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Binding energy of excitons in an infinitely deep spherical quantum dot under intense THz laser field

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Abstract. We study the effects of intense THz laser field on the ground-state binding energy of heavy hole excitons confined in GaAs spherical quantum dots. The calculation is performed using the variational method in the framework of the single band effective mass theory. Our results show that (i) the laser electric field lowers the binding energy for all quantum dot radii, making the exciton clustered near the centre of the dot, (ii) the binding energy is mainly due to the dressed potential making the kinetic part insensitive to the field and (iii) the behaviour of the exciton, under the approximations used, can be modelled by a unique set of plots, depending on the material only via its excitonic units.

Keywords. Exciton; quantum dot; laser field; dressed potential; binding energy; variational method.

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1. Introduction

Over the last decades, confined excitons in quantum dots have been largely investigated experimentally and theoretically for a wide variety of II–VI and III–V semiconductor compounds because of their original properties that allow many interesting applications, namely, producing artificial atoms and molecules, single-electron transistors, quantum dot lasers [1] and quantum-bit [2]. The base of these applications is the large dependence of the exciton binding energy on different and adjustable parameters: the radius of the dot, the effective masses of the carriers, the height and the shape of the confining potential caused by the matrix material in which the exciton is embedded [3–5]. Various external actions, such as magnetic field [6], electric field [7,8] and hydrostatic pressure [9] have already been considered. Recently, some researchers have shown interest in intense terahertz (THz) laser effects on excitons in bulk semiconductor [10,11] and in GaInNAs/GaAs quantum wells [12]. In the former case, calculation of near absorption and transient concludes that the excitons are stabilised against the field ionisation [11]. This counterintuitive effect was confirmed by Lima [10]. By computing the binding energy of excitons in bulk GaAs semiconductor, it is found that this decreases with increasing field intensity and leads to a quarter of the exciton Rydberg energy [10]. In GaInNAs/GaAs quantum wells, Yesilgul [12] found similar trends for all the widths of the well and showed that the intense THz laser field creates an additional geometric confinement on the ground state of the exciton. This work is an extension of these studies, and the purpose of this work is to examine the case of quantum dot excitons under intense THz laser field which, to our knowledge, have not been studied yet.

2. Theory

Let us consider an exciton $X(e, h)$ confined in a spherical quantum dot of radius (R) embedded in an insulating matrix. The Hamiltonian H_0 of the exciton is as follows:

$$H_0 = T_e + T_h + V_c(0) + V_e + V_h, \tag{1}$$

where T_e (T_h) is the kinetic energy for the electron (hole), $V_c(0)$ is the Coulomb interaction between the two particles and V_e (V_h) is the potential confinement for the electron (hole). In the two-bands effective mass approximation, the Hamiltonian H_0 reads as

$$H_0 = -\frac{\Delta_e}{1+\sigma} - \frac{\sigma\Delta_h}{1+\sigma} - \frac{2}{r_{eh}} + V_e + V_h, \tag{2}$$

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where excitonic units (e.u.) are used, that is, the 3D-exciton effective Bohr radius $a^* = \varepsilon\hbar^2/\mu e^2$ for length and the 3D-Rydberg $R^* = \mu e^4/2\epsilon^2\hbar^2$ for energy with $\sigma = m_e/m_h$, $\mu = m_e m_h/(m_e + m_h)$, m_e (m_h) is the electron (hole) effective mass and ε is the relative dielectric constant of the material. We restrict our study in this work to an infinitely deep well:

$$V_i = \begin{cases} 0, & r_i < R \\ \infty, & r_i \geq R \end{cases}. \tag{3}$$

In the presence of intense laser field of amplitude (F_0) and angular frequency (ω) at sufficiently high frequencies, the combined action of the field and the Coulomb interaction between the electron and the hole is equivalent to the effect of a unique so-called 'dressed potential' $V_c(\alpha)$, as has been established by Lima [10] (in the case of bulk material), which is given as

$$V_c(\alpha) = -\left(\frac{1}{|\vec{r}_e - \vec{r}_h + \alpha\vec{k}|} + \frac{1}{|\vec{r}_e - \vec{r}_h - \alpha\vec{k}|}\right), \tag{4}$$

where $\vec{r}_e$ ($\vec{r}_h$) denotes the position vector of the electron (hole) with respect to the centre of the dot and $\alpha = eF_0/\mu\omega^2$ is the laser field parameter, which can be viewed as the excursion amplitude of the relative particle in its vibration in the laser field and $\vec{k}$ is the unity vector along the direction of polarisation of the field. For a given laser source whose power is I (in kW/cm^2), the following practical formula is useful [11]:

$$F_0 \text{ (in kV/cm)} \approx 0.868\sqrt{I}/\sqrt[4]{\varepsilon}.$$

Assuming that the dressed potential model (4) is applicable to the confined excitons, the work seeks to solve the Schrödinger equation:

$$H_\alpha \psi(\vec{r}_e, \vec{r}_h) = E\psi(\vec{r}_e, \vec{r}_h) \tag{5}$$

with

$$H_\alpha = H_0 + V_c(\alpha) - V_c(0). \tag{6}$$

The task of directly solving this equation is so difficult because the variables cannot be separated. That is why approximation methods are required. Hereafter, we adopt the general variational method, which can give at least qualitative results. The variational method minimises the energy operator value $\langle\psi|H_\alpha|\psi\rangle$ with respect to variational parameters included in a chosen trial function ψ, which represents the ground state of the system.

Taking into account the correlation between the electron and the hole and having in mind the form of the solution in the absence of the field ($\alpha = 0$), we choose ψ, in the first approximation, as follows:

$$\psi = N\varphi(r_e)\varphi(r_h)(1 + \beta Z)\varphi_{eh}, \tag{7}$$

where $Z = z_e - z_h$ is the relative position between the electron and the hole along the polarisation direction of the field,

$$\varphi(r) = \frac{\sin(kr)}{kr},$$

where $k = \pi/R$ is the one-particle wave function in the dot, N is the normalisation coefficient given by $\langle\psi|\psi\rangle = 1$. $\varphi_{eh} = \exp(-\lambda r_{eh})$ is the term which describes the spatial correlation between the electron and the hole, β and λ are the variational parameters. The factor $(1+\beta Z)$ is introduced in order to take into account the distortion caused by the electric field. The binding energy for the ground state of the exciton is then given by

$$E_b = E_e + E_h - \min_{\beta,\lambda}\langle\psi|H|\psi\rangle, \tag{8}$$

where $E_e(E_h)$ is the energy of the electron (hole) in an infinitely deep spherical well $E_i = \hbar^2\pi^2/2m_i^*R^2$ which leads (in excitonic units) to

$$E_e + E_h = k^2. \tag{9}$$

In order to solve eq. (3), we introduce the complete Hylleraas [13] coordinates ($r_e, r_h, r_{eh}, z_e, z_h$).

Thus, the kinetic operator reads as

$$T = -\frac{1}{1+\sigma}(T_{re} + \sigma T_{rh}) - \frac{1}{1+\sigma}(T_{ze} + \sigma T_{zh}) \tag{10}$$

where $i = e, h$.

$$T_{ri} = \frac{\partial^2}{\partial r_i} + \frac{2}{r_i}\frac{\partial}{\partial r_i} + \frac{(r_i^2 + r_{ij}^2 + r_j^2)}{r_i r_{ij}}\frac{\partial^2}{\partial r_{ij}\partial r_i} + \frac{2}{r_{ij}}\frac{\partial}{\partial r_{ij}}, \tag{11}$$

$$T_{zi} = \frac{\partial^2}{\partial z_i^2} + \frac{2z_i}{r_i}\frac{\partial^2}{\partial z_i \partial r_i} + 2\frac{(z_i - z_j)}{r_{ij}}\frac{\partial^2}{\partial r_{ij}\partial z_i}. \tag{12}$$

In these coordinates, the elementary volume is given by

$$d\tau = \frac{8\pi r_h dr_h r_e dr_e r_{eh} dr_{eh}\, dz_e dz_h}{\sqrt{4\left(r_e^2 - z_e^2\right)\left(r_h^2 - z_h^2\right) - \left(r_e^2 + r_h^2 - r_{eh}^2 - 2z_e z_h\right)^2}} \tag{13}$$

and the integration over the coordinates is done in domains:

$$0 < r_e, r_h \leq R;\ |r_e - r_h| \leq r_{eh} \leq r_e + r_h;$$

$$-r_e \leq z_e \leq r_e;\ Z_1 \leq z_h \leq Z_2,$$

where Z_1 and Z_2 are the roots of the denominator expression in eq. (12) with respect to z_h. Let us note that, according to the symmetry of the problem, the order of integration over z-coordinates can be inverted without

affecting the result on the condition of interchanging e and h indices. After elementary transformations,

$$d\tau = d\tau_r d\tau_z \tag{14}$$

with

$$d\tau_r = 4\pi r_h dr_h dr_e r_{eh} dr_{eh} \tag{15}$$

$$d\tau_z = \frac{dz_e dz_h}{\sqrt{(z_h - Z_1)(Z_2 - z_h)}} \tag{16}$$

and

$$Z_1 + Z_2 = S = z_e \left(1 + \frac{r_h^2 - r_{eh}^2}{r_e^2}\right);$$

$$Z_1 Z_2 = P = \frac{r_e^2}{4z_e^2} S^2 - \left(1 - \frac{z_e^2}{r_e^2}\right) r_h^2. \tag{17}$$

Even under these simplifications, the problem remains unsolvable analytically. Thus, it is necessary to support the resolution by using computational techniques. Let us consider at first the potential term of eq. (4):

$$V_c(\alpha) = -A^{-1/2}\left[(1+z)^{-1/2} + (1-z)^{-1/2}\right], \tag{18}$$

where

$$A = r_{eh}^2 + \alpha^2; \quad z = \frac{2\alpha}{A} Z; \quad r_{eh} = |\vec{r}_e - \vec{r}_h|. \tag{19}$$

As $0 \leq z < 1$, power series development of the term between brackets around $z = 0$ may be used and, practically, it is proved that the 10th order of the development is sufficient to obtain quite accurate results. The calculation of the potential energy $\langle\psi|V_c(\alpha)|\psi\rangle$ is then solved by analytically computing integrals over z-coordinates in terms of elementary mathematics. On the other hand, taking into account the symmetry in exchanging (z_e, r_e) with (z_h, r_h) when performing integrations in calculating the kinetic energy, we obtain

$$T = \left[k^2 - \lambda^2\right] + 4\lambda\beta^2 N^2 L + N^2\lambda F + 2\lambda N^2 K - \frac{1-\sigma}{1+\sigma} 2N^2\beta^2 P, \tag{20}$$

where

$$L = \int \frac{Z^2}{r_{eh}} \varphi_0^2 d\tau; \quad K = 8\pi^2 \int \frac{\varphi_0^2}{r_{eh}} d\tau_r, \tag{21}$$

$$P = \int \varphi_0 \varphi_{eh}^2 \varphi_h \frac{z_e}{r_e} \frac{d\varphi_e}{dr_e} Z d\tau, \tag{22}$$

$$F = \int r_{eh} \frac{1}{\varphi_e r_e} \frac{d\varphi_e}{dr_e} (1 + \beta^2 Z^2) \varphi_0^2 d\tau, \tag{23}$$

$$N^2 = \left[\langle\varphi_0|\varphi_0\rangle + \beta^2 \langle\varphi_0|Z^2\varphi_0\rangle\right]^{-1}. \tag{24}$$

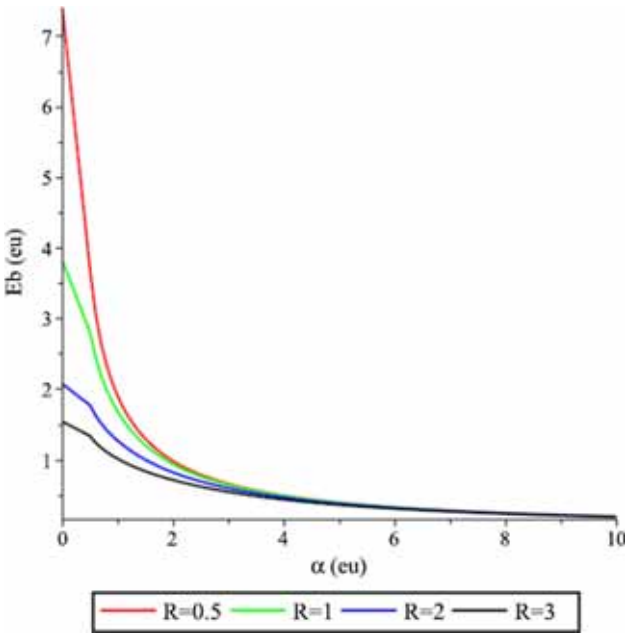

Figure 1. Binding energy of the exciton in GaAs vs. the field parameter α for various radii of the quantum dot (e.u.).

3. Results and discussion

Calculations of the binding energy for the confined excitons were performed for GaAs characterised by its σ parameter and its excitonic units R^* and a^*. Integrations over r_e, r_h and r_{eh} were calculated using Gauss-Legendre [14] method within Maple platform. For minimising the energy, several standard numerical methods were tested leading to the same results. The binding energy of the QD-exciton under laser field was then computed for different values of the field intensity parameter α from 0 to 10 e.u. and for various values of R ranging from $0.5a^*$ (the strong confinement regime) to $3a^*$ (quasi-3D-exciton). The result is shown in figure 1. Several interesting points can be noted: (i) The exciton binding energy decreases with the increase in laser field, because the Coulombic interaction between the electron and the hole decreases. For large enough dot dimensions, the laser field sensitivity of the binding energy is observed to be very weak. We can explain this behaviour of the curves as follows: The geometric confinement has a major effect on the exciton in narrow quantum wells. For this reason, any change in the geometric confinement significantly affects the binding energy, (ii) for high intensity values of the filed ($\alpha > 5$ e.u.), the system becomes insensitive to the confinement and the binding energy tends towards the limit $R^*/5$ when $\alpha \to \infty$ which is close to the limit $R^*/4$ found by Lima in the case of bulk exciton [10],

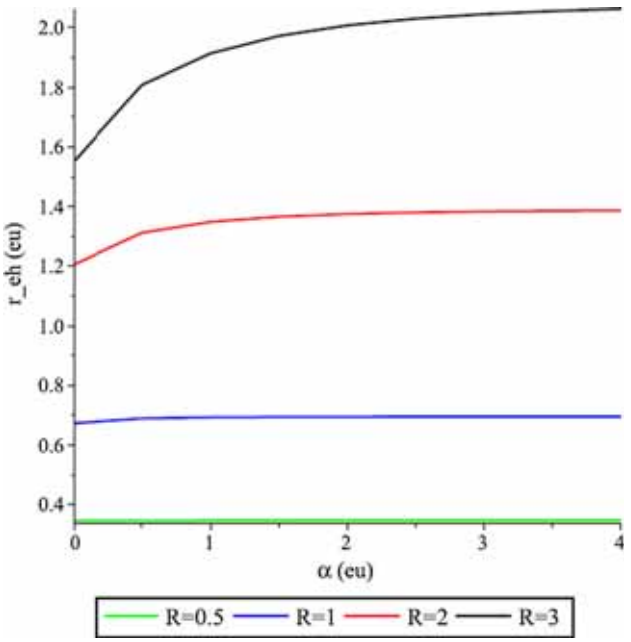

Figure 2. Variations of the spatial extension of the exciton (r_{eh}) vs. the field parameter (α) for various radii of the dot in GaAs.

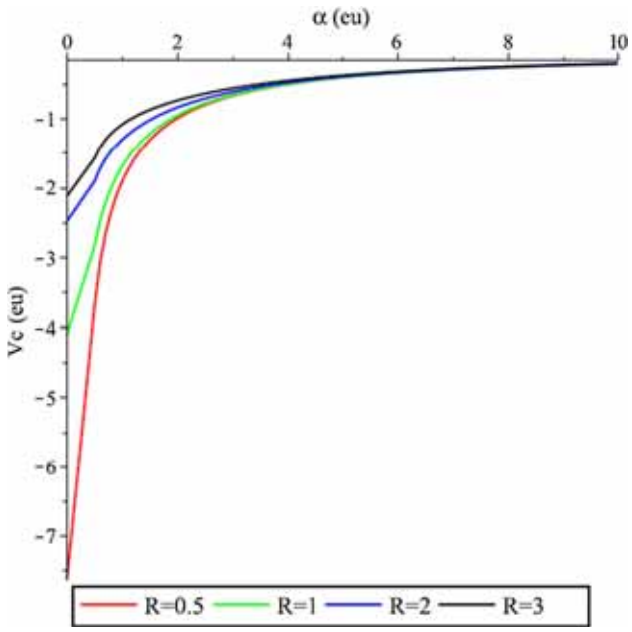

Figure 3. Dressed potential of the exciton vs. the field parameter (α) in GaAs quantum dot for various radii of the dot (e.u.)

(iii) for negligible confinement ($R = 3$) and $\alpha = 0$ the binding energy approaches the limit value $1.5R^*$ which is one half higher than the limit $1R^*$ found by the same authors in the purely 3D-exciton case [10]. These results show that the exciton remains stabilised against the field ionisation and predict an infrared shift in its photoluminescence edge spectra. For $\alpha > 5$, the field effect drastically reduces the confinement effect making the exciton a bulk one. Furtheremore, by drawing the variations of the spatial extension of the exciton r_{eh} vs. the field intensity as shown in figure 2, we notice that the shape of the exciton, for low radii, is quasi-field-independent making the electron and the hole clustered to the centre of the dot. For larger dots, the shape of the exciton expands slightly when increasing the field intensity from 0 to 2 and then stablises for higher values of the field intensity making electron and hole more distant. But in all the cases, this separation does not exceed 35% of the diameter of the dot. In order to check these properties, we have calculated the relative contribution of the kinetic energy and the dressed potential to the binding energy of the exciton. Figure 3 shows how the dressed potential varies with increasing intensity of the field. Unexpected behaviour is highlighted: all the curves are close to those obtained for E_b by inverting the sign which means that the kinetic part of the binding energy is negligible. Indeed, plot of T vs. α, shown in figure 4, reveals the kinetic energy for any given radius R following the simple relation $TR^2 \approx \pi^2$ or $T \approx k^2$

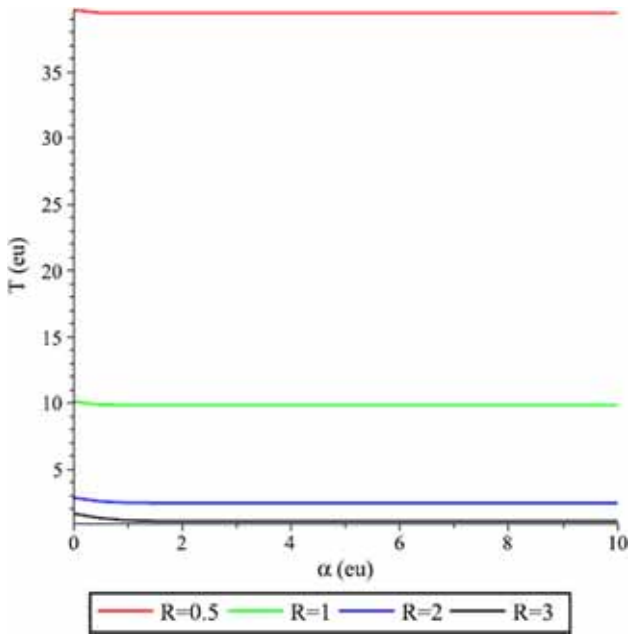

Figure 4. Variation of kinetic energy with laser field for different quantum dot radii.

which leads effectively to $E_b \approx -V_c$ (eqs (8) and (9)) as shown in figure 3. Subsequently, and according to eq. (20), the expression of E_b (in excitonic units) is σ independent and then, it may be used for all materials satisfying the approximations of our model. Finally,

before ending, we have to note that these results depend mainly on the choice of the trial function and testing a more advanced expression with higher power degree polynomial in Z would be more relevant. However, our work establishes the first contribution in the area and gives original results which we are extending by deeper and more elaborate studies to the case of finite confinement potential.

4. Conclusion

We have studied the quantum dot exciton under intense THz laser field in the dressed potential approximation. The binding energy and the spatial extension of the exciton are established and calculated in the framework of the variational method. The results show that the field lowers the binding energy for all quantum dot radii of the dot and makes the exciton clustered near the centre of the dot. Furthermore, the binding energy is mainly due to the dressed potential making the kinetic part insensitive to the field. This result leads us to conclude that the behaviour of the exciton, under the approximations used, can be modelled by a unique set of plots depending on the material only via its excitonic units.

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