Polaron binding energy and effective mass in the GaAs film

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Abstract. The binding energy and effective mass of a polaron in a GaAs film deposited on the Al₀.₃Ga₀.₇As substrate are studied theoretically by using the fractional-dimensional space approach. Our calculations show that the polaron binding energy and mass shift decrease monotonously with increasing the film thickness. For the film thicknesses with \( L_w \leq 70\,\text{Å} \) and the substrate thicknesses with \( L_b \leq 200\,\text{Å} \), the different values of the substrate thickness influence the polaron binding energy and mass shift in the GaAs film. The polaron binding energy and mass shift increase monotonously with increasing the substrate thickness. For the film thickness with \( L_w \geq 70\,\text{Å} \) or the substrate thicknesses with \( L_b \geq 200\,\text{Å} \), the different values of the substrate thickness have no significant influence on the polaron binding energy and mass shift in the GaAs film deposited on the Al₀.₃Ga₀.₇As substrate.

1. Introduction
The film is an important low-dimensional structure. It is important for applications in the electronic and optoelectronic devices. One of the effects that has attracted the attention of a considerable amount of researchers is the polaron effect. In particular, the GaAs film deposited on the Al₀.₃Ga₀.₇As substrate is an important low-dimensional heterostructure. It is well known that the electron–LO phonon interaction leading to the polaron effect may be significantly modified by the confinement. These modifications in the polaron effect can strongly influence the optical and transport properties of such weak polar low-dimensional systems. Consequently, a wide variety of theoretical models has been proposed by different researchers. However, most of the models have tedious calculations [1-5]. Of particular interest to this paper is the original approach proposed by He [6,7]. In this approach the anisotropic (or confined) interactions in real three-dimensional (3D) space are treated as isotropic (or unconfined) ones in an effective fractional-dimensional environment, which dimension constitutes a measure of the degree of anisotropy (or confinement) of the actual physical system. The main advantage of this approach lies in the fact that all information about a perturbation (confinement or anisotropy) can be introduced in a single value—the dimensionality. Thus given this simple value, the real system can be modeled in a simple analytical way. In the last few years, the fractional-dimensional space approach has been successfully used in modelling exciton [8-12], magnetoexciton [13,14], biexciton [15-17] and impurity states [11,18-24] in semiconductor heterostructures. The Stark shift of excitonic complexes [25], the refractive index [26] and electron–phonon effects on excitons...
in quantum well structures [27] have also been studied within the fractional-dimensional space approach. In recent years, some researchers have used the fractional-dimensional space approach to treat the polaron problems in low-dimensional structures, and obtained an easy estimation of the polaron corrections with a good accuracy [28-33].

We have studied the effects of confined longitudinal and interface optical phonons on excitons in an asymmetric quantum well [34]. In this paper, we extend the fractional-dimensional space approach to the case of a polaron confined to a GaAs film deposited on the Al$_{0.3}$Ga$_{0.7}$As substrate by using a consistent set of material parameters as discussed by Smondyrev et al. [35]. As functions of the film thickness, the polaron binding energy and mass shift are calculated. This paper is organized as follows. In Section 2 the theoretical basis of the fractional-dimensional model for polarons in symmetric [28-30] and asymmetric [31] quantum wells, is extended to the case of polarons confined in our GaAs–Al$_{0.3}$Ga$_{0.7}$As system. Numerical results and discussion are in Section 3, and conclusions are in Section 4.

2. Theoretical framework

For a polaron in a GaAs film deposited on the Al$_{0.3}$Ga$_{0.7}$As substrate and the case of no electron escaping from the GaAs–Al$_{0.3}$Ga$_{0.7}$As system, the potential of the system is characterized by

\[
V(z) = \begin{cases} 
V_w (= 0) & \text{if } 0 \leq z \leq L_w, \\
V_b & \text{if } L_w < z < L_w + L_b, \\
\infty & \text{otherwise},
\end{cases}
\]

(1)

where $L_w$ and $L_b$ represents the film thickness and substrate thickness, respectively. The subscripts $w$ and $b$ label the film (GaAs) and substrate (Al$_{0.3}$Ga$_{0.7}$As) regions, respectively. The potential energy function of the system is displayed in Fig. 1.

Within the fractional-dimensional space approach, the actual confined polaron is modeled through an unconfined effective fractional-dimensional polaron. The electron self-energy due to the electron–LO phonon interaction in the weak-coupling approximation can be calculated within second-order perturbation theory [28-31], where the polaron binding energy was given by

\[
\Delta E = \alpha \hbar \omega_{LO} G_1(D)
\]

(2)
and the polaron effective mass by

$$m^* = \frac{m}{1 - \alpha G_2(D)}.$$  \hspace{1cm} (3)

In Eqs. (2) and (3) $D$ represents the dimensionality, $\alpha$ the Fröhlich constant, $\omega_{LO}$ the LO phonon limit frequency in the non-dispersive approximation, and $m$ is the electron effective mass. The $D$-dependent functions $G_1(D)$ and $G_2(D)$ are given by

$$G_1(D) = \frac{\sqrt{\pi} \Gamma[(D-1)/2]}{2 \Gamma[D/2]}$$ \hspace{1cm} (4)

and

$$G_2(D) = \frac{\sqrt{\pi} \Gamma[(D-1)/2]}{4 D \Gamma[D/2]},$$ \hspace{1cm} (5)

respectively. In Eqs. (4) and (5) $\Gamma(x)$ represents the Gamma function.

The set of equations (2)-(5) determines the polaron corrections in a fractional-dimensional bulk. It is straightforward to check that these equations recover the well-known forms in both the exact two-dimensional (2D) and three-dimensional (3D) limits.

The dimensional parameter $D$ that guarantees the mapping of the actual system into the fractional-dimensional environment can be calculated through the relation [28-31]

$$D = 3 - \exp[-\xi],$$ \hspace{1cm} (6)

where $\xi$ represents the ratio of the length of confinement to the effective characteristic length of interaction. The effective length that characterizes the electron–phonon interaction is the polaron diameter $2R_p$ (with $R_p = \sqrt{\hbar/2m\omega_{LO}}$ being the polaron radius), while the length of confinement is characterized by an effective film thickness $L_w^*$ that takes account of the carrier penetration into the substrate. In the case of our system we have

$$L_w^* = L_w + \frac{1}{k_b}$$ \hspace{1cm} (7)

and Eq. (6) reduces to

$$D = 3 - \exp \left[-\frac{L_w^*}{2R_p}\right].$$ \hspace{1cm} (8)

In Eq. (7) $k_b$ represent the electron wave vector in the substrate.

After solving the Schrödinger equation

$$\left[ -\frac{\hbar^2}{2} \frac{d}{dz} \left( \frac{1}{m(z)} \frac{d}{dz} \right) + V(z) \right] \psi = E\psi$$ \hspace{1cm} (9)

that describes the motion of the single electron confined in the GaAs film deposited on the $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ substrate potential [Eq. (1)], $m(z)$ represent the electron $z$-dependent effective mass

$$m(z) = \begin{cases} m_w & \text{if} \quad 0 \leq z \leq L_w, \\ m_b & \text{if} \quad L_w < z < L_w + L_b, \end{cases}$$ \hspace{1cm} (10)

the value of $k_b$ can be obtained from the relation

$$k_b = \sqrt{\frac{2m_b(V_b - E)}{\hbar}}.$$ \hspace{1cm} (11)

$E$ represents the electron ground-state energy in our GaAs–$\text{Al}_x\text{Ga}_{1-x}\text{As}$ system.
In the GaAs film deposited on Al$_{0.3}$Ga$_{0.7}$As substrate system, the material parameters that characterize the polaron properties differ when passing from the film to the substrate region. In order take account of this fact, we may assign to the effective fractional-dimensional bulk an average of the material parameters over the polaron positions. Our effective fractional-dimensional electron–phonon interaction is then characterized by the following set of mean parameters:

\[
\begin{align*}
    m^{-1} &= \sum_{i=w,b} \frac{P_i}{m_i}, \\
    \omega_{LO} &= \sum_{i=w,b} \omega_i P_i, \\
    \alpha &= \left[ \sum_{i=w,b} \left( \frac{P_i \omega_i}{\omega_{LO}} \sqrt{\frac{m \omega_{LO}}{m_i \omega_i}} \right) \right]^2, \\
    R_p &= \left[ \sum_{i=w,b} \left( \frac{P_i \omega_i}{\omega_{LO}} \sqrt{\frac{\alpha_i R_{pi}}{\alpha}} \right) \right]^2, \\
    R_{pi} &= \sqrt{\frac{\hbar}{2m_i \omega_i}}.
\end{align*}
\]

In Eqs. (12)-(15) $\alpha_i$ and $\omega_i$ represent the Fröhlich constants and the phonon frequencies in the different regions, and

\[
\begin{align*}
    P_w &= \int_0^{L_w} |\psi(z)|^2 dz, \\
    P_b &= 1 - P_w
\end{align*}
\]

denote the probabilities of finding the single electron in the film (GaAs) and substrate (Al$_{0.3}$Ga$_{0.7}$As) regions, respectively. The binding energy and the effective mass of a polaron in a GaAs film deposited on the Al$_{0.3}$Ga$_{0.7}$As substrate can then be computed in a very simple way from Eqs. (2), (3) and (8) and assuming the material parameter mean values defined in Eqs. (12)-(16). As functions of the film thickness and the substrate thickness, the polaron binding energy and mass shift are calculated. The numerical results and discussion are given in the following section.

3. Numerical results and discussion

The fractional dimension in the GaAs film deposited on the Al$_{0.3}$Ga$_{0.7}$As substrate as a function of the film thickness and the substrate thickness is displayed in Fig. 2. For very large film thicknesses the system behaves as a GaAs bulk and consequently the fractional dimension has the limit value $D = 3$. When the film thickness decreases, the system becomes more and more confined, the polaron turns more and more compressed, and the effective dimension decreases, reaching a minimum $D \approx 2.58$ for the film thickness $L_w \approx 42 \text{Å}$. Once the film thickness is reduced and less than the polaron size, the polaron wave function will penetrate into the substrate so that the fractional dimension increases suddenly. The results show that in the region $L_w \leq 50 \text{Å}$ and $L_b \leq 150 \text{Å}$, the different values of the substrate thickness influence the fractional dimension in the GaAs film. The fractional dimension increases slowly with increasing
the substrate thickness. In the region $L_w \geq 50\text{Å}$ or $L_b \geq 150\text{Å}$, the different values of the substrate thickness have no significant influence on the fractional dimension in the GaAs film.

The fractional-dimensional polaron binding energy as a function of the film thickness and substrate thickness in the GaAs film deposited on the Al$_{0.3}$Ga$_{0.7}$As substrate is calculated and displayed in Fig. 3. It is seen that the polaron binding energy decreases monotonously with increasing the film thickness. The polaron binding energy decreases rapidly for narrow film thicknesses, but decreases slowly for large film thicknesses. Our calculations show that in the region $L_w \leq 70\text{Å}$ and $L_b \leq 200\text{Å}$, the different values of the substrate thickness influence the polaron binding energy in the GaAs film. The polaron binding energy in the GaAs film increases slowly with increasing the substrate thickness. In the region $L_w \geq 70\text{Å}$ or $L_b \geq 200\text{Å}$, the different values of the substrate thickness have no significant influence on the polaron binding energy in the GaAs film.

Figure 2. The fractional dimension as a function of the film thickness and the substrate thickness in the GaAs film deposited on the Al$_{0.3}$Ga$_{0.7}$As substrate.

Figure 3. The fractional-dimensional polaron binding energy as a function of the film thickness and substrate thickness in the GaAs film deposited on the Al$_{0.3}$Ga$_{0.7}$As substrate.
The fractional-dimensional polaron effective mass as a function of the film thickness and substrate thickness in the GaAs film deposited on the Al$_{0.3}$Ga$_{0.7}$As substrate can be appreciated in Fig. 4, where the film thickness and the substrate thickness dependence of the polaron mass shift $\delta m = \Delta m / \Delta m_{\text{in}}$ is displayed. Notice that, $\delta m$ represents the ratio of the mass shift ($\Delta m = m^* - m$) to that in the film material ($\Delta m_{\text{in}} = m_{w}^* - m_{w}$). For brevity, from now on we will refer to $\delta m$ just as the polaron mass shift. It is seen that the variation trend of the polaron mass shift is quite similar to the polaron binding energy in the GaAs film as a function of the film thickness and substrate thickness.

4. Conclusions
In conclusion, we have extended the fractional-dimensional space approach, in which the real confined polaron in the GaAs film deposited on Al$_{0.3}$Ga$_{0.7}$As system is modeled into an effective fractional-dimensional environment in which the polaron behaves unconfined and the fractional dimension is a measure of the degree of confinement of the real system, to the study of a polaron in a GaAs film deposited on the Al$_{0.3}$Ga$_{0.7}$As substrate. The fractional-dimensional space approach allows us an estimation of the polaron binding energy and mass shift as functions of the film thickness and substrate thickness in a very simple way, avoiding the tedious and complicated calculations arising in the standard treatments. It is shown that the polaron binding energy and mass shift decrease monotonously with increasing the film thickness. For the film thicknesses with $L_w \leq 70\,\text{Å}$ and the substrate thicknesses with $L_b \leq 200\,\text{Å}$, the different values of the substrate thickness influence the polaron binding energy and mass shift in the GaAs film. The polaron binding energy and mass shift increase monotonously with increasing the substrate thickness. For the film thickness with $L_w \geq 70\,\text{Å}$ or the substrate thicknesses with $L_b \geq 200\,\text{Å}$, the different values of the substrate thickness have no significant influence on the polaron binding energy and mass shift in the GaAs film deposited on the Al$_{0.3}$Ga$_{0.7}$As substrate.

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