Weak-coupling optical polaron in QW-confined media

1991 J. Phys.: Condens. Matter 3 4357

(http://iopscience.iop.org/0953-8984/3/24/005)

J. Phys.: Condens. Matter 3 (1991) 4357–4364. Printed in the UK

Weak-coupling optical polaron in QW-confined media

T Yıldırım†§ and A Erçelebi‡

† Department of Physics, Middle East Technical University, 06531 Ankara, Turkey
‡ Department of Physics, Bilkent University, 06533 Bilkent, Ankara, Turkey

Received 21 December 1990

Abstract. The ground state of the Fröhlich polaron is retrieved as a function of the degree of confinement in a three-dimensional quantum well with tunable barrier potentials. A unified overview of the binding energy interpolating between all possible confinement geometries is provided within the framework of the second-order perturbation theory.

1. Introduction

In the last two decades much attention has been focussed on the study of polarons of reduced dimensionality in the context of quantum-well confined semiconductor structures. Of particular interest is the quasi-two-dimensional (Q2D) optical polaron, with most emphasis devoted to its strict two-dimensional (2D) characterization within the framework of an idealized approximation, accounting for the almost-planar aspect of an electron in a thin quantum well and yet interacting with the bulk LO-phonon modes of the well material [1, 2]. The common theoretical prediction led by the relevant works in the literature [1–5] is that the electron interacts more effectively with the phonons in two dimensions and consequently certain polaron quantities scale by rather large factors over their corresponding bulk values. The ground state binding, for instance, becomes deepened by a factor of $\frac{1}{2}\pi$ at weak coupling, and by $\frac{3}{8}\pi^2 \simeq 3.7$ under the strong coupling (adiabatic) approach. Similar features show up for further other quantities like the effective polaron mass or the mean phonon density accompanying the electron. Going on further to quasi-one-dimensionally (Q1D) confined configurations, such as for instance the quantum-well wire (QWW) geometry, the electron phonon coupling becomes even stronger with much larger polaronic binding than in comparable Q2D systems [6]. The role the confinement effects play in pronounced phonon coupling can readily be confirmed by making further reference to the magnetopolaron problem where it has been well established that the phonon coupling-induced corrections in the energy levels grow larger with increasing degree of localization brought about by the magnetic field (cf [7]).

In this work we focus our attention on the ground-state property of the confined polaron and present a comprehensive review through a description interpolating between integer space limits. We adopt a rather simple model of an electron immersed

§ Present address: Department of Physics, University of Pennsylvania, Philadelphia, PA 19104-6391, USA.

0953-8984/91/244357+08$03.50

in the field of bulk LO-phonons and bounded within an anisotropic potential box with parabolic potential barriers, i.e., $V(\rho, z) = \frac{1}{2}(\kappa_1\rho^2 + \kappa_2 z^2)$. Such a choice for the confining potential, besides facilitating the calculations, is also compatible with the usual harmonic description of the rapidly fluctuating electron due to random scattering in the phonon field. The respective force constants κ_1 and κ_2 in the potential will be treated as tunable parameters refering to the degree of confinement in the x–y and z directions. By varying κ_1 and/or κ_2 from zero to values much larger than unity one can display a unifying picture tracing the transition from the bulk to various confinement geometries, namely the quasi-two- and quasi-one-dimensional limits as well as the quantum well box (QWB) case.

It should be noted that for the present we take the confined electron as interacting with the bulk phonon modes only, and refrain from including any modifications such as those due to phonon confinement, the polaron-induced band non-parabolicity or the loss of validity of the effective mass approximation in thin quantum wells. Our concern is primarily to give a clear view of the bulk phonon effects as a function of the dimensionality stripped from all other perturbing quantities.

Since in the most commonly studied compound materials (such as GaAs, for instance) the electron–phonon coupling is rather weak, an appropriate approach is to treat the Fröhlich interaction as a perturbation. In the following we restrict our considerations solely to the weak-coupling regime. A discussion of the same model within the strong-coupling polaron theory has already been provided in a previous paper [8] with which we shall make some correspondence in the next section.

2. Theory and discussion

Using units for which $2m^* = \hbar = \omega_{\mathrm{LO}} = 1$, the Hamiltonian describing the confined electron coupled to LO-phonons is given by

$$H = H_{\mathrm{e}} + \sum_{Q} a_Q^{\dagger} a_Q + H_{\mathrm{e-ph}} \tag{1}$$

where

$$H_{\mathrm{e}} = p^2 + p_z^2 + \tfrac{1}{4}(\omega_1^2\rho^2 + \omega_2^2 z^2) \tag{2}$$

is the electron part, and

$$H_{\mathrm{e-ph}} = \sum_{Q} V_Q [a_Q \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{\rho}) \exp(\mathrm{i}q_z z) + \mathrm{HC}] \tag{3}$$

is the Fröhlich interaction. In the above, (ρ, z) and $(\boldsymbol{p}, p_z)$ denote the electron position and momentum, and $\omega_i = \sqrt{\kappa_i/m^*\omega_{\mathrm{LO}}^2}$ $(i = 1, 2)$ stand for the dimensionless measures of the degree of confinement in the transverse $(x$–$y)$ and longitudinal (z) directions. The interaction amplitude is related to the electron–phonon coupling constant α and the phonon wavevector $\boldsymbol{Q} = (\boldsymbol{q}, q_z)$ through $V_Q = \sqrt{4\pi\alpha}/Q$.

Depending on the so called bulk-phonon approximation we first make correspondence with the Q2D slab- and Q1D wire-like confining geometries. A general view in the overall range of ω_1 and ω_2 will be presented at the end of this section.

2.1. Q2D and Q1D confinements

Setting $\omega_1 = 0$ and varying ω_2 from zero to infinity one can trace the bulk polaron properties go over to those of a strictly 2D-polaron. On the other hand, deleting the confining potential along the z-axis ($\omega_2 = 0$) and fixing ω_1 at non-zero finite values, the theory reflects the Q1D-description in a QWW-like tubular structure. In the following we shall use ω to mean $\omega_1(\omega_2)$ when $\omega_2(\omega_1) = 0$.

We first derive the binding energy and the polaron mass in the slab-like confinement. Writing $V(\rho, z) = \frac{1}{4}\omega^2 z^2$, the unperturbed wave equation for the electron is given by

$$H_e \Phi_{k,\nu}(\rho, z) = \epsilon_\nu(k)\Phi_{k,\nu}(\rho, z) \qquad \nu = 0, 1, 2, \ldots \tag{4}$$

where

$$\Phi_{k,\nu}(\rho, z) = \frac{1}{\sqrt{2^\nu \nu!}}\left(\frac{\omega}{2\pi}\right)^{1/4} H_\nu\left(\sqrt{\frac{\omega}{2}}z\right)\exp(-\tfrac{1}{4}\omega z^2)\phi_k(\rho) \tag{5}$$

with H_ν denoting the Hermite polynomial of degree ν. Since $\alpha \ll 1$, we assume the electron to be almost free in the transverse directions and thus utilize a plane wave representation for its motion parallel to the x–y plane, i.e., we take $\phi_k(\rho) \sim \exp(\mathrm{i}k\cdot\rho)$. The corresponding energy eigenvalues of equation (4) are then given by

$$\epsilon_\nu(k) = (\nu + \tfrac{1}{2})\omega + k^2 . \tag{6}$$

We begin by expressing the general total wavefunction in a product form of the electron and phonon parts, i.e. $\Psi_{\text{total}} = \Phi_{k,\nu}(\rho, z)\varphi_{\text{ph}}$. For the ground state we take the electron to be in the lowest subband ($\nu = 0$) and select φ_{ph} as the phonon vacuum $|0\rangle$ simply due to that at low temperatures ($kT \ll \hbar\omega_{\text{LO}}$) there will be no effective phonons.

The first non-vanishing contribution to the ground-state energy comes from the term which is of second order in the interaction amplitude, i.e.

$$\Delta E_g^{(2)} = -\sum_Q \sum_{k'} \sum_\nu \frac{|\langle\Phi_{k',\nu}|\langle 1_Q|H_{e-ph}|0\rangle|\Phi_{k,0}\rangle|^2}{\epsilon_\nu(k') - \epsilon_0(k) + 1} . \tag{7}$$

With the form (3) for the Fröhlich interaction, the above equation can be written alternatively as

$$\Delta E_g^{(2)} = -\sum_Q V_Q^2 \sum_{k'} \sum_\nu \frac{|\langle\phi_{k'}|\exp(-\mathrm{i}q\cdot\rho)|\phi_k\rangle|^2}{\omega\nu + 1 + k'^2 - k^2}|h_\nu(q_z)|^2 \tag{8}$$

where

$$h_\nu(q_z) = \frac{1}{\sqrt{2^\nu \nu!}}(\frac{\omega}{2\pi})^{1/2}\int_{-\infty}^{\infty} \mathrm{d}z\, \exp(-\mathrm{i}q_z z)H_\nu\left(\sqrt{\frac{\omega}{2}}z\right)\exp(-\tfrac{1}{2}\omega z^2)$$

$$= \frac{(-\mathrm{i})^\nu}{\sqrt{\nu!}}\left(\frac{q_z^2}{\omega}\right)^{\nu/2}\exp\left(-\frac{q_z^2}{2\omega}\right). \tag{9}$$

Projecting out the k' summation we obtain

$$\Delta E_g^{(2)} = -\sum_Q V_Q^2 \sum_\nu \frac{1}{\nu!}\frac{1}{\omega\nu + 1 + q^2 - 2k\cdot q}\left(\frac{q_z^2}{\omega}\right)^\nu \exp\left(-\frac{q_z^2}{\omega}\right). \tag{10}$$

It should be noted that due to the term q^2 in the energy denominator the contributions to the $\boldsymbol{Q}$ summation fall off rather rapidly when this term becomes large compared to the phonon energy. There is therefore an efficient contribution of the virtual phonons to the polaron energy only when q is not too large. In this regard, for small electron momentum ($\boldsymbol{p} \simeq 0$), the term $2\boldsymbol{k}\cdot\boldsymbol{q}$ will also be small. Thus, expanding the summand in equation (10) in a power series up to seond order in $\boldsymbol{k}\cdot\boldsymbol{q}$ we obtain

$$\Delta E_g^{(2)} = -\sum_{Q} V_Q^2 \exp\left(-\frac{q_z^2}{\omega}\right) \sum_{\nu} \frac{1}{\nu!}\left(\frac{q_z^2}{\omega}\right)^{\nu} \left(\frac{1}{\omega\nu + 1 + q^2} + \frac{(2\boldsymbol{k}\cdot\boldsymbol{q})^2}{(\omega\nu + 1 + q^2)^3}\right). \tag{11}$$

Using the identity

$$\sum_{\nu=0}^{\infty} \frac{1}{\nu!} \frac{\beta^{\nu}}{(a\nu + b)^{n+1}} = \frac{1}{n!} \int_0^{\infty} \mathrm{d}\eta\, \eta^n \mathrm{e}^{-b\eta} \exp(\beta \mathrm{e}^{-a\eta}) \qquad n = 0, 1, 2, \ldots \tag{12}$$

and defining

$$\varrho_Q = \exp[-\tfrac{1}{2}(q^2 + q_z^2/\sigma)\eta] \tag{13}$$

with

$$\sigma = \frac{\omega\eta}{1 - \mathrm{e}^{-\omega\eta}} \tag{14}$$

the ground-state energy, $E_g = \frac{1}{2}\omega + k^2 + \Delta E_g^{(2)}$, can be written as

$$E_g = \frac{1}{2}\omega - \varepsilon_p + k^2(1 - \mu) \tag{15}$$

where

$$\varepsilon_p = \sum_{Q} V_Q^2 \int_0^{\infty} \mathrm{d}\eta\, \mathrm{e}^{-\eta} \varrho_Q^2 \tag{16}$$

and

$$\mu = \sum_{Q} V_Q^2 q^2 \int_0^{\infty} \mathrm{d}\eta\, \eta^2 \mathrm{e}^{-\eta} \varrho_Q^2 . \tag{17}$$

In the above, ε_p is the polaron binding energy and μ the polaronic contribution to the composite inertia of the electron together with the concomitant cloud of virtual phonons, i.e. $m_p/m^* = (1 - \mu)^{-1} \simeq 1 + \mu$.

For the QWW-like tubular confinement we take the transverse part of the electron wavefunction as consisting of harmonic oscillator states written in a product form in the variables x and y, and use a plane wave description along the axis of the tube. We find that the corresponding expressions for ε_p and μ are almost identical to those derived for the slab geometry. The only modifications are that in equations (13), (16) and (17), $q_z^2(q^2)$ replaces $q^2(q_z^2)$, and a factor of 2 multiplies the right-hand side of equation (17).

For $\omega = 0$ and $\omega \to \infty$ the analytic evaluation of the integrals in equations (16) and (17) are readily available. In the former case $\sigma = 1$ and we obtain the results relevant to the bulk polaron. For the binding energy we have

$$\varepsilon_p^{(3D)} = \sum_{Q} V_Q^2 \int_0^{\infty} \mathrm{d}\eta\, \mathrm{e}^{-\eta} \exp[-(q^2 + q_z^2)\eta] = \sum_{Q} \frac{V_Q^2}{1 + Q^2} = \alpha . \tag{18}$$

Similarly, equation (17) reduces to

$$\mu^{(3D)} = \sum_Q V_Q^2 q^2 \int_0^\infty d\eta\, \eta^2 e^{-\eta} \exp[-(q^2 + q_z^2)\eta] = \sum_Q V_Q^2 q^2 \frac{2}{(1+Q^2)^3} = \frac{\alpha}{6}. \tag{19}$$

In the strict 2D limit ($\omega \to \infty$), σ^{-1} tends to zero, and the corresponding integrals simplify to

$$\varepsilon_p^{(2D)} = \sum_Q \frac{V_Q^2}{1+q^2} = \frac{\pi}{2}\alpha. \tag{20}$$

and

$$\mu^{(2D)} = \sum_Q V_Q^2 q^2 \frac{2}{(1+q^2)^3} = \frac{\pi}{8}\alpha. \tag{21}$$

In figure 1 we provide plots of the binding energy and the phonon contribution to the effective mass as functions of the degree of confinement. We note that with increasing barrier slopes of the confining potential, the binding in the wire-like confinement rapidly becomes much deeper than in the Q2D configuration, which follows essentially from the fact that in the wire geometry the polaron becomes highly localized towards the wire axis due to confinement coming from all transverse directions.

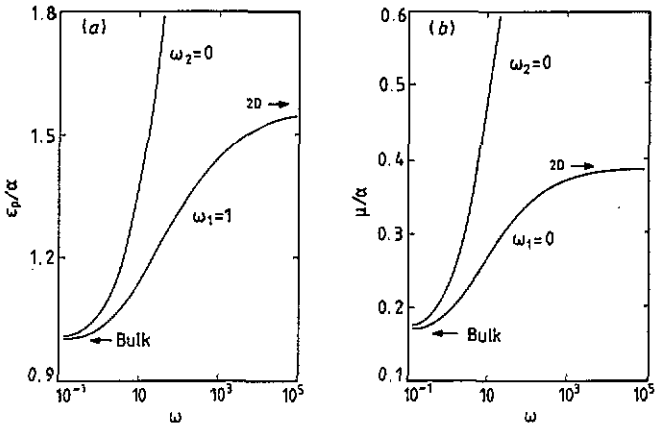

Figure 1. (*a*) the binding energy ε_p, and (*b*) the phonon correction to the effective mass μ as functions of the degree confinement for the slab- ($\omega_1 = 0$) and wire-like ($\omega_2 = 0$) confinement geometries.

2.2. Confinement in the overall range of ω_1 and ω_2

For a total overview interpolating between all possible extremes of the effective dimensionality we refer back to equation (2) and revise the perturbation calculation when ω_1 and ω_2 are both non-zero in general. The binding energy thus obtained is given by the same expression as in equation (16) where now ϱ_Q reads as

$$\varrho_Q = \exp\left[-\frac{1}{2}\left(\frac{q^2}{\sigma_1} + \frac{q_z^2}{\sigma_2}\right)\eta\right] \tag{22}$$

with

$$\sigma_i = \frac{\omega_i \eta}{1 - \exp(-\omega_i \eta)} \qquad i = 1, 2. \tag{23}$$

Projecting out the summations over the wavevector components we obtain

$$\varepsilon_p = \frac{\alpha}{\sqrt{\pi}} \int_0^\infty d\eta\, e^{-\eta} \sqrt{\frac{\sigma_2}{\eta}}\, \frac{\tan^{-1}\gamma}{\gamma} \tag{24}$$

where

$$\gamma = \sqrt{\sigma_2/\sigma_1 - 1} \tag{25}$$

Correspondingly, the first order perturbation correction to the polaron ground state can be obtained as

$$\delta\Psi^{(1)} = \sum_Q V_Q v_Q^* a_Q^\dagger |0\rangle \Phi_g \tag{26}$$

where Φ_g refers to the lowest bound-state wavefunction of the unperturbed electron, and

$$v_Q = \int_0^\infty d\eta\, e^{-\eta} \exp\left(-\frac{q^2 - q^2(\eta)}{2\omega_1} - \frac{q_z^2 - q_z^2(\eta)}{2\omega_2}\right) \exp[i\boldsymbol{Q}(\eta)\cdot\boldsymbol{r}] \tag{27}$$

in which

$$\boldsymbol{Q}(\eta) = \{q(\eta), q_z(\eta)\} = \{q\exp(-\omega_1\eta), q_z\exp(-\omega_2\eta)\}\,. \tag{28}$$

It should be remarked that in equation (26) only the lowest subband shows up explicitly, and the electron states above the ground level take part in the theory somewhat implicitly through the parameter v_Q. A glance at equation (27) reveals that v_Q consists of a Gaussian-type bounded structure and a plane-wave counterpart, both of which are related to the degree of confinement through the modified wavevector $\boldsymbol{Q}(\eta)$. In fact, it is only by means of $\boldsymbol{Q}(\eta)$ that a detailed interbalance is set up between the two aspects (localized and free) of the problem, since the way ω_1 and ω_2 enter the theory is through $q(\eta)$ and $q_z(\eta)$.

In the limit $\alpha \ll 1$, the electron is only very weakly coupled to the phonon field, and if additionally the confining potential is turned off, an appropriate description of the electron should be a plane-wave representation in all directions. Indeed, when, $\omega_1 = \omega_2 = 0$, the Gaussian structure in the polaron wavefunction is totally removed and v_Q reduces to $\exp(i\boldsymbol{Q}\cdot\boldsymbol{r})$. For a confined qeometry ($\omega_1, \omega_2 \gg 1$) however, the situation is just the opposite where the theory imparts most dominance to the localized counterpart of the problem. In this extreme, the energy levels are distantly separated and those above the ground level do not yield any significant contribution. Alternatively, this can be seen from the perturbation expansion (cf equation (10)): the term with quantum numbers all zero leads to the smallest energy denominator and hence to the largest contribution in the perturbation series. Making reference to the slab-like confinement ($\omega_1 = 0$), for instance, we see that as ω_2 is increased to large values, the dominant z profile turns out to be that of the lowest bound state (Gaussian) alone, and eventually when ω_2 becomes infinite the waveform conforms to $\delta(z)$, thus restricting the electronic motion in a sheet of zero thickness. This readily reflects our results in that $q_z(\eta)$ in equation (27) and the factor σ_2^{-1} in equation (22) tend to zero, resulting in a complete removal of any z-dependence in the dynamical behaviour of the electron, compatible with the strict 2D characterization [1] of the confined polaron. In all these respects, we observe that the exponential weights $\exp(-\omega_1\eta)$ and

$\exp(-\omega_2\eta)$, which scale q and q_z play an essential role in determining the plane-wave aspect of the electron, or equivalently the percent enrollment of the subbands lying above the ground level.

Before giving our numerical results we would like to comment further on the implications of the present equations. It should be noted that the binding energy expression given through equations (22)–(25) bears a close structural resemblance to that obtained previously for the strongly coupled polaron within the same confining potential [8], and moreover, for large values of ω_1 and ω_2, the resemblence becomes an identity. This follows essentially from the fact that when $\omega_1, \omega_2 \gg 1$, the perturbation series can be approximated by its leading term, i.e., $\Delta E_g^{(2)} = -\sum_Q f_Q^2$, where $f_Q = V_Q\langle\Phi_g|\exp(-iQ\cdot r)|\Phi_g\rangle$ is the optimal fit to the conventional displaced oscillator transformation, $\exp\sum_Q f_Q(a_Q - a_Q^\dagger)$, of the strong-coupling polaron theory (cf [8]). In this regard, we thus note that high degrees of confinement raise the possibility that, in spite of a small coupling constant, a pseudo-strong coupling can be reached.

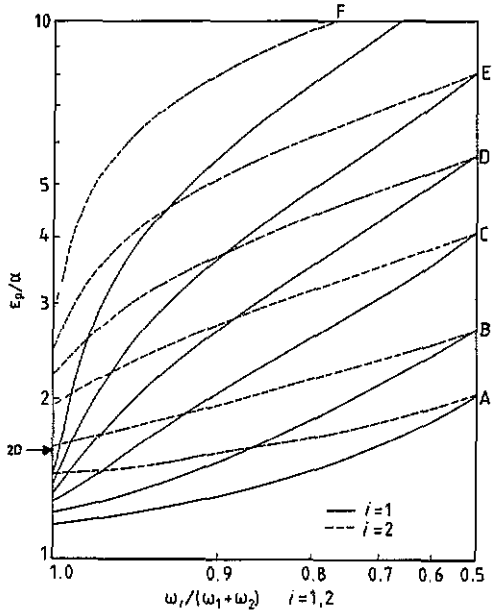

Figure 2. The binding energy as a function of the effective dimensionality. The succession of full (broken) curves A, B, C, D, E and F are for fixed values of $\omega_2(\omega_1) =$ 10, 20, 50, 100, 200 and 500 with ω_1 (ω_2) varied, respectively. The intercepts on the left margin refer to the slab- (wire-)like configurations, and those on the right margin yield the binding energy values in the spherically symmetric ($\omega_1 = \omega_2$) confinement.

In order to achieve a general insight into the enhancement in the phonon coupling in reduced dimensionalities, we integrate equation (24) numerically over the entire range of the degree of confinement. For the Q2D-configuration with $\omega_2 = 10$ we obtain $\varepsilon_p/\alpha \simeq 1.16$. For the case of a wire geometry with $\omega_1 = 10$ the binding gets deeper by a factor of about 1.44, and for the spherically symmetric confinement ($\omega_1 = \omega_2 = 10$) we have $\varepsilon_p/\alpha \simeq 2.02$. The corresponding values when ω_1 and/or $\omega_2 = 100$ are 1.33, 2.23 and 5.72. In figure 2 we provide a unified display of the polaron binding over a reasonably broad range of ω_1 and ω_2 covering all interesting extremes

of the confinement geometry. The intercepts of the full (broken) curves on the left margin give the binding energy values in the Q2D- (Q1D-)dimensional configurations, and going over to the right margin the binding is observed to get much stronger since now the polaron becomes squeezed symmetrically in all directions (reflecting a QW-box- or QW-dot-type localization of the polaron).

In conclusion, we have reviewed the ground-state property of the optical polaron in low-dimensional geometries and have provided a unifying insight into the electron phonon interaction as a function of the degree of confinement at weak coupling. We remark that in certain compound semiconductor structures, such as those consisting of elements from columns II and VI of the periodic table, the relevant coupling constants cannot be regarded as sufficiently small ($\alpha \simeq 0.4$ for CdTe, for instance) for the perturbation approach to be totally dependable. In its most general form the problem may thus involve a vague strong-coupling counterpart, making it neccessary to adopt powerful interpolating theories that account for the percent involvement of the weak- and strong-coupling aspects simultaneously. This, however, is beyond the scope of the present work and will be the subject of a future paper.

References

[1] Das Sarma S and Mason B A 1985 *Ann. Phys., NY* **163** 78
[2] Peeters F M and Devreese J T 1987 *Phys. Rev.* B **36** 4442
[3] Huybrechts W J 1978 *Solid State Commun.* **28** 95
[4] Xiaoguang Wu, Peeters F M and Devreese J T 1985 *Phys. Rev.* B **31** 3420
[5] Larsen D M 1987 *Phys. Rev.* B **35** 4435
[6] Degani M H and Hipólito O 1988 *Solid State Commun.* **65** 1185
[7] Peeters F M and Devreese J T 1985 *Phys. Rev.* B **31** 3689
[8] Yıldırım T and Erçelebi A 1991 *J. Phys.: Condens. Matter* **3** 1271