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Effective carrier interaction in semiconductor thin films: A model-independent formula

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ABSTRACT

It is shown that the effective carrier interaction in semiconductor thin films, which is essentially of a non-Coulomb type, depends on the layer thickness but it is not sensitive to the form of quantum well. As a consequence the analytical expression for the effective 2D interaction potential, obtained using the parabolic quantum well model, can be used as a general (model-independent) formula. As an example, we have considered the electrons localized in a quantum dot. It is demonstrated that, when the quantum well confinement is much stronger than the lateral one, the results obtained using the 2D approach with the effective potential are in a good agreement with the full 3D calculations.

1. Introduction

Fast development of the semiconductor technology has made possible to fabricate the heterostructures consisting of various thin ($\sim 10\,\mathrm{nm}$) semiconductor/insulator layers (films). By inserting a semiconductor between two insulator layers, one obtains a realization of the quantum well for electrons (and holes) in the semiconductor (see e.g. Refs. [1,2]). The thickness of this quantum well is for an order of magnitude or more larger than the lattice constant, allowing the effective mass approximation, but it is small enough that at low temperatures only the quantum state with the lowest energy ε_1 (the ground state of the quantum well) is occupied by electrons (see the bottom of Fig. 1). Then, in the direction perpendicular to the film (z-axis) the electrons in the semiconductor perform only the zero-point motion, i.e. essentially they can only move laterally (*xy*-plane) in the layer. If we additionally confine this two-dimensional (2D) electron gas laterally, we shall obtain the 'zero-dimensional' system called quantum dot (QD), see Fig. 1. For the electrons dynamics in a QD, beside the full 3D confinement, the electron-electron (e-e) correlations are essential (see e.g. Ref. [5,3,4] for a review). For this reason these systems are sometimes called 'artificial atoms'. Since the lateral size of QDs created in thin films is typically few hundreds nanometers, i.e. for an order of magnitude larger than the layer thickness, the concept of 2D electron gas can be extended to these systems. As a consequence the usual theoretical approach for QDs formed in thin film heterostructures is two-dimensional [6,7]. A similar conclusion holds for the electron-hole (e-h) bound systems (excitons) created in such layers. If the exciton Bohr radius is much larger than the thickness d (the so-called strong confinement regime) the 2D approximation may be satisfactory [1,2]. The 2D approach, of course, breaks down when the effective lateral confinement becomes comparable to the perpendicular one. Then the full three-dimensional (3D) approach becomes necessary [10,11]. In typical samples, however, the thickness effects can be included either using the full 3D approach (see e.g. Ref. [12] for two-electron QDs) or through the effective e-e (or e-h) interaction within the 2D model (the quasi-3D model, see below). A modification of the latest approximation when the interaction between electrons keeps the Coulomb-type form, the so-called effective charge approximation, has been considered recently in the case of two-electron QDs [13,10].

2. Quantum well models and the probability distribution for the zero point motion

Certainly, the simplest quantum well models are: (i) the one-dimensional (1D) infinite square well (the hard wall model)

$$V_\perp = \begin{cases} 0, & |z| < d/2 \\ \infty, & |z| \geq d/2, \end{cases} \tag{1}$$

where d is the layer thickness, and (ii) the parabolic well $V_\perp = \frac{1}{2} m^* \omega_\perp^2 z^2$ (linear harmonic oscillator), where m^* and $\omega_\perp$ are the electron (hole) effective mass and the perpendicular characteristic frequency, respectively. These two potentials can be understood as the hard/soft wall limiting cases keeping in mind

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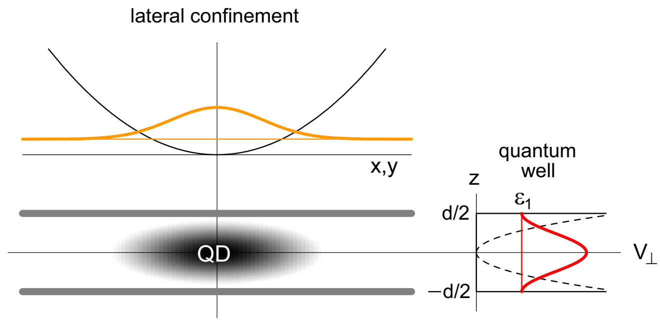

Fig. 1. The localization of a QD in the semiconductor layer of the thickness d (bottom left) and schematic plots showing the corresponding lateral (top) and perpendicular (right) confinements, as well as the lowest levels (thin orange/red lines) and the probability distributions (thick orange/red lines). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

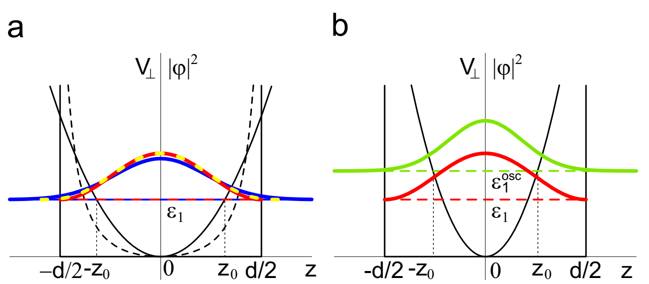

Fig. 2. The ground state energy levels (ε_1) and the corresponding probability distributions (thick lines) for the square well (red lines) and parabolic (blue/green lines) models in the cases: (a) when $\omega_\perp = \omega_1$ and (b) when $\omega_\perp$ is given by Eq. (3) with $c = 3.85$. An example of the quantum well (black dashed line), which form is between the parabolic and the square well, and the corresponding ground state probability distribution (yellow dashed line) are shown for the case (a). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

that a more realistic model may have a form between (i) and (ii) (see Fig. 2a). The hard wall model is widely used because it is able to describe thickness effects in the majority of typical samples. Contrary, the parabolic one corresponds rather to specific samples based, for example, on $GaAs/Al_xGa_{1-x}As$ heterostructures where the parabolic shape is caused by the varying Al content x along the growth direction (z-axis) [8,9]. From the mathematical point of view, however, the second model is more suitable because in many cases it provides analytical solutions (particularly for QDs where the lateral confinement is also parabolic). For this reason in this paper we inspect the applicability of the parabolic model for typical samples, too, and compare the results obtained in these two (i/ii) cases. Unfortunately, there is no general relation between the parameter $\omega_\perp$ and the layer thickness d. Namely, one fixed value for $\omega_\perp$ can be used only in a restricted energy domain. In the following we show how the value $\omega_\perp$ can be estimated from the layer thickness d, under the assumption that electrons occupy only the ground state of the well.

The period of classical motion for a particle of the mass m^* and energy ε confined in the square well defined by Eq. (1) is $T = d\sqrt{2m^*/\varepsilon}$. Thus, the frequency of this periodic motion is $\omega = 2\pi/T = (\pi/d)\sqrt{2\varepsilon/m^*}$. Since the lowest energy level in the 1D infinite square well is $\varepsilon_1 = \pi^2\hbar^2/(2m^*d^2)$, the associated frequency will be

$$\omega_1 = \frac{\pi^2\hbar}{m^*d^2} \tag{2}$$

and we can write $\varepsilon_1 = \frac{1}{2}\hbar\omega_1$. Clearly, if we choose in the parabolic model the parameter $\omega_\perp = \omega_1$, two models will be characterized by the same ground state energy. Besides, for this choice, the probability distributions $|\varphi(z)|^2$, where $\varphi(z)$ are the corresponding ground state wave functions, are also similar (see Fig. 2 a). Emphasize that the corresponding distribution for any quantum well, which form is between the limiting cases (i) and (ii), will be also close to these two (i/ii) distributions. An example is the potential $V_\perp = (A/d^2)\tan^2(\kappa\pi z/d)$ $(-d/2\kappa < z < d/2\kappa)$ which is for certain values of the parameters A and κ (a continuous family) characterized by the same ground state energy ε_1 as the models (i) and (ii). (Note that for $A \to 0$ and $\kappa \to 1$ this potential reduces to the infinite square well potential.) The latest potential, for $A = 2$ and $\kappa = 0.8435$, and the corresponding probability distribution are shown in Fig. 2 a (dashed lines).

Even better agreement between the probability distributions for the models (i) and (ii) can be obtained if we choose

$$\omega_\perp = \frac{c^2\hbar}{m^*d^2} \tag{3}$$

with $c \approx 3.85$ (see Fig. 2 b). For this value the ground state probability distribution approximately vanishes at $z = \pm d/2$ in the parabolic model, too. (In fact, the parameter c is matched precisely to this value after introducing the screening function below.) Note that relation (3) finally reduces to $d = cz_0$, where $z_0 = \sqrt{\hbar/m^*\omega_\perp}$ is the harmonic oscillator characteristic length. A disadvantage is that the ground state energy in the latest case overestimates the square well value, i.e. $\frac{1}{2}\hbar\omega_\perp > \frac{1}{2}\hbar\omega_1$ (see Fig. 2 b). However, since for small d the electrons occupy only the lowest level of the quantum well (at least at low temperatures), this zero-point-motion energy will produce only a constant energy shift in the total energy.

3. Dynamical screening

Another, less trivial, effect of the sample thickness is the reduction (dynamical screening) of the Coulomb interaction (e-e/e-h) comparing to that in the pure 2D model [13]. In the following we show that, if the condition (3) holds, the considered two models give almost identical screening rates.

In order to justify this statement let us consider N electrons in a semiconductor layer, which are additionally confined laterally by a parabolic trap with the characteristic frequency $\omega_0 \ll \omega_\perp$, i.e. consider an anisotropic axially symmetric QD (see Fig. 1). If we add, besides, a perpendicular magnetic field the lateral confinement remains the parabolic, but with the effective frequency $\Omega = (\omega_0^2 + \omega_L^2)^{1/2}$ which depends on magnetic field through the Larmor frequency $\omega_L = eB/2m^*$. Another effect of the field is the constant term $-\omega_L L_z$ in the Hamiltonian, where $L_z = \sum_i l_{z_i}$ is the z-projection of the total angular momentum and l_{z_i} are the projections of the individual electrons angular momenta. In principle the lateral and perpendicular motions may be coupled by the confining potential [14]. However, for the sake of simplicity we shall assume that this coupling can be neglected. Then the corresponding 3D Hamiltonian (using cylindrical coordinates) reads

$$H = \sum_{i=1}^{N}\left(\frac{p_{\rho_i}^2}{2m^*} + \frac{l_{z_i}^2}{2m^*\rho_i^2} + \frac{1}{2}m^*\Omega^2\rho_i^2 - \omega_L l_{z_i}\right) + \sum_{i=1}^{N}\left(\frac{p_{z_i}^2}{2m^*} + V_\perp(z_i)\right) + V_C, \tag{4}$$

where $\rho_i = (x_i^2 + y_i^2)^{1/2}$, $\varphi_i = \arctan(y_i/x_i)$, z_i are the i-th electron coordinates and p_{ρ_i}, $p_{\varphi_i} \equiv l_{z_i}/\rho_i$, p_{z_i} are the conjugated momenta. In that case the coupling between the lateral and perpendicular motions comes only from the Coulomb term describing the interaction (repulsion) between electrons

$$V_C = \sum_{i=1}^{N}\sum_{j=i+1}^{N}\frac{k}{r_{ij}}, \tag{5}$$