determined by this term.

It is worthy knowing that, restricting the electron charge fluctuations to be just on the surface, the present model conforms to that for strictly two-

dimensional magnetopolaron [11]. Imposing an infinitely large value for β in equation (21), the strong coupling ground state energy simplifies to

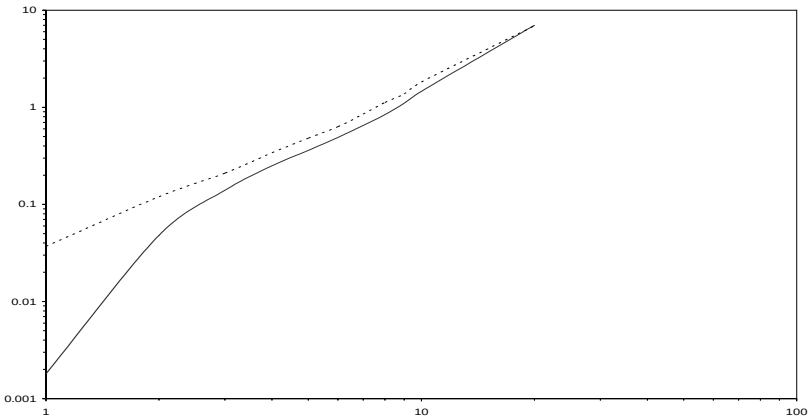
$$E_g = \sigma^{-2} + \left(\tfrac{1}{4}\Omega\sigma\right)^2 \sqrt{\frac{\pi}{2}}\alpha\sigma^{-1}. \qquad (28)$$

For strong coupling and weak magnetic field $\left(\Omega/\alpha^2 \langle\langle 1\right)$, the dominant contribution come from the first and the third terms in equation (28). Minimization of the dominant part gives

$$E_g = -\frac{\pi}{8}\alpha^2\left[1-\left(2\Omega/\pi\alpha^2\right)^2\right] \qquad (29)$$

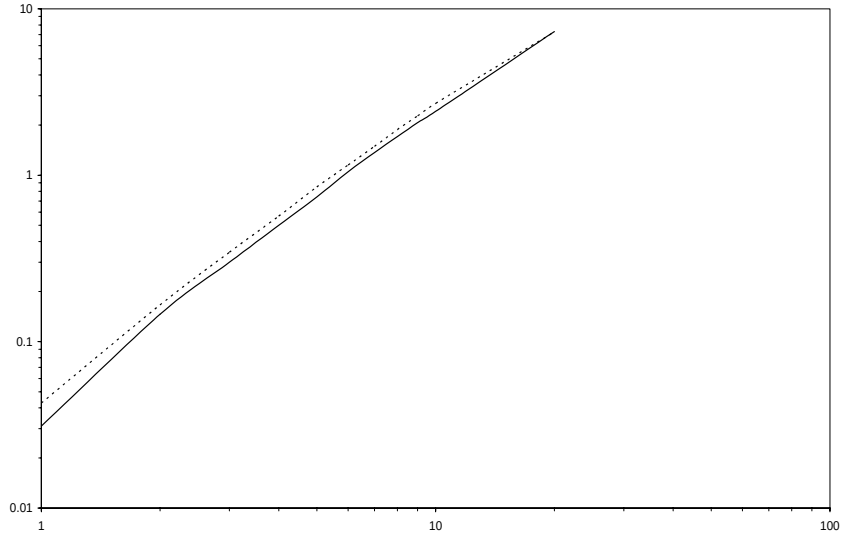
Which is the two-dimensional analogue of the corresponding bulk value [12].

In order to find an optimization for the energy in equation (16) in the overall range of the magnetic field one requires numerical techniques. Figure (1) shows the dependence of the binding energy $\left(E_b = E_g - \tfrac{1}{2}\Omega\right)$ on α using the strong coupling and the extended theories disregarding the magnetic field effect. To show the effect of the magnetic field on the problem, figure (2) represents the binding energy as a function of α for for $\Omega = 4$ From the two figures it is concluded that the two theories are in close quantitative agreement for large values of α Furthermore, in spite of small values of α, the problem show up a pseudo strong coupling counterpart at high magnetic fields. For $\alpha = 1$ the discrepancies between the two theories are found to be 55% and 27% for $\Omega = 0$ and $\Omega = 4$ respectively. The corresponding percentages for $\alpha = 10$ are 17% and 7%.



α

Figure 1. The binding energy as a function of α with zero magnetic field. The solid and the dashed lines corresponding to the strong coupling and the extended theories, respectively.



α

Figure 2. The binding energy as a function of α with Ω=4. The solid and the dashed lines corresponding to the strong coupling and the extended theories, respectively.

CONCLUSION:

The present work retrieves the problem of an exterior surface polaron under the effect of an external magnetic field using a variational procedure intended to be valid for the overall range of the coupling constant. In spite of small α, the problem show up a pseudo strong coupling counterpart at high magnetic field

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