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Ground state energy of excitons in quantum dot treated variationally via Hylleraas-like wavefunction

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In this work, the effects of quantum confinement on the ground state energy of a correlated electron–hole pair in a spherical and in a disc-like quantum dot have been investigated as a function of quantum dot size. Under parabolic confinement potential and within effective mass approximation Ritz's variational method is applied to Hylleraas-like trial wavefunction. An efficient method for reducing the main effort of the calculation of terms like $r_{\rm eh}^k \exp(-\lambda r_{\rm eh})$ is introduced. The main contribution of the present work is the introduction of integral transforms which provide the calculation of expectation value of energy and the related matrix elements to be done analytically over single-particle coordinates instead of Hylleraas coordinates.

Keywords: exciton, parabolic confinement, variational method, Hylleraas coordinates
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1. Introduction

Progress in modern nanofabrication techniques made it possible to grow low-dimensional semiconductor systems where the size and composition could be controlled well. Structures where the strong confinement is imposed in all three spatial dimensions are referred to as quantum dot (QD).[1] Dynamical confinement by application of external field on electrons and holes implements of complete quantization of their free motion[2] that make it possible to observe quantum size effect (QSE) in these quasi-zero-dimensional systems.[3] Because of the quantum size effect, quantum dots show many new physical features which differs from bulk systems.

Modern technologies, such as self-organized growth or molecular beam epitaxy, allow scientists to fabricate QDs up to 10 nm where size, shape and properties are well controlled in experiments.[4] Since the natural length scale of QDs is about a few nanometres, they contain finite number of carriers. Thus QDs have discontinuous energy spectra.[5] So the increased interest has been focused on Coulomb states of few-particles where quantum mechanical effect can be strongly observed.[6] This is an attractive area not only for technological application in optoelectronic devices, such as quantum dot lasers, but also for the fundamental researches.

Optical methods are convenient experimental tools for studying the properties of quantum dots. One type of elementary excitations in quantum dots are excitons which play a central role on semiconductor optical properties.[7−9] In quasi-zero-dimensional quantum dot systems, the different quantum confinement dramatically changes the optical and electronic properties of the system. Correspondingly, the excitonic spectrum is expected to be strongly affected which improves the electron–hole interaction.[10]

Theoretical investigations of excitons in QDs have been in strong interest of researches in last two decades. Many studies have been carried out on the electron–hole pair in nanocrystals from various points of view. Among these, variational studies assuming a model of a spherical quantum dot with an effective-mass approximation have been widely used to gain insight into the essential features of quantum size effects.[11−14] Generally, infinite barriers have been considered as a confinement potential of excitons. Exact numerical analysis of the exciton problem has been done by Hu and coworkers[15] where excitonic ground state wavefunction is expanded in terms of single-particle wavefunctions. There are also pa-

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pers where non-spherical quantum dots, such as boxes, square flat plates and cylindrical shapes, have been investigated.[3,12,16,17]

In contrast to various works done on excitonic states in spherical quantum dots, the works on parabolic confinement are relatively low in numbers.[7,18−20] It has been demonstrated theoretically that far-infrared light is strongly absorbed for bare parabola frequencies for electrons confined in quantum dot.[21−23] These theoretical predictions are consistent with experimental measurements done on QDs.[24] The evidence that bare potential in many quantum dots has a parabolic form is basic electrostatic models.[25] Sikorski and Merkt[26] envisaged that the parabolic model is suitable approach for a few electron quantum dots.

In this work, we calculated the ground state energy of an exciton in two-dimensional (2D) and three-dimensional (3D) quantum dot by using variational method with Hylleraas-like trial wavefunction. We introduced here an computationally efficient approach for the calculation of the expectation value of ground state energy by means of the integral representations for the terms like $r_{\rm eh}^k \exp(-\lambda r_{\rm eh})$. This approach provided the calculation of integrals to be done over single-particle coordinates instead of Hylleraas coordinates.

The paper is organized as follows. In Section 2, we briefly describe the formalism and the method used for variational calculation of the ground state energy of an exciton in a quantum dot. The results for the ground state energy are presented in Section 3. Finally in Section 4, we summarize the main conclusions of this work.

2. Theory and method

Within the framework of the effective mass approximation, Hamiltonian of a system composed of electron and hole pair confined in a spherical or disc-like quantum dot can be written as

$$\hat{H} = -\frac{\hbar^2}{2m_{\rm e}}\boldsymbol{\nabla}_{\rm e}^2 - \frac{\hbar^2}{2m_{\rm h}}\boldsymbol{\nabla}_{\rm h}^2 + V(r_{\rm e}) + V(r_{\rm h}) - \frac{e^2}{4\pi\varepsilon r_{\rm eh}}. \quad (1)$$

Here $m_{\rm e}$ ($m_{\rm h}$) and $\boldsymbol{r}_{\rm e}$ ($\boldsymbol{r}_{\rm h}$) are isotropic effective mass of electron (hole) and position vectors, respectively and $r_{\rm eh} = |\boldsymbol{r}_{\rm e} - \boldsymbol{r}_{\rm h}|$ indicates the distance between electron and hole. Also here, ε is the dielectric constant of the medium where particles move. In terms of simplicity distortion of Coulomb interaction formed due to difference between dielectric constants of quantum dot and matrix material has been neglected. In the model presented in this work unscreened $V(r_i)$, $(i = {\rm e}, {\rm h})$, confinement potential with strength ω_0 for $i^{\rm th}$ particle has been considered as parabolic. So the spherical symmetric potential experienced by both of electron and hole is chosen to be

$$V(r_i) = \frac{1}{2} m_i \omega_0^2 r_i^2, \qquad (i = {\rm e}, {\rm h}). \quad (2)$$

Assumption of identical parabola frequency for the different charge carriers indicates that the range of electron and hole potentials are approximately the same. This is not a bad approximation for the materials like GaAs.[18] Therefore it is expected to have great overlap between electron and hole wavefunctions and strong Coulomb interaction.

By defining new parameters, $\mu = 1/(m_{\rm e}^{-1} + m_{\rm h}^{-1})$ as the reduced effective mass, $\sigma_i = m_i/\mu$ as the dimensionless effective mass of electron $(i = {\rm e})$ and hole $(i = {\rm h})$, we choose effective Bohr radius $a_x^\star = 4\pi\varepsilon\hbar^2/\mu e^2$ as the length scale and effective Hartree energy $E_H^\star = \hbar^2/\mu a_x^{\star 2}$ as the energy scale. These new definitions lead to the dimensionless Hamiltonian of the system to be

$$\frac{\hat{H}}{E_H^\star} = -\frac{1}{2\sigma_{\rm e}}\boldsymbol{\nabla}_{\tilde{r}_{\rm e}}^2 - \frac{1}{2\sigma_{\rm h}}\boldsymbol{\nabla}_{\tilde{r}_{\rm h}}^2 + \tilde{V}(\tilde{r}_{\rm e}) + \tilde{V}(\tilde{r}_{\rm h}) - \frac{1}{\tilde{r}_{\rm eh}}, \quad (3)$$

where $\tilde{V}(\tilde{r}_i) = \frac{1}{2}\sigma_i W^2 \tilde{r}_i^2$, $(i = {\rm e}, {\rm h})$ is dimensionless confinement potential and $\tilde{r}_j$ $(j = {\rm e}, {\rm h}, {\rm eh})$ represent dimensionless coordinates. For simplicity, in what follows we shall use 'tildeless' representation of coordinates unless otherwise is stated, $l_0 = \sqrt{\hbar/\mu\omega_0}$ is the characteristic length of quantum dot and dimensionless parameter W is defined as $W = (a_x^\star/l_0)^2$. It is clear that $W^{-1/2}$ is related with the confinement region of the exciton in a parabolic quantum dot.

The Hamiltonian in Eq.(3) includes six independent spherical coordinates. Using Hylleraas coordinate system which explicitly includes $r_{\rm eh}$ interparticle distance is very convenient for this problem.[27] In this coordinate system six degrees of freedom are classified into two groups named 'inner' and 'outer'. Outer coordinates are chosen as three Euler angles that denote the plane spanned by $\boldsymbol{r}_{\rm e}$ and $\boldsymbol{r}_{\rm h}$ vectors. It is appropriate to adopt $r_{\rm e} \equiv |\boldsymbol{r}_{\rm e}|$, $r_{\rm h} \equiv |\boldsymbol{r}_{\rm h}|$ and $r_{\rm eh} \equiv |\boldsymbol{r}_{\rm e} - \boldsymbol{r}_{\rm h}|$

as the inner coordinates. After taking away the outer coordinates, Schrödinger equation reduces to the form including only inner coordinates.[28,29] Due to the spherical symmetry of the system, complete description of the ground state can be obtained by using these inner coordinates.

The wavefunction expanded in terms of generalized Hylleraas basis set has been used in variational treatment of three-body Coulomb systems with optimization techniques chosen according to the desired accuracy.[30] Owing to the correlated character of these functions it is sufficient to use rather low expansions to reach the accurate energies of free two-electron and three-body molecular systems for describing their ground state. In this connection the accuracy of both energy and wavefunctions can be improved by systematic increase of expansion. Our ansatz to find the appropriate wavefunction describing exciton in quantum dot confined by parabolic potential is chosen in the form of

$$\Phi\left(r_{\mathrm{e}}, r_{\mathrm{h}}, r_{\mathrm{eh}}\right) = \sum_{N} C_N \, \Psi^N\left(r_{\mathrm{e}}, r_{\mathrm{h}}, r_{\mathrm{eh}}\right), \tag{4}$$

where

$$\Psi^N\left(r_{\mathrm{e}}, r_{\mathrm{h}}, r_{\mathrm{eh}}\right) = \phi\left(r_{\mathrm{e}}\right)\phi\left(r_{\mathrm{h}}\right) \mathrm{e}^{-\lambda r_{\mathrm{eh}}} \, r_{\mathrm{e}}^{n_{\mathrm{e}}} \, r_{\mathrm{h}}^{n_{\mathrm{h}}} \, r_{\mathrm{eh}}^{n_{\mathrm{eh}}}. \tag{5}$$

The basis function $\phi\left(r_i\right)$ is chosen to be solution of the non-interacting system in the form of

$$\phi\left(r_i\right) = \mathrm{e}^{-\gamma W \sigma_i \frac{r_i^2}{2}}, \qquad (i = \mathrm{e}, \mathrm{h}). \tag{6}$$

The trial wavefunction, Eq.(4), is spanned by $\mathrm{N} \equiv \{n_{\mathrm{e}}, n_{\mathrm{h}}, n_{\mathrm{eh}}\}$ which corresponds to the powers of coordinates r_{e}, r_{h} and r_{eh}, respectively. $\phi\left(r_{\mathrm{e}}\right)\phi\left(r_{\mathrm{h}}\right)$ product in Eq.(5) defines the ground state of uncorrelated electron–hole pair in parabolic confinement with strength W. The next term, $\mathrm{e}^{-\lambda r_{\mathrm{eh}}}$, describes the Coulombic correlation between electron and hole. And finally $r_{\mathrm{e}}^{n_{\mathrm{e}}} r_{\mathrm{h}}^{n_{\mathrm{h}}} r_{\mathrm{eh}}^{n_{\mathrm{eh}}}$ product is introduced in order to take into account the spatial correlations where the integers n_{e}, n_{h}, n_{eh} are positive or equal to zero. λ and γ are used as the variational parameters. For simplicity, in what follows we shall drop the $(r_{\mathrm{e}}, r_{\mathrm{h}}, r_{\mathrm{eh}})$ dependence of $\Psi^N\left(r_{\mathrm{e}}, r_{\mathrm{h}}, r_{\mathrm{eh}}\right)$.

Having this trial wavefunction, the ground state energy of an exciton in 3D and 2D QD system can be found by using Ritz's variational principle. The linear $C_{n_{\mathrm{e}},n_{\mathrm{h}},n_{\mathrm{eh}}}$ expansion coefficients and nonlinear γ and λ parameters in the wavefunction are defined to minimize the average value of energy:

$$\langle E(\gamma,\lambda)\rangle = \langle \Phi|\hat{H}|\Phi\rangle / \langle \Phi|\Phi\rangle. \tag{7}$$

Optimization with respect to the C_N linear expansion coefficients in Eq.(4) is a generalized eigenvalue problem, $\boldsymbol{HC} = E\boldsymbol{SC}$. Here $\boldsymbol{H}$ consists of kinetic term, Coulomb interaction and confinement potential, and $\boldsymbol{S}$ is the norm with respect to the Ψ^N. $\boldsymbol{C}$ stands for the column matrix of $C_{n_{\mathrm{e}},n_{\mathrm{h}},n_{\mathrm{eh}}}$ coefficients.

Elements of $\boldsymbol{S}$ overlap matrix are given by

$$\begin{aligned} S_{M,N} &= \langle \Psi^M | \Psi^N \rangle \\ &= \iint \mathrm{d}\boldsymbol{r}_{\mathrm{e}} \mathrm{d}\boldsymbol{r}_{\mathrm{h}} \, \Psi^{M\star} \Psi^N. \end{aligned} \tag{8}$$

Using the definition of vector operator del expressed in Hylleraas-type coordinates as

$$\boldsymbol{\nabla}_i = \hat{r}_i \frac{\partial}{\partial r_i} + \sum_{j \neq i} \hat{r}_{ij} \frac{\partial}{\partial r_{ij}} \tag{9}$$

and interaction potential $U(r_{\mathrm{eh}}) = -1/r_{\mathrm{eh}}$, elements of $\boldsymbol{H}$ Hamiltonian matrix can be evaluated as follows:

$$\begin{aligned} H_{M,N} &= \langle \Psi^M | \hat{H} | \Psi^N \rangle \\ &= \iint \mathrm{d}\boldsymbol{r}_{\mathrm{e}} \mathrm{d}\boldsymbol{r}_{\mathrm{h}} \left[\frac{1}{2\sigma_{\mathrm{e}}} \boldsymbol{\nabla}_{r_{\mathrm{e}}} \Psi^{M\star} \cdot \boldsymbol{\nabla}_{r_{\mathrm{e}}} \Psi^N + \Psi^{M\star} V\left(r_{\mathrm{e}}\right) \Psi^N \right] \\ &\quad + \iint \mathrm{d}\boldsymbol{r}_{\mathrm{e}} \mathrm{d}\boldsymbol{r}_{\mathrm{h}} \frac{1}{2\sigma_{\mathrm{e}}} \frac{(r_{\mathrm{e}}^2 - r_{\mathrm{h}}^2 + r_{\mathrm{eh}}^2)}{2 r_{\mathrm{e}} r_{\mathrm{eh}}} \left(\frac{\partial \Psi^{M\star}}{\partial r_{\mathrm{e}}} \frac{\partial \Psi^N}{\partial r_{\mathrm{eh}}} + \frac{\partial \Psi^{M\star}}{\partial r_{\mathrm{eh}}} \frac{\partial \Psi^N}{\partial r_{\mathrm{e}}} \right) \\ &\quad + \iint \mathrm{d}\boldsymbol{r}_{\mathrm{e}} \mathrm{d}\boldsymbol{r}_{\mathrm{h}} \left[\frac{1}{2\sigma_{\mathrm{h}}} \boldsymbol{\nabla}_{r_{\mathrm{h}}} \Psi^{M\star} \cdot \boldsymbol{\nabla}_{r_{\mathrm{h}}} \Psi^N + \Psi^{M\star} V\left(r_{\mathrm{h}}\right) \Psi^N \right] \\ &\quad + \iint \mathrm{d}\boldsymbol{r}_{\mathrm{e}} \mathrm{d}\boldsymbol{r}_{\mathrm{h}} \frac{1}{2\sigma_{\mathrm{h}}} \frac{(r_{\mathrm{h}}^2 - r_{\mathrm{e}}^2 + r_{\mathrm{eh}}^2)}{2 r_{\mathrm{h}} r_{\mathrm{eh}}} \left(\frac{\partial \Psi y^{M\star}}{\partial r_{\mathrm{h}}} \frac{\partial \Psi^N}{\partial r_{\mathrm{eh}}} + \frac{\partial \Psi^{M\star}}{\partial r_{\mathrm{eh}}} \frac{\partial \Psi^N}{\partial r_{\mathrm{h}}} \right) \\ &\quad + \iint \mathrm{d}\boldsymbol{r}_{\mathrm{e}} \mathrm{d}\boldsymbol{r}_{\mathrm{h}} \left[\frac{1}{2} \boldsymbol{\nabla}_{r_{\mathrm{eh}}} \Psi^{M\star} \cdot \boldsymbol{\nabla}_{r_{\mathrm{eh}}} + \Psi^{M\star} U\left(r_{\mathrm{eh}}\right) \Psi^N \right]. \end{aligned} \tag{10}$$

General procedure for the evaluation of integrals in order to determine ground state energy working with wavefunctions expressed in Hylleraas coordinates is to use the coordinates $u = r_{12}$, $s = r_1 + r_2$ and $t = r_1 - r_2$. Integrals in type of $I = \int F(r_1, r_2) f(r_{12}) \mathrm{d}^3 r_1 \mathrm{d}^3 r_2$ are calculated in terms of Hylleraas coordinates as $I = 8\pi^2 \int F(r_1, r_2) r_1 \mathrm{d}r_1 r_2 \mathrm{d}r_2 \int_{|r_1 - r_2|}^{(r_1 + r_2)} f(r_{12}) r_{12} \mathrm{d}r_{12}$.[31] In this work unlike the general procedure mentioned above, the Fourier transforms have been used for the terms including interparticle distance r_{eh}.

The Fourier transforms for 3D spherical quantum dot are defined as[32,33]

$$\frac{\mathrm{e}^{-\lambda r}}{r} = \frac{1}{2\pi^2} \int \frac{\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}}{(\lambda^2 + q^2)} \mathrm{d}\boldsymbol{q} \tag{11}$$

and

$$\frac{1}{r_{\mathrm{eh}}} = \frac{1}{2\pi^2} \int \frac{\mathrm{e}^{\mathrm{i}\boldsymbol{R}\cdot(\boldsymbol{r}_{\mathrm{e}} - \boldsymbol{r}_{\mathrm{h}})}}{R^2} \mathrm{d}\boldsymbol{R}. \tag{12}$$

Utilization of this transform leads to the general integral representations for the terms in the form of $(\mathrm{e}^{-\lambda r_{\mathrm{eh}}} r_{\mathrm{eh}}^k)$, ($k \in \mathbb{Z}$ and λ is a parameter) which avoid the use of general integration technique for Hylleraas coordinates. The obtained integral representations are

$$\begin{aligned} &\int \mathrm{d}\Omega_{\mathrm{e}} \int \mathrm{d}\Omega_{\mathrm{h}}\ \mathrm{e}^{-\lambda r_{\mathrm{eh}}}\, r_{\mathrm{eh}}^{(p-1)} \\ &= 32\pi \int_0^\infty \mathrm{d}q\ \frac{\sin(qr_{\mathrm{e}})}{r_{\mathrm{e}}}\ \frac{\sin(qr_{\mathrm{h}})}{r_{\mathrm{h}}} \\ &\quad \times Q_{3\mathrm{D}}[q, \lambda, p], \end{aligned} \tag{13}$$

where

$$Q_{3\mathrm{D}}[q, \lambda, p] = (-1)^p \frac{\partial^p}{\partial \lambda^p} \left[\frac{1}{(q^2 + \lambda^2)} \right] \quad p = 0, 1, 2, ...$$

and $\Omega_i, (i = \mathrm{e}, \mathrm{h})$ are solid angles describing spatial orientation of electron and hole. Since these integral representations separate coordinates of electron and hole from each other, the integrations over r_{e} and r_{h} in Eqs.(8) and (10) lead to the integrals in similar form for each carrier. These separated integrals, we name them $G_{3\mathrm{D}}$, are calculated analytically and have the general form in terms of hypergeometric (${}_1\mathrm{F}_1$) and gamma (Γ) functions as

$$\begin{aligned} &G_{3\mathrm{D}}(q, \gamma, \sigma, W, m, n, k) \\ &= \frac{1}{2} q (W\gamma\sigma)^{\frac{1}{2}(-k-m-n-2)} \Gamma\left(\frac{1}{2}(k + m + n + 2)\right) \\ &\quad \times {}_1\mathrm{F}_1\left(\frac{1}{2}(k + m + n + 2); \frac{3}{2}; -\frac{q^2}{4W\gamma\sigma}\right). \end{aligned} \tag{14}$$

Initially, integrations over r_{e} and r_{h} coordinates are performed analytically for $S_{M,N}$ and $H_{M,N}$, then the numerical procedure is applied for the integrations over q variable introduced in Eq.(13).

Under these definitions, equations (13) and (14), the elements of $\boldsymbol{S}$ matrix for 3D are obtained according to the expression given below

$$\begin{aligned} S_{M,N}^{3\mathrm{D}} = 32\pi &\int_0^\infty \mathrm{d}q\, Q_{3\mathrm{D}}(q, 2\lambda, m_{\mathrm{eh}} + n_{\mathrm{eh}} + 1) \\ &\times G_{3\mathrm{D}}(q, \gamma, \sigma_{\mathrm{e}}, W, m_{\mathrm{e}}, n_{\mathrm{e}}, 1) \\ &\times G_{3\mathrm{D}}(q, \gamma, \sigma_{\mathrm{h}}, W, m_{\mathrm{h}}, n_{\mathrm{h}}, 1). \end{aligned} \tag{15}$$

By using the length definitions of A_{nd}, B_{nd}, C_{nd} and D_{nd} defined in Appendix, the elements of $\boldsymbol{H}$ matrix are calculated as follows:

$$\begin{aligned} H_{M,N}^{3\mathrm{D}} = 32\pi &\int_0^\infty \mathrm{d}q\, [Q_{3\mathrm{D}}(q, 2\lambda, m_{\mathrm{eh}} + n_{\mathrm{eh}} - 1) D_{3\mathrm{D}} \\ &+ Q_{3\mathrm{D}}(q, 2\lambda, m_{\mathrm{eh}} + n_{\mathrm{eh}}) C_{3\mathrm{D}} \\ &+ Q_{3\mathrm{D}}(q, 2\lambda, m_{\mathrm{eh}} + n_{\mathrm{eh}} + 1) B_{3\mathrm{D}} \\ &+ Q_{3\mathrm{D}}(q, 2\lambda, m_{\mathrm{eh}} + n_{\mathrm{eh}} + 2) A_{3\mathrm{D}}]. \end{aligned} \tag{16}$$

Procedure similar to the Fourier transforms in three-dimension can be applied to 2D disc-like QD. Using the definition for two-dimension

$$\frac{\mathrm{e}^{-\lambda r}}{r} = \frac{1}{(2\pi)} \int_0^\infty \mathrm{d}\boldsymbol{q} \frac{\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}}{\sqrt{q^2 + \lambda^2}}, \tag{17}$$

we obtain the integral representations,

$$\begin{aligned} &\int \mathrm{d}\theta_{\mathrm{e}} \int \mathrm{d}\theta_{\mathrm{h}}\, \mathrm{e}^{-\lambda r_{\mathrm{eh}}} r_{\mathrm{eh}}^{(p-1)} \\ &= (2\pi)^2 \int_0^\infty \mathrm{d}q q \mathrm{J}_0(qr_{\mathrm{e}}) \mathrm{J}_0(qr_{\mathrm{h}}) Q_{2\mathrm{D}}[q, \lambda, p], \end{aligned} \tag{18}$$

where

$$Q_{2\mathrm{D}}[q, \lambda, p] = (-1)^p \frac{\partial^p}{\partial \lambda^p} \left[\frac{1}{\sqrt{q^2 + \lambda^2}} \right] \quad p = 0, 1, 2, ...$$

and J_0 is a spherical Bessel function. Analytical expression for the integrals in similar form over the separated electron and hole coordinates is found in terms of hypergeometric (${}_1\mathrm{F}_1$) and gamma (Γ) functions as follows:

$$\begin{aligned} &G_{2\mathrm{D}}(q, \gamma, \sigma, W, m, n, k) \\ &= \frac{1}{2} (W\gamma\sigma)^{\frac{1}{2}(-k-m-n-1)} \Gamma\left(\frac{1}{2}(k + m + n + 1)\right) \\ &\quad \times {}_1\mathrm{F}_1\left(\frac{1}{2}(k + m + n + 1); 1; -\frac{q^2}{4W\gamma\sigma}\right). \end{aligned} \tag{19}$$

The evaluation of the matrix elements in two-dimension is similar to the calculation in three-dimension. Using the definitions for A_{nd}, B_{nd}, C_{nd} and D_{nd} given in the Appendix, the matrix elements of $\boldsymbol{S}$ and $\boldsymbol{H}$ in two-dimension are

$$S^{2D}_{M,N} = (2\pi)^2 \int_0^\infty \mathrm{d}q\; q\, Q_{2D}(q, 2\lambda, m_{eh} + n_{eh} + 1) \times G_{2D}(q, \gamma, \sigma_e, W, m_e, n_e, 1) G_{2D}(q, \gamma, \sigma_h, W, m_h, n_h, 1), \quad (20)$$

$$H^{2D}_{M,N} = (2\pi)^2 \int_0^\infty \mathrm{d}q\, q\, [Q_{2D}(q, 2\lambda, m_{eh} + n_{eh} - 1) D_{2D} + Q_{2D}(q, 2\lambda, m_{eh} + n_{eh}) C_{2D} + Q_{2D}(q, 2\lambda, m_{eh} + n_{eh} + 1) B_{2D} + Q_{2D}(q, 2\lambda, m_{eh} + n_{eh} + 2) A_{2D}]\,. \quad (21)$$

3. Results and discussion

We have performed calculations for the ground state energy of exciton in parabolic quantum dot by means of the Hylleraas-like wavefunction in Eq.(4), which spans powers of $\{n_e, n_h, n_{eh}\}$ for the corresponding coordinates r_e, r_h and r_{eh} and is commensurate with the condition $(n_e + n_h + n_{eh}) \leq 3$. Due to the built-in correlated character of the wavefunction, relatively low expansions are sufficient to ensure a good accuracy without lengthening calculation time. We have calculated the ground state energies for different radii of quantum dot for both heavy- and light-hole. Also the effects of parabolic confinement potential for different quantum dot shapes (3D spherical and 2D disc-like) have been investigated.

In this section we present the numerical results for the parameters appropriate to GaAs quantum dot. We choose dielectric constant $\varepsilon = 13.1$, electron effective mass $m_e = 0.067\, m_0$, and hole effective mass $m_{lh} = 0.090\, m_0$ for light-hole (lh) and $m_{hh} = 0.377\, m_0$ for heavy-hole (hh) where m_0 indicates free electron mass.[7,19]

In Fig.1 we present our variational calculation results for the light- and heavy-hole exciton ground state energies in 2D (disc-like) quantum dot as a function of single-particle confinement potential energy, $\hbar\omega_0$. The variational parameters λ and γ vary in the ranges between 1.9–2.0 and 0.9–1.0, respectively. In principle, for more realistic calculations one should consider the finite thickness of disc-like QD. However, we assume that the confinement in vertical direction is very strong, so the small corrections arisen from the finite thickness can be ignored.

The decrease in confinement potential, in other words the increase in quantum dot radius, leads to monotonically decrease in ground state energy of the exciton. This is due to the decrease of individual confinement energies of the electron and hole states. The confinement of exciton for larger quantum dot radius is getting weaker and the behaviour of the exciton resembles to the bulk material.

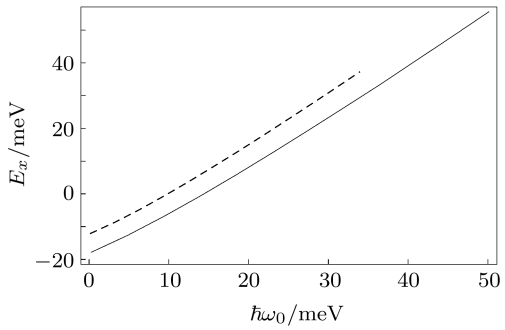


Fig.1. Ground state energy of 2D exciton in GaAs quantum dot as a function of a single-particle confinement potential energy. The solid curve here is for heavy-hole exciton while dashed curve is for light-hole exciton.

As seen in Fig.1, the energy of light-hole exciton for the same quantum dot radius is greater than that of heavy-hole. The effect of quantum confinement appears more for the electron and light-hole pair than the electron and heavy-hole pair, as expected from lighter charge carriers.[7] Halonen and co-workers[19] calculated the ground state energies for 2D hydrogenic heavy-hole exciton in GaAs by the method of numerical diagonalization. They needed 500 basis states for the expansion of the wavefunction of the system in terms of the eigenfunctions of the non-interacting electron–hole pair to describe accurately the ground state of the system. Que[34] reported the results for the energies of the exciton in 2D disc-like QD obtained by configuration interaction method, where more than 20 basis states were used. Our results, obtained with relatively low number of expansions, are in good agreement with the previous theoretical calculations of Refs.[9,19,34,35], indicating that the chosen variational wavefunction Eq.(4) is suitable for the exciton states confined in parabolic QDs.

To further our investigation of the behaviour of the exciton ground state trapped in GaAs QD, in Fig.2, we plot the ground state energy of the exciton in 3D spherical parabolic QD as a function of confinement potential. We found the variational parameters λ and γ of 3D exciton in the range of 0.6–0.8 and 0.8–1.1, respectively. Although the general behaviour of

3D exciton is similar to the 2D disc-like system, there is an obvious quantitative difference in energy values. It is clear that the effect of the effective mass of hole on the system energy is less than that of the 2D exciton. As seen in Figs.1 and 2 the light-hole exciton calculation stops earlier than the heavy-hole exciton. The reason for this is, simply, we have used the same W value for both calculation.

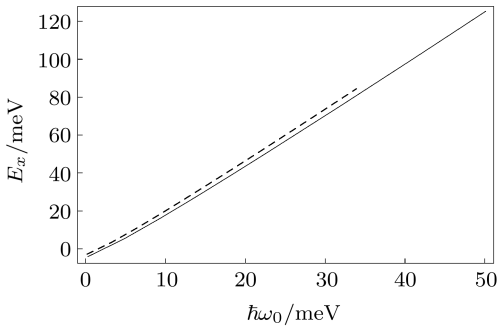


Fig.2. Ground state energy of 3D exciton in GaAs quantum dot as a function of single-particle confinement potential energy. The solid curve is for heavy-hole exciton while the dashed curve is for light-hole exciton.

Additionally, in order to compare the effect of confinement on the shape of excitonic systems, we present the behaviour of ground state energy of the heavy-hole exciton in parabolic quantum dot for 2D disc-like and 3D spherical quantum dot as a function of radius of nanocrystal in Fig.3. The energy decreases rapidly with increasing QD radius both for 2D and 3D excitons with a quantitative difference. For smaller values of radius, the energy of exciton is more sensitive to the size of the dot. Increasing exciton energies are obtained in the case of narrower QD where the effect of quantum confinement is more pronounced. In this case spatial overlap between electron and hole increases, which leads to the enhancement of Coulomb binding energy. Against this for larger QD radius the confinement comes weaker so the energy of the exciton resembles that of its bulk.

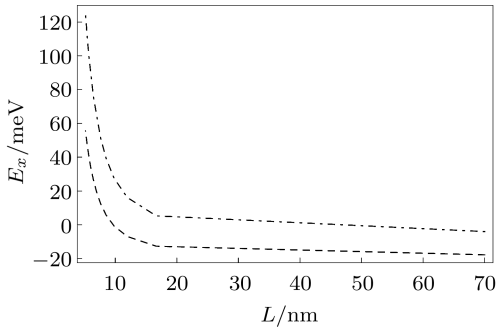


Fig.3. Ground state energy of 2D and 3D heavy-hole exciton in GaAs as a function of quantum dot radius. The dashed curve shows the results for 2D exciton and the dot-dashed curve for 3D exciton.

The energy of 2D disc-like QD is lower than the value of 3D spherical QD for the same radius. The reason of this situation is the enhanced effective confinement of electron and hole in 2D disc-like QD. This result is in agreement with the results given by Xie.[9]

4. Conclusion

In this paper we introduced the integral representations for the terms as $r_{\rm eh}^k \exp(-\lambda r_{\rm eh})$ and calculated variationally the ground state energies of excitons in 2D and 3D parabolic QD by using Hylleraas-like trial wavefunction. The advantage of our choice of the wavefunction, (4), is that the most of the integrations in matrix elements are calculated analytically, by using integral representations in Eqs.(13) and (18), without time-consuming numerical calculations. Inevitable numerical procedure has been invoked at the last stage of the calculations. In the present work, to ensure the validity of our method, dependencies of the ground state energy as a function of confinement potential and effective mass ratios for the exciton in 2D disc-like and 3D spherical quantum dot have been investigated. Explicit incorporation of interparticle distance in the wavefunction made it possible to accomplish reasonable accurate energies with relatively low expansions. Calculations for an exciton in 2D or 3D quantum dot lead to qualitatively similar but quantitatively different results for ground state energies as expected. Comparison with the previous theoretical works, as mentioned in Section 3, revealed a good agreement for ground state energies, confirming that the chosen trial wavefunction (4) and the method presented in this work describes accurately the exciton states confined in parabolic quantum dot.

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Appendix

If the subscript nd indicates dimension of space, 2D or 3D, definitions used for calculation of the elements of matrix $\boldsymbol{H}$ are given below:

$$\begin{aligned}
A_{\rm nd} = &\left(-\frac{m_{\rm h}}{4\sigma_{\rm h}} - \frac{n_{\rm h}}{4\sigma_{\rm h}}\right)\lambda G_{\rm nd}(q,\gamma,\sigma_{\rm e},W,m_{\rm e},n_{\rm e},1)G_{\rm nd}(q,\gamma,\sigma_{\rm h},W,m_{\rm h},n_{\rm h},-1)\\
&+\left(-\frac{m_{\rm e}}{4\sigma_{\rm e}} - \frac{n_{\rm e}}{4\sigma_{\rm e}}\right)\lambda G_{\rm nd}(q,\gamma,\sigma_{\rm e},W,m_{\rm e},n_{\rm e},-1)G_{\rm nd}(q,\gamma,\sigma_{\rm h},W,m_{\rm h},n_{\rm h},1)\\
&+W\gamma\lambda G_{\rm nd}(q,\gamma,\sigma_{\rm e},W,m_{\rm e},n_{\rm e},1)G_{\rm nd}(q,\gamma,\sigma_{\rm h},W,m_{\rm h},n_{\rm h},1), \qquad \text{(A1)}\\
B_{\rm nd} = &\left(-\frac{m_{\rm e}W\gamma}{2} - \frac{m_{\rm eh}W\gamma}{2} - \frac{m_{\rm h}W\gamma}{2} - \frac{n_{\rm e}W\gamma}{2} - \frac{n_{\rm eh}W\gamma}{2} - \frac{n_{\rm h}W\gamma}{2} + \frac{\lambda^2}{2}\right)\\
&\times G_{\rm nd}(q,\gamma,\sigma_{\rm e},W,m_{\rm e},n_{\rm e},1)G_{\rm nd}(q,\gamma,\sigma_{\rm h},W,m_{\rm h},n_{\rm h},1)\\
&+\left(\frac{m_{\rm e}n_{\rm e}}{2\sigma_{\rm e}} + \frac{m_{\rm eh}n_{\rm e}}{4\sigma_{\rm e}} + \frac{m_{\rm e}n_{\rm eh}}{4\sigma_{\rm e}}\right)G_{\rm nd}(q,\gamma,\sigma_{\rm e},W,m_{\rm e},n_{\rm e},-1)G_{\rm nd}(q,\gamma,\sigma_{\rm h},W,m_{\rm h},n_{\rm h},1)\\
&+\left(\frac{1}{2}W^2\sigma_{\rm e} + \frac{1}{2}W^2\gamma^2\sigma_{\rm e}\right)G_{\rm nd}(q,\gamma,\sigma_{\rm e},W,m_{\rm e},n_{\rm e},3)G_{\rm nd}(q,\gamma,\sigma_{\rm h},W,m_{\rm h},n_{\rm h},1)\\
&+\left(\frac{m_{\rm h}n_{\rm h}}{2\sigma_{\rm h}} + \frac{m_{\rm eh}n_{\rm h}}{4\sigma_{\rm h}} + \frac{m_{\rm h}n_{\rm eh}}{4\sigma_{\rm h}}\right)G_{\rm nd}(q,\gamma,\sigma_{\rm e},W,m_{\rm e},n_{\rm e},1)G_{\rm nd}(q,\gamma,\sigma_{\rm h},W,m_{\rm h},n_{\rm h},-1)\\
&+\left(\frac{1}{2}W^2\sigma_{\rm h} + \frac{1}{2}W^2\gamma^2\sigma_{\rm h}\right)G_{\rm nd}(q,\gamma,\sigma_{\rm e},W,m_{\rm e},n_{\rm e},1)G_{\rm nd}(q,\gamma,\sigma_{\rm h},W,m_{\rm h},n_{\rm h},3), \qquad \text{(A2)}\\
C_{\rm nd} = &\left(-\kappa - \frac{m_{\rm eh}\lambda}{2} - \frac{n_{\rm eh}\lambda}{2} - \frac{m_{\rm e}\lambda}{4\sigma_{\rm e}} - \frac{n_{\rm e}\lambda}{4\sigma_{\rm e}} - \frac{m_{\rm h}\lambda}{4\sigma_{\rm h}} - \frac{n_{\rm h}\lambda}{4\sigma_{\rm h}}\right)\\
&\times G_{\rm nd}(q,\gamma,\sigma_{\rm e},W,m_{\rm e},n_{\rm e},1)G_{\rm nd}(q,\gamma,\sigma_{\rm h},W,m_{\rm h},n_{\rm h},1)\\
&+\left(\frac{m_{\rm e}\lambda}{4\sigma_{\rm e}} + \frac{n_{\rm e}\lambda}{4\sigma_{\rm e}}\right)G_{\rm nd}(q,\gamma,\sigma_{\rm e},W,m_{\rm e},n_{\rm e},-1)G_{\rm nd}(q,\gamma,\sigma_{\rm h},W,m_{\rm h},n_{\rm h},3)\\
&+\left(\frac{m_{\rm h}\lambda}{4\sigma_{\rm h}} + \frac{n_{\rm h}\lambda}{4\sigma_{\rm h}}\right)G_{\rm nd}(q,\gamma,\sigma_{\rm e},W,m_{\rm e},n_{\rm e},3)G_{\rm nd}(q,\gamma,\sigma_{\rm h},W,m_{\rm h},n_{\rm h},-1), \qquad \text{(A3)}\\
D_{\rm nd} = &\left(\frac{m_{\rm eh}n_{\rm eh}}{2} + \frac{m_{\rm eh}n_{\rm e}}{4\sigma_{\rm e}} + \frac{m_{\rm e}n_{\rm eh}}{4\sigma_{\rm e}} + \frac{m_{\rm eh}n_{\rm h}}{4\sigma_{\rm h}} + \frac{m_{\rm h}n_{\rm eh}}{4\sigma_{\rm h}}\right)\\
&\times G_{\rm nd}(q,\gamma,\sigma_{\rm e},W,m_{\rm e},n_{\rm e},1)G_{\rm nd}(q,\gamma,\sigma_{\rm h},W,m_{\rm h},n_{\rm h},1)\\
&+\left(-\frac{m_{\rm eh}n_{\rm e}}{4\sigma_{\rm e}} - \frac{m_{\rm e}n_{\rm eh}}{4\sigma_{\rm e}}\right)G_{\rm nd}(q,\gamma,\sigma_{\rm e},W,m_{\rm e},n_{\rm e},-1)G_{\rm nd}(q,\gamma,\sigma_{\rm h},W,m_{\rm h},n_{\rm h},3)\\
&+\left(-\frac{m_{\rm eh}n_{\rm h}}{4\sigma_{\rm h}} - \frac{m_{\rm h}n_{\rm eh}}{4\sigma_{\rm h}}\right)G_{\rm nd}(q,\gamma,\sigma_{\rm e},W,m_{\rm e},n_{\rm e},3)G_{\rm nd}(q,\gamma,\sigma_{\rm h},W,m_{\rm h},n_{\rm h},-1). \qquad \text{(A4)}
\end{aligned}$$

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