Application of the variations calculus on energy spectra of shallow hydrogen-like impurities and excitons in GaAs/AlGaAs quantum wells

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Abstract

A variational calculus method is applied for hydrogen-like impurities states and exciton states in Al-GaAs/GaAs quantum wells within the effective masses approach. The Hamiltonian is separated into radial and transversal parts to be considered and optimized using trial wavefunctions. The results satisfy the well-known cases of three-dimensional and two-dimensional hydrogen. The donor and exciton bound energy is shown to decrease while widening the quantum well. The non-symmetrical donor position also decreases the bound energy.

1 Introduction

Donor and acceptor energy spectra determination in the quantum well (QW) structures has a consistent interest combining theoretical accent and practical issues. Impurity ionisation energy defines the spatial charge distribution in heterostructures, while the excitonic spectra governs the optical properties near the QW band gap region1.

This paper focuses on shallow hydrogen-like impurities and excitons in single QW structures of GaAs/AlGaAs in assumption of the effective mass approach. The developed variations calculus method minimizes lateral part of the Hamiltonian, in contrast to the typical calculation based on the total Hamiltonian functional minimization 2,3. The wavefunction is assumed as a product of 2D trial and a function of spatial coordinate across the QW.

The obtained differential equations were solved numerically using the variations calculus and applied for 1s, 2p0 and 2p± states of hydrogen-like impurity and exciton in GaAs/AlGaAs QW as described in Section 2. Energy spectra dependencies on the QW width, depth and the impurity position were considered in Section 3.

2 Calculation procedure

2.1 Donor states

2.1.1 Trial wavefunction choice

Abrupt QW is placed normally to the z direction. Thus the hamiltonian describing the electron in the box QW potential $U(z)$ and the donor Coulombic field is

$$\hat{H} = -\frac{\hbar^2}{2m_{\text{eff}}} \nabla^2 + U(z) - \frac{e^2}{\epsilon |x - x_b|},$$

where $x_b = \{0, 0, b\}$ aims the donor position. Since now we operate dimensionless units. The axial symmetry is benefited in a cylindrical coordinates $(\rho, \phi, z)$, where $\hat{H}$ becomes

$$\hat{H} = -\nabla^2 + U(z) - \frac{2}{\sqrt{\rho^2 + (z - b)^2}}. \quad (2.1)$$

The Shrödinger equation $\hat{H}\Psi = E\Psi$ determines a total wavefunction $\Psi$. We consider this as a product of 2D trial and a function of spatial coordinate across the QW $\Psi(\rho, \phi, a, z) = F(\rho, \phi, a) \xi(z)$, where $a$ is a variation parameter, $F(\rho, \phi, a)$ notes an trial 2D part operating in a QW plane $(x, y)$ and being independent on $z$, while the last term $\xi(z)$ defines the wavefunction along $z$ axis. The 2D part is bounded at the infinite range and symmetrical.

| State | 2D wavefunction part |
|-------|----------------------|
| $1s$  | $A_{1s} \exp(-\rho/a)$ |
| $2p_0$| $A_{2p} \exp(-\rho/a)$ |
| $2p_-$| $A_{2p} - \rho \cos\phi \exp(-\rho/a)$ |
| $2p_+$| $A_{2p} + \rho \cos\phi \exp(-\rho/a)$ |

Table 1: Trial radial parts of wavefunction
The pre-exponential factor \( A \) is chosen to satisfy the unite propability of the particle presence in heterostructure
\[
\int_0^{+\infty} \int_{-\pi}^{\pi} |F(\rho, \phi, a)|^2 \rho d\rho d\phi = 1. \tag{2.2}
\]

### 2.1.2 Shrödinger equation solution

The Shrödinger equation \( \hat{H} \Psi = E \Psi \) is multiplied with a 2D ansatz \( F(\rho, \phi, a) \) and integrated over the QW plane \((x, y)\). Using \( \hat{L} = -\nabla^2 \) condition one obtains another operator equation for the longitudinal wavefunction part \( \xi(z) \)
\[
\hat{K}(a, z) \xi(z) = E \xi(z),
\]
where \( \hat{K} \) is a mean hamiltonian value over the ansatz function \( F(\rho, \phi, a) \). For a \( n \)-th state, this one yields

\[
\hat{K}_n(a, z) = \int_0^{+\infty} \int_{-\pi}^{\pi} F_n(\rho, \phi, a) \hat{H} F_n(\rho, \phi, a) \rho d\rho d\phi =
\]

\[
= \int_0^{+\infty} \int_{-\pi}^{\pi} F_n(\rho, \phi, a) \left\{- \frac{1}{\rho} \nabla_{\rho} + \nabla_{\varphi}^2 + \frac{1}{\rho^2} \nabla_{\varphi}^2 + \nabla_z^2 \right\} +
\]

\[
+ U(z) - \frac{2}{\sqrt{\rho^2 + (z-b)^2}} \right\} F_n(\rho, \phi, a) \rho d\rho d\phi =
\]

\[
= -\nabla_z^2 + U(z) + I_n(a, z).
\]

The problem is reduced to a 1D Shrödinger equation with additional potential term \( I_n(a, z) \). The subject of the variation procedure related to a parameter is to detect the minimal value of \( I_n(a, z) \) for any given \( z \) by varying \( a = a_{\min}(z) \). Finally, the effective operator is

\[
\hat{K}_n(a, z) = -\nabla_z^2 + U(z) + W_n(z),
\]
where \( W_n(z) = I_n(a_{\min}(z), z) \) and acts as additional effective potential. Its profile depends only on state considered and does not involve the QW parameters. Figure 2.1 depicts \( W_n(z) \) profile for \( n = 1s, 2p_0 \) and \( 2p_{\pm} \) states.

1D Shrödinger equation
\[
[-\nabla_z^2 + U(z) + W_n(z)] \xi(z) = E \xi(z)
\]
was solved numerically in a routine approach. Here we neglect the difference in lattice periods and effective carrier masses within the materials of the heterostructure. The strains are also out of the scope due to the matched AlGaAs/GaAs material choice.

![Figure 2.1: Effective potential \( W_n(z) \) profile for (a) \( n = 1s, 2p_0 \) and (b) \( 2p_{\pm} \) states.](image)

### 2.2 Exciton states

The hamiltonian for an excition problem operates with the electron \( z_e \) and hole \( z_h \) coordinates and comprises twice more degrees of freedom
\[
\hat{H} = -\frac{\hbar^2}{2m_{e,\text{eff}}} \nabla_e^2 - \frac{\hbar^2}{2m_{h,\text{eff}}} \nabla_h^2 +
\]

\[
+ U_e(z_e) + U_h(z_h) - \frac{e^2}{\epsilon |x_e - x_h|},
\]

After switching to the mass center and performing variational procedure as in section 2.1.2, the problem reduces to 1D case regarding \( z_e \) and \( z_h \), while effective potential \( W_n(z) \) becomes equal to the one of donor case
\[
[-\eta_e \nabla_e^2 - \eta_h \nabla_h^2 + U_e(z_e) + U_h(z_h) + W_n(z_e - z_h)] \xi = E \xi,
\]
where notation \( \eta_e = \mu/m_e, \eta_h = \mu/m_h \) are used and \( \mu = 1/(m_e^{-1} + m_h^{-1}) \) is the dimensionless reduced exciton mass.

### 3 Results and discussion

To verify the variational procedure, the calculation approach was applied to well-known 3D and 2D hydrogen problem. The well depth was set to \( U(z) = 0 \) and \( U(z) = -\infty \) respectively, to obtain \( E_0 \) and \( E_1 \) energies. The results in the Rydberg units are presented in Table 2 and indicate appropriate accuracy.

|          | \( E_0 \)/Ry | \( E_1 \)/Ry | \( dE_0 \) | \( dE_1 \) |
|----------|--------------|--------------|------------|------------|
| Our solution | -1.083       | -0.249       | 8.3 %      | 0.4 %      |
| Exact solution | -1.000       | -0.250       | -          | -          |

Table 2: The variational procedure accuracy.
The bound energy dependencies of the QW width were considered in assumption the donor was positioned in the AlGaAs/GaAs well center. As shown in Fig. 3.1-3.2, the decrease in the well width increases the binding energy of the donor electron and exciton energy as well. This is attributed to severe wavefunction concentration in the narrow QW [4, 5].

Then we considered the donor to be shifted away the QW center. Figures 3.3. and 3.4. illustrate the results. The displacement decreases the bound energy and provokes significant disturbance while reaching the QW border. The intermixing of $1s$ and $2p_0$ states occurs near 30 Å position and may be interpreted as computational feature, so that $1s$ should prevail the $2p_0$ after 30 Å as formerly. The general decrease indicates the wavefunction diffusion from the QW region.

After that the exciton state was calculated in dependence on the QW width. Similarly to the donor problem, the increase in width causes the wavefunction diffusion and lowers the bound energy of exciton, as shown in Figures 3.5. and 3.6.

4 Conclusions

The developed variation method was applied for energy spectra calculations for shallow hydrogen-like impurities and excitons in single GaAs/AlGaAs quantum wells. The results for $1s$, $2p_0$ and $2p_\pm$ states rather satisfy the theoretical results for typical cases.

Shrinking the well width increases the binding energy of the donor electron and exciton energy as well. The shift of impurity away of QW center decreases the electron binding energy.
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Note

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