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The ground-state description of the optical polaron versus the effective dimensionality in quantum-well-type systems

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Abstract. Within the framework of the strong-coupling polaron theory the ground-state binding energy and the effective mass of the electron–LO phonon system is retrieved as a function of the effective dimensionality in a quantum-well confinement. The geometry we use is a three-dimensional parabolic potential box, the barrier slopes of which can be tuned so as to yield a unified characterization interpolating between the bulk, the quasi-two- and one-dimensional limits as well as the quantum-well box case.

1. Introduction

Recently, increasing attention has been focused on the study of polarons of reduced dimensionality in the context of quantum-well confined structures. Particular emphasis has been devoted to the strict two-dimensional (2D) optical polaron consisting of a surface electron interacting with the LO branch of the surface phonon modes of an ionic or polar crystal (Huybrechts 1978, Wu *et al* 1985, Larsen 1987). Another aspect of the 2D characterization of the optical polaron is that it finds its relevance as an approximating model accounting for the almost-two-dimensional dynamical behavior of an electron within the confining barriers of a thin semiconductor quantum well and yet interacting with the bulk LO phonon modes of the well material (Das Sarma and Mason 1985, Peeters *et al* 1987). The common theoretical prediction reached by all the works pertaining to 2D-polaron properties is that in switching from the bulk to the case of two-dimensionally confined structures the electron–phonon coupling gets substantially stronger and, consequently, certain polaron quantities scale to considerably pronounced values (Peeters *et al* 1987). The polaron binding energy, for instance, is deepened by a factor of $\pi/2$ in the weak-coupling regime, and by $3\pi^2/8$ within the framework of the strong-coupling approximation. The same feature is true for other quantities like the effective polaron mass or the mean density of phonons clothing the electron.

The purpose of this paper is to display a unifying and comprehensive theoretical presentation yielding an explicit track of the electron–phonon interaction effects as a function of the effective dimensionality. For the present we focus our discussions on the strongly coupled polaron in its lowest bound state in a confined medium. We utilize a simple model consisting of an optical polaron within an *anisotropic harmonic oscillator-type* confining potential given in usual polaron units ($\hbar = 2m = \omega_{\mathrm{LO}} = 1$)

by

$$V(\rho, z) = \tfrac{1}{4}(\omega_1^2 \rho^2 + \omega_2^2 z^2) \tag{1}$$

where

$$\omega_i = (k_i / m\omega_{\mathrm{LO}}^2)^{1/2}$$

in which $k_i (i = 1, 2)$ denotes the respective force constants in the x, y and the z directions. Such a choice for the confining potential is appealing in the sense that the effective dimensionality can be adjusted by varying the dimensionless frequencies ω_1 and ω_2 so as to provide a broad insight into the effect of degree of confinement on the ground-state property of the polaron. By shifting ω_1 and ω_2 from zero to values much larger than unity one can trace the transition from the bulk to the two-dimensional slab-like confinement ($\omega_1 = 0, \omega_2 \gg 1$) or else, to the quasi-one-dimensional quantum-well wire (QWW)-like behaviour ($\omega_1 \gg 1, \omega_2 = 0$).

2. Theory and results

Under the traditional displaced oscillator transformation of the strong-coupling formalism

$$H \longrightarrow H' = \mathrm{e}^{-S} H \mathrm{e}^{S} \qquad S = \sum_Q f_Q (a_Q - a_Q^\dagger) \tag{2}$$

the polaron Hamiltonian is

$$H' = \boldsymbol{P}^2 + V(\rho, z) + \sum_Q f_Q^2 - \sum_Q V_Q f_Q (\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}} + \mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}}) + \sum_Q a_Q^\dagger a_Q + \sum_Q [(V_Q \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}} - f_Q) a_Q + \mathrm{HC}] \tag{3}$$

where $\boldsymbol{P} = (\boldsymbol{p}, p_z)$ and $\boldsymbol{r}$ denote the electron momentum and position, and f_Q is a variational parameter describing the depth and the profile of the lattice potential well induced by the mean charge density fluctuations of the electron. The interaction amplitude is related to the electron–phonon coupling constant α and the phonon wavevector $\boldsymbol{Q} = (\boldsymbol{q}, q_z)$ through $V_Q = \sqrt{4\pi\alpha}/Q$.

Compatible with the anisotropy in the potential (1) we introduce different adjustable parameters λ_1 and λ_2 for the dynamic description of the electron. We implicitly assume Gaussian spreads by utilizing the linear combination of the coordinates and momenta of the electron as operators:

$$b_\mu = \sqrt{\frac{1}{\lambda_1}} \left(p_\mu - \mathrm{i}\frac{\lambda_1}{2} x_\mu \right) \qquad b_z = \sqrt{\frac{1}{\lambda_2}} \left(p_z - \mathrm{i}\frac{\lambda_2}{2} z \right) \tag{4}$$

where the index μ refers to the x and y directions.

Defining the ground state $|0\rangle$ by

$$b_\mu |0\rangle = b_z |0\rangle = 0 \qquad a_Q |0\rangle = 0 \qquad \langle 0|0\rangle = 1 \tag{5}$$

and performing the minimization of $E_g = \langle 0|H'|0\rangle$ with respect to f_Q we obtain

$$f_Q = V_Q \sigma_Q \qquad \sigma_Q = \langle 0|e^{\pm i Q\cdot r}|0\rangle = \exp\left(-\frac{q^2}{2\lambda_1} - \frac{q_z^2}{2\lambda_2}\right) \tag{6}$$

and for the polaron binding energy, relative to the subband level, we have

$$\varepsilon_p = \omega_1 + \tfrac{1}{2}\omega_2 - E_g \tag{7}$$

where

$$E_g = \tfrac{1}{2}(\lambda_1 + \omega_1^2/\lambda_1) + \tfrac{1}{4}(\lambda_2 + \omega_2^2/\lambda_2) - \frac{\alpha}{\sqrt{\pi}}\sqrt{\frac{\lambda_1\lambda_2}{\lambda_2 - \lambda_1}}\tan^{-1}\sqrt{\frac{\lambda_2}{\lambda_1} - 1}. \tag{8}$$

For $\omega_1 = \omega_2 = 0$ the binding energy is readily available. In this limit we obtain $\lambda_1 = \lambda_2 = 4\alpha^2/9\pi$, and $\epsilon_p^{(3D)} = \alpha^2/3\pi$, i.e. the bulk value. When either ω_1 or ω_2 is comparable with the polaron size, the boundary effects start to become significant and the system enters a regime of reduced dimensionality. Setting $\omega_1 = 0$ and increasing ω_2 we obtain the binding energies in a Q2D slab-like structure and, in particular, when ω_2 becomes infinite we arrive at the strict 2D-characterization of the polaron wherein $\lambda_2 = \omega_2 \to \infty$, $\lambda_1 = \pi\alpha^2/4$, and for the binding energy we obtain $\epsilon_p^{(2D)} = (8/\pi)\alpha^2$. On the other hand, deleting the confining potential along the z axis totally ($\omega_2 = 0$) and fixing ω_1 at non-zero finite values, the theory reflects the Q1D description of the optical polaron in a QWW-like tubular structure. In figure 1 we display the binding energy as a function of the degree of confinement, i.e. as a function of either ω_1 or ω_2, respectively for the wire- and slab-like configurations. We note that with increasing barrier slopes of the confining potential, the binding energy for the wire geometry rapidly becomes much larger than in the Q2D configuration, which follows essentially from the fact that in the wire geometry the polaron cloud is squeezed towards the wire axis in all transverse directions resulting in a much stronger effective electron–phonon coupling than for the slab-like configuration. A more general and comprehensive presentation of how the binding becomes enhanced by the reduction in the effective dimensionality is given in figure 2 where we provide a total overview of the binding energy in the overall range of ω_1 and ω_2 interpolating between all extremes, including the quantum-well box (QWB) case. It is observed that in the case when the ratio ω_1/ω_2 approaches unity either from above or from below (respectively for ω_1 being held fixed and ω_2 varied, or ω_2 held fixed and ω_1 varied), the binding becomes much deeper than in the Q2D or Q1D limits since now the polaron becomes squeezed in all directions. For instance, for the Q2D confinement with $\alpha = 5$ and $\omega_2 = 1$ we obtain $\epsilon_p/\epsilon_p^{(3D)} = 1.16$. For the case of a wire with $\omega_1 = 1$ the binding gets deeper by a factor of about 1.33 and for a spherically symmetric confinement ($\omega_1 = \omega_2 = 1$) we have $\epsilon_p/\epsilon_p^{(3D)} = 1.49$. The corresponding values when $\alpha = 5$ and ω_1 and/or $\omega_2 = 10$, are 1.73, 2.64 and 3.66.

The variational model used in this work can be extended to yield the effective polaronic mass in various limits of the confinement geometry. The procedure consists of the variation of the Hamiltonian under the constraint that the relevant component of the total momentum

$$P = \boldsymbol{P} + \sum_Q Q a_Q^\dagger a_Q \tag{9}$$

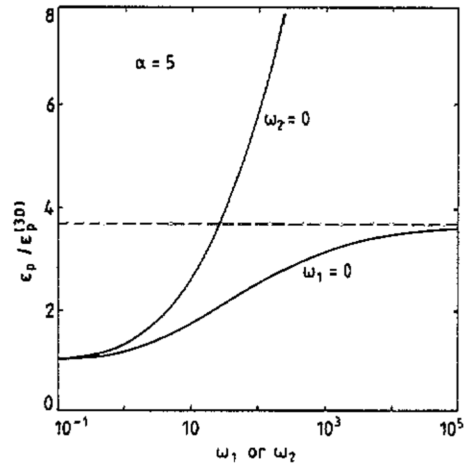

Figure 1. The binding energy against the degree confinement for the slab-like ($\omega_1 = 0$) and the wire-like ($\omega_2 = 0$) configurations. The horizontal broken line refers to the energy value in the 2D limit.

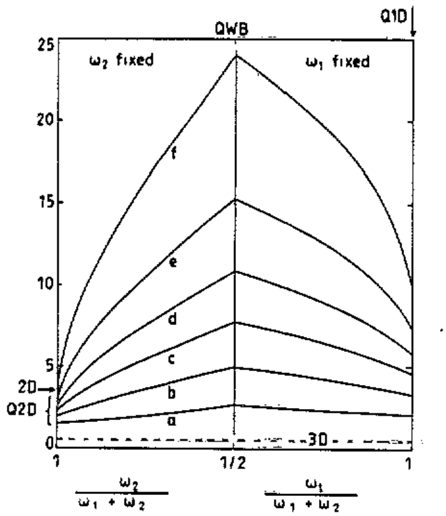

Figure 2. The binding energy as a funtion of the effective dimensionality. The succession of curves a, b, c, d, e and f are for fixed values of either ω_1 or $\omega_2 = 5, 20, 50, 100, 200, 500$ with $\omega_1(\omega_2)$ held fixed and $\omega_2(\omega_1)$ varied in the right (left) part of the figure. The central vertical line refers to the spherically symmetric confinement, whereas the intercepts on the left and the right margins give the binding energy value for the slab and the wire geometries. ($\alpha = 5$).

is conserved. In what follows we shall take $\langle 0|e^{-S} P e^{S}|0\rangle = 0$.

We first refer to the z direction. For the electron momentum we write

$$p_z = \frac{\sqrt{\lambda_2}}{2}(b_z + b_z^\dagger + \pi_z) \tag{10}$$

with π_z introduced as a further variational parameter in the theory so as to account for the composite inertia of the electron dressed by the cloud of virtual phonons.

Minimization of the functional

$$\phi(\lambda_1, \lambda_2; v_z, \pi_z, f_Q) \equiv \langle 0|e^{-\mathcal{S}}(H - v_z \mathcal{P}_z)e^{\mathcal{S}}|0\rangle \tag{11}$$

yields $\pi_z = v_z/\sqrt{\lambda_2}$, and equation (6) scales to

$$f_Q = V_Q \sigma_Q (1 - v_z q_z)^{-1} \tag{12}$$

wherein the Lagrange multiplier v_z is to be identified as the polaron velocity (see, e.g. Parker *et al* 1974).

Substituting the optimal fits for π_z and f_Q back into equation (11) we find

$$\phi(\lambda_1, \lambda_2; v_z) = \langle 0|H'|0\rangle - \tfrac{1}{4}v_z^2 + \sum_Q V_Q^2 \sigma_Q^2 [1 - (1 - v_z q_z)^{-1}]. \tag{13}$$

For the case where $\langle 0|e^{-\mathcal{S}}\mathcal{P}_z e^{\mathcal{S}}|0\rangle = 0$, the last two terms in this expression are identically zero which, however, should not be disregarded *a priori* in order to keep trace of the effective mass. Retaining terms up to second order in v_z, equation (13) can be written alternatively as

$$\phi(\lambda_1, \lambda_2; v_z) = \langle 0|H'|0\rangle - \tfrac{1}{4}v_z^2 - \sum_Q (v_z q_z)^2 V_Q^2 \sigma_Q^2 \tag{14}$$

from which we identify the polaronic mass $m_{\mathrm{p}}^{(z)}$ as

$$\begin{aligned} m_{\mathrm{p}}^{(z)}/m &= 1 + 4\sum_Q q_z^2 V_Q^2 \sigma_Q^2 \\ &= 1 + 2\alpha(\lambda_1^2\lambda_2^3/\pi)^{1/2}(\lambda_2 - \lambda_1)^{-1}[1 - (\lambda_2/\lambda_1 - 1)^{-1/2}\tan^{-1}(\lambda_2/\lambda_1 - 1)^{1/2}]. \end{aligned} \tag{15}$$

In order to calculate the mass in the directions perpendicular to the z axis we retrieve the same formulation, where now p_z is replaced by the transverse momentum, i.e. $p_\mu = \frac{1}{2}\sqrt{\lambda_1}(b_\mu + b_\mu^\dagger + \pi_\mu), \mu = x, y$, and the corresponding functional to be minimized is

$$\phi(\lambda_1, \lambda_2; \boldsymbol{v}, \boldsymbol{\pi}, f_Q) \equiv \langle 0|e^{-\mathcal{S}}\left(H - \boldsymbol{v}\cdot\boldsymbol{p} - \boldsymbol{v}\cdot\sum_Q \boldsymbol{q} a_Q^\dagger a_Q\right)e^{\mathcal{S}}|0\rangle. \tag{16}$$

With optimal $\boldsymbol{\pi}$ and f_q, equation (16), up to order v^2, conforms to

$$\phi(\lambda_1, \lambda_2; \boldsymbol{v}) = \langle 0|H'|0\rangle - \tfrac{1}{4}v^2 - \sum_Q (\boldsymbol{v}\cdot\boldsymbol{q})^2 V_Q^2 \sigma_Q^2 \tag{17}$$

implying

$$\begin{aligned} m_{\mathrm{p}}^{(xy)}/m &= 1 + 2\sum_Q q^2 V_Q^2 \sigma_Q^2 \\ &= 1 + \alpha(\lambda_1^2\lambda_2^3/\pi)^{1/2}(\lambda_2 - \lambda_1)^{-1} \\ &\quad \times [(\lambda_1/\lambda_2 - \lambda_1)^{-1/2}\tan^{-1}(\lambda_2/\lambda_1 - 1)^{-1/2} - \lambda_1/\lambda_2] \end{aligned} \tag{18}$$

for the polaronic mass in the x, y directions.

From equation (15) or (18) the bulk polaron mass can be achieved analytically as a function of α simply by considering the asymptotic limit where both λ_1 and λ_2 approach the same value, $\lambda = 4\alpha^2/9\pi$, which minimizes the ground-state energy. For the 3D mass we thus obtain

$$m_{\mathrm{p}}^{(3\mathrm{D})}/m = 1 + \frac{2\alpha}{3\sqrt{\pi}}\lambda^{3/2} \simeq \frac{16}{81\pi^2}\alpha^4. \tag{19}$$

A further well established extreme is the strict two-dimensional characterization of the polaron ($\omega_1 = 0, \omega_2 \gg 1$) where in equation (18) $\lambda_2 \to \infty$ and $\lambda_1 = \pi\alpha^2/4$, yielding

$$m_{\mathrm{p}}^{(2\mathrm{D})}/m = 1 + \frac{\sqrt{\pi}\alpha}{2}\lambda_1^{3/2} \simeq \frac{\pi^2}{16}\alpha^4.$$

In figure 3 we display the effective mass as a function of either ω_1 or ω_2, respectively, for when the polaron is taken to be bounded within QWW-like ($\omega_2 = 0$) or Q2D slab-like ($\omega_1 = 0$) potentials. Starting from the bulk value (19), the effective polaron mass in the Q1D and Q2D geometries becomes considerably pronounced with shrinking wire radius or decreasing slab width. In the slab configuration the effective mass displays an asymptotic profile and eventually conforms to the limiting value (20), whereas in the tubular confinement the enhancement in the mass is at a much faster rate accompanied by an ever growing density of virtual phonons.

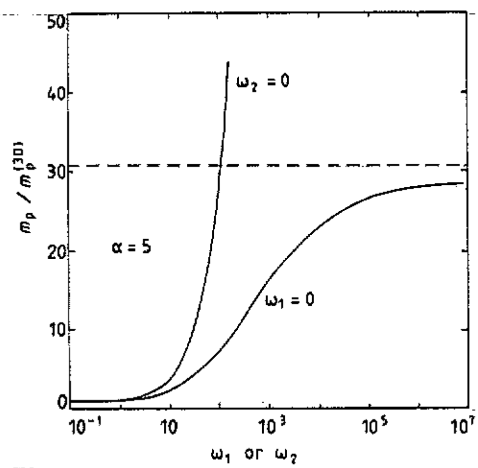

Figure 3. The effective polaron mass versus the degree of confinement for the slab-like ($\omega_1 = 0$) and the wire-like ($\omega_2 = 0$) geometries. The horizontal broken line refers to the polaron mass in the strict 2D-limit.

In this report we have retrieved the basic qualitative features of the strongly coupled polaron in confined structures and have given a wide theoretical insight into the electron–phonon interaction effects as a function of the effective dimensionality. A remark concerning the reliability of the values derived in this work is that in actual materials of interest the electron–phonon coupling is rather weak and consequently the theory we have adopted fails to reflect a totally dependable characterization of the problem. One further remark is that high degrees of localization in reduced dimensionalities lead to an enhancement in the effective phonon coupling which in turn brings about the possibility that, in spite of a small coupling constant, the problem may as well have a strong-coupling counterpart coming from confinement effects. The problem in its most general form is therefore somewhat involved and requires an interpolating theory accounting for both the strong- and weak-coupling aspects all at once.

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