Efficient Modeling of Coulomb Interaction Effect on Exciton in Crystal-Phase Nanowire Quantum Dot

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Abstract- **The binding energy and oscillation strength of the ground-state exciton in type-II quantum dot (QD) is calculated by using a post Hartree-Fock method known as the configuration interaction (CI) method which is significantly more efficient than conventional methods like ab initio method. We show that the Coulomb interaction between electron and holes in these structures considerably affects the transition dipole moment which is the key parameter of optical quantum gating in STIRAP (stimulated Raman adiabatic passage) process for implementing quantum gates [1], [2].**

I. INTRODUCTION

Numerous works have been devoted to studying microscopic modeling of excitons in nanostructured QDs because of their appealing potential for quantum information processing applications [1], [2]. However, previous modeling methods such as ab initio or tight binding methods are numerically demanding as they would not be efficient for engineering and designing of quantum devices. In this paper we use a different method for modeling excitons in type-II crystal-phase QDs which reduces computational complexity and allows for fast design and optimization of quantum devices.

Type-II crystal-phase QDs are formed by two different crystal phases: wurtzite (WZ) and zinc-blende (ZB) in growth direction [3]. As is shown in Fig. 1, conduction and valance band of ZB section has lower energy compare to WZ sections. This Type-II band edge structure makes the electron to be confined in ZB section and the hole in WZ section. While a lot of work has been devoted to studying Type-I QD to understand exciton phenomenon [1], however there have been few works to study excitons in crystal phase Type-II QDs. In this paper, we calculate exciton binding energy and oscillation strength through a full CI description of the few particle electron-hole system.

II. MODELING COULOMB INTERACTION

Our system is an exciton, consisting of an electron and a hole. Then the full Hamiltonian of the system within the framework of an envelope function and effective mass approximation is described as:

$$\hat{H} = \hat{H}_0 + \hat{H}_c \qquad (1)$$

Where $\hat{H}_0 = \hat{H}_e + \hat{H}_h$ is the Hamiltonian in three dimention for non-interacting electrons and holes such that:

$$\hat{H}_k = -\frac{\hbar^2}{2m_k}\nabla^2 + V_T^k(r,\theta) + V_{QW}^k(z) \qquad (2)$$

Where $k \in e$ or h, for electron and holes; m_k is the effective mass; ∇ is 3D laplacian operator; the first term of (2) is the kinetic energy of electron (hole); $V_{QW}^k(z)$ and $V_T^k(r,\theta)$ are the confinement potentials for electron (hole) in the growth and in-plane directions, respectively; and $\hat{H}_c$ in (1) is the Hamiltonian for Coulomb interaction between electron and hole in the QD structure. The representation of this operator in terms of creation and annihilation operators is [1]:

$$\hat{H}_c = \frac{1}{2}\sum_{nm}\iint \frac{q^2}{4\pi\varepsilon}\frac{\hat{\psi}_m^\dagger(r)\hat{\psi}_n^\dagger(r')\hat{\psi}_n(r')\hat{\psi}_m(r)}{|r-r'|}drdr' \qquad (3)$$

Here, ε is the dielectric constant of material; $\hat{\psi}_{m/n}^\dagger(r)$ and $\hat{\psi}_{m/n}(r)$ are field operators which create or annihilate an electron/hole, respectively at position $r:(r,\theta,z)$ such that: $|\phi\rangle = \int dr\, \phi(r)\psi^\dagger(r)|vac\rangle = \int dr\, \phi(r)|r\rangle$. This Few-particle Hamiltonian in (3) which contains all possible electron-electron, hole-hole and electron-hole interactions is expanded within the basis of the energetically lowest single-particle states obtained by solving Schrodinger equation: $\hat{H}_k\phi(r) = E_k^{nlm}\phi(r)$. We assume that there exists solution of the wavefunction that takes the form: $\phi(r) = R(r,\theta)Z(z)$.

Fig. 1. Type-II single well Nanowire QD and its band structure
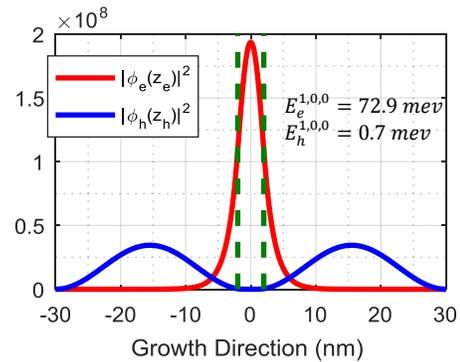
Fig. 2. Ground state probability densities along the growth direction for electron in conduction band and hole in valance band potential

The transverse part of these single-particle wavefunctions by considering $V_T^j(r, \theta)$ as an infinite quantum well potential with zero wavefunction boundary in the radius of the wire would be $R(r, \theta) = A J_{m_k}(l_k r) e^{im_k \theta}$ with l and m being solution parameters (quantum numbers). The energy of the particles in the transverse direction is found from the zeros of the Bessel function and the radius of the wire. The wavefuction along the growth direction, $Z(z)$, with the potential $V_{QW}^k(z)$ being the single well band structure shown in Fig. 1 is a piecewise function defined differently in each WZ/ZB part. The ground state probability densities of electron in conduction band and hole in valance band for a structure with $d = 4\ nm$ are shown in Fig. 2. Now Hamiltonian $\hat{H}_c$ in (3) could be written within Hilbert state of the single-particle electron-hole excitations $|ij\rangle$ which is: $|ij\rangle = |e_i\rangle|h_j\rangle$ where i and j are correspond to three quantum number $n_{i/j} l_{i/j} m_{i/j}$ for electron and hole respectively. We have used this notation just for simplicity. Then the Coulomb interaction matrix elements of the neutral exciton from (3) could be calculated as:

$$\langle ij|\hat{H}_c|i'j'\rangle$$
$$= \iint \frac{-e^2}{4\pi\varepsilon} \frac{\phi_e^{i'*}(r)\phi_h^{j'*}(r')\phi_e^i(r)\phi_h^j(r')}{|r - r'|} dr dr' \tag{4}$$

By calculating matrix elements of Coulomb interaction from (4) and summing it up with matrix elements H_0 according to (1), the energy and wavefunction of exciton are found by diagonalizing the Hamiltonan H. Excitons energies are eigenvalues of H, and exciton wavefunctions are, $\Psi(r_e, r_h) =$

$\sum_{i,j} C_{i,j}\ \phi_e^i(r_e)\phi_h^j(r_h)$ where C coefficients are eigenvector elements of the corresponding Eigen energy.

Fig. 3a and 3b show the ground state exciton wavefunction $|\Psi(z_e, z_h)|^2$, with considering coulomb interaction and without considering it, respectively, in the electron and hole coordinates in the growth direction. This figures show how Coulomb interaction makes hole state more localized. The band structure with well width is 2 nm and the binging energy of exciton is 4.9 meV.

Oscillation strength which is an important parameter in the study of the optical transitions intensity [3] and in the realizing of qubit operations [1], [2], is related to the amplitude of finding electron and hole on the same site as:

$$f = \frac{E_P}{\hbar\omega_0}\left|\int dr \Psi(r, r)\right|^2 \tag{5}$$

Where m_0 is the bare electron mass, ω_0 is the exciton optical transition frequency and E_P is called Kane energy. Fig. 4 shows f_{excCI}/f_{exc} dependence on well width ,d. Here f_{excCI} and f_{exc} are the exciton oscillation strength when we have considered Coulomb interaction and have neglected it, respectively. It shows that Coulomb interaction significantly enhances oscillation strength in these type-II structures.

III. CONCLUSION

We investigated how Coulomb interaction affects ground state exciton state in Crystal phase Type-II QD by employing a CI method which is a fast and efficient method for designing and engineering of quantum devices.

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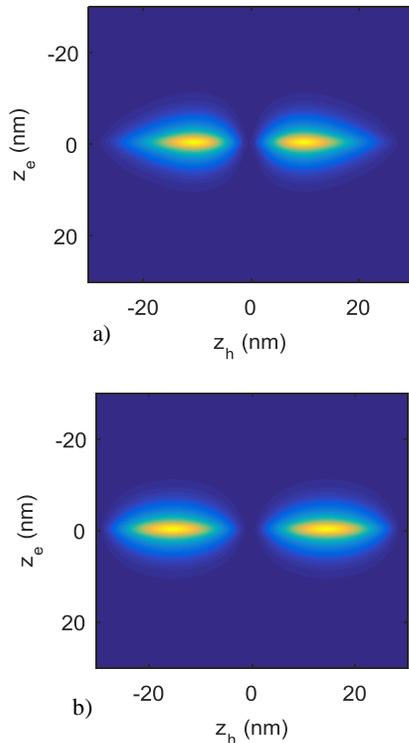
Fig. 3. Ground state exciton wavefunction a) with considering Coulomb interaction b) without considering Coulomb interaction. In this calculation we have just considered ground state of single-particle electron and hole states in radial direction.
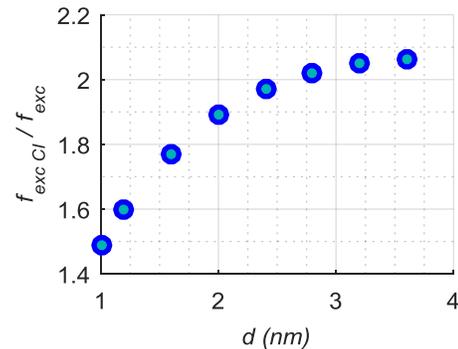
Fig. 4. Calculated dependence of ground state exciton oscillation strength on well width d