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Analysis of Exciton Binding Energy in Bulk and Quantum Well Semiconductor Structures

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ABSTRACT

We estimate Bohr radius and binding energy of exciton in bulk as well as quantum well for semiconductors with non-parabolic energy band structure. Kane type dispersion relation is used to incorporate such band non-parabolicity. Exciton binding energy in various III-V semiconductors are calculated for two different expressions of non-parabolicity factor α, and results are compared with those for parabolic energy bands. In presence of band non-parabolicity, exciton binding energies are found to increase in quantum wells, whereas such variation is almost insignificant in bulk semiconductors.

KEYWORDS: Exciton, Binding Energy, Band non-parabolicity, III-V semiconductors.

INTRODUCTION

Exciton plays a key role in a wide range of opto-electronic devices used in optical communication systems or optical computers. Confinement of carriers leads to higher value of exciton binding energy in Quantum well (QW) or other low-dimensional systems. The energy spectrum and wave-functions of quantum confined excitons are strongly different from those of bulk excitons. The density of states changes from a smooth parabola in three dimensions to a stair case in two-dimensional (2D) system, which in turn, enhances the optical properties. Such enhancement of optical absorption and emission results in well-defined exciton lines in QWs [1] even at room temperature. Dingle et al. [2] were the first to observe enhanced excitonic effects in the quantum well structure, while Miller et al. [3] measured such increase in exciton binding energy in these structures. Bastard et al.[4] and Greene et al.[5,6] assumed confinement of the carriers in either an infinite or finite square quantum well and estimated binding energy of the exciton using variational technique. Leavitt and Little [7] presented a general method for calculating the exciton binding energies in various complex quantum confined semiconductor structures. In recent time, self-consistent approach is tried out [8], which is very effective for wide band-gap material and can be extended to asymmetric QW.

Excitonic absorption in QWs can be greatly varied by application of electric field along the direction of growth of the well and this phenomenon is termed as Quantum Confined Stark Effect (QCSE). In fact, strong modulation is obtained when absorption edge is dominated by excitonic effects. This is put to practical use in high performance semiconductor electro-optic modulators. Such devices based on zinc blende III-V semiconductors are being extensively used for data transmission, photonic switching and optical interconnects. At present, visible /ultraviolet electro-absorption modulators based on wide band gap nitride semiconductors viz. GaN films and GaN/AlGaN multiple Quantum wells [9] are being developed and characterized.

In general, the energy dispersion relation is assumed ideally to be parabolic. But the deviation of experimental results from the theoretical ones indicates the presence of non-ideal conditions. One such condition originates from band non-parabolicity. In semiconductors, the energy bands are parabolic only at the vicinity of allowed band edge. In bulk materials, higher energy states occupied by the carrier within conduction and valence bands may lie far away from the band-edge where assumption of parabolic energy band is no more valid. Such band non-parabolicity is more prominent in case of quantum structures, where carriers even in the ground states leave the band edges due to quantum size effect. Excitonic states are, therefore, expected to be profoundly influenced by the band non-parabolicity and are worth investigating.

In the present work, we calculate binding energy of the ground excitonic state in bulk semiconductor and in QW, the simplest quantum confined semiconductor structure, in presence of band non-parabolicity. In order to obtain exciton binding energy in bulk, we begin with the Schrödinger equation and use Kane dispersion relation to include non-parabolicity effect in it. The similar formulation is followed for 2D structure. From the derived results, exciton binding energies for various semiconductors are estimated using different expressions of non-parabolicity factor.

KANE DISPERSION MODEL

In parabolic approximation, the $E-k$ dispersion relation can be written as

$$E=\frac{\hbar^2k^2}{2m^*} \tag{1}$$

with m^* being the carrier effective mass, $\hbar k$ the crystal momentum and $\hbar$ the Dirac's constant. However at higher energies i.e. for states away from the band extrema, the parabolic approximation is rather unsatisfactory. Therefore, the energy bands in III-V direct band gap semiconductors can be described by the Kane dispersion relation [10], which considerably modifies the parabolic approximation. According to the Kane model, energy in a non-parabolic conduction band is represented as,

$$E(k)[1+\alpha E(k)] = \frac{\hbar^2 k^2}{2m^*} \tag{2}$$

from which the energy can be expressed, retaining terms only up to 4th order of k, as

$$E(k) = \frac{\hbar^2 k^2}{2m^*} - \alpha\left(\frac{\hbar^2 k^2}{2m^*}\right)^2 \tag{3}$$

where non-parabolicity factor α, is given by [11],

$$\alpha = \left(1-\frac{m^*}{m_0}\right)^2\left(\frac{3+4x+2x^2}{3+5x+2x^2}\right)\frac{1}{E_g} \tag{4}$$

In the above equation, $x = \frac{\Delta}{E_g}$, where Δ is the spin-orbit splitting, E_g is the band gap energy, m^* and m_0 are the effective and free electron masses. In its simplest form, α is taken to be reciprocal of the band gap energy E_g i.e.

$$\alpha = \frac{1}{E_g} \tag{5}$$

In order to find out the ground excitonic state in bulk materials in presence of band non-parabolicity, we adopt the standard scheme [12] for deriving exciton energy in bulk semiconductors with parabolic energy bands.

EXCITONS IN BULK

A general form of Schrödinger equation, dependent on the position co-ordinates of both electrons and holes (r_e and r_h) in bulk semiconductors with parabolic *E*-*k* dispersion relation, is given [12] as,

$$\left[E_g - \frac{\hbar^2}{2m_e^*}\nabla_e^2 - \frac{\hbar^2}{2m_h^*}\nabla_h^2 - \frac{e^2}{4\pi\epsilon(r_e - r_h)}\right]\psi(r_e, r_h) = E\psi(r_e, r_h) \tag{6}$$

where m_e^* and m_h^* are respectively electron and hole effective masses and ϵ is permittivity of the semiconductor.

Separation of the wave-function into centre of mass co-ordinate ($R = \frac{m_e^* r_e + m_h^* r_h}{M}$) and relative co-ordinate ($r = r_e - r_h$), followed by transformation from the co-ordinates (r_e, r_h) to (R, r), yields the Schrödinger equation involving relative motion of the electron-hole pair forming the exciton as,

$$\left(E_g - \frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{e^2}{4\pi\varepsilon r}\right)\psi(r) = E_r\psi(r) \tag{7}$$

where, $\nabla_r^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$, $r = \sqrt{(x^2+y^2+z^2)}$ is the electron-hole separation,
M is total mass of exciton i.e. ($m_e^* + m_h^*$), μ is the reduced mass given by the relationship ($\frac{1}{\mu} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$).

To incorporate the effect of band non-parabolicity, we employ the Kane Dispersion relation to modify equation (7) as,

$$\left[-\frac{\hbar^2}{2\mu}\nabla_r^2 - \alpha\left(\frac{\hbar^2}{2\mu}\right)^2\nabla_r^4 - \frac{e^2}{4\pi\epsilon r}\right]\psi = (E_r - E_g)\psi \tag{8}$$

Next, in order to transform Cartesian co-ordinates into plane polar co-ordinates, we represent $\frac{\partial\psi}{\partial x} = \frac{x}{r}.\frac{\partial\psi}{\partial r}$, and thereby, $\frac{\partial^2\psi}{\partial x^2} = \frac{x^2}{r^2}\frac{\partial^2\psi}{\partial r^2} + \frac{1}{r}\frac{\partial\psi}{\partial r} - \frac{x^2}{r^3}\frac{\partial\psi}{\partial r}$.

Similar forms of $\frac{\partial^2\psi}{\partial y^2}$ and $\frac{\partial^2\psi}{\partial z^2}$, along with $\frac{\partial^2\psi}{\partial x^2}$, yield

$$\nabla_r^2\psi = \frac{\partial^2\psi}{\partial r^2} + \frac{2}{r}\frac{\partial\psi}{\partial r} \tag{9}$$

Thus we finally get

$$\nabla_r^4\psi = \frac{4}{r}\frac{\partial^3\psi}{\partial r^3} + \frac{\partial^4\psi}{\partial r^4} \tag{10}$$

Using expressions (9) and (10) in equation (8), we get the final form of the Schrödinger equation, which is to be solved by variational technique.

Coulombic interaction between the electron-hole pair is considered to be of Hydrogenic type. Hence, it is a standard practice to choosea spherically symmetric wavefunction $\psi \sim \exp\left(\frac{-\mathrm{r}}{\lambda}\right)$ as the trial wave function, where λ is the variational parameter. Use of the ground excitonic wave function modifies the Schrödinger equation as,

$$\left[\frac{1}{\lambda^2} + \frac{\alpha\hbar^2}{2\mu\lambda^4} + \frac{2\mu}{\hbar^2}\left(E_r - E_g\right)\right]\psi + \frac{1}{r}\left[-\frac{2}{\lambda} - 4\frac{\alpha\hbar^2}{2\mu\lambda^3} + \frac{2\mu}{\hbar^2}\frac{e^2}{4\pi\epsilon}\right]\psi = 0 \tag{11}$$

As $r \to 0$, the above equation diverges. Therefore, the second term must vanish which leads to

$$\lambda^3 - \frac{4\pi\epsilon\hbar^2}{\mu e^2}\lambda^2 - \left(\frac{\alpha\hbar^2}{\mu}\right)\left(\frac{4\pi\epsilon\hbar^2}{\mu e^2}\right) = 0 \tag{12}$$

Solution of the above equation gives the proper value of λ and is expressed here as λ_{3D}. It ,is practically the exciton Bohr radius for bulk semiconductor with non-parabolic energy band structures.
Use of the resulting λ_{3D} in the first term of equation (11) yields the desired exciton binding energy that can be expressed as,

$$E_B^{(3D)} = \frac{\hbar^2}{2\mu\lambda_{3D}^2} + \alpha\left(\frac{\hbar^2}{2\mu\lambda_{3D}^2}\right)^2 \tag{13}$$

To get the results for bulk semiconductors with parabolic energy bands, we put $\alpha = 0$ in equations (12) and (13). This yields the ground state Bohr radius as,

$$\lambda = \frac{4\pi\epsilon\hbar^2}{\mu e^2} \tag{14}$$

and the corresponding binding energy (E_B) as,

$$E_B = \frac{\mu e^4}{32\pi^2\hbar^2\epsilon^2} \tag{15}$$

which are the standard results.

EXCITONS IN QUANTUM WELL

It is already pointed out that in a QW, the ground states of both electron and hole lie away from the band extrema, and thereby, make the consideration of band non-parabolicity relevant. As in very narrow wells, the above effect becomes much more pronounced, we assume our model to be strictly two-dimensional. The excitons in such QWs are also 2D in nature.
The Schrödinger equation involving relative motion of the electron-hole pair, in presence of band non-parabolicity, is expressed here as

$$\left[-\frac{\hbar^2}{2\mu}\nabla_{r_\perp}^2 - \alpha\left(\frac{\hbar^2}{2\mu}\right)^2\nabla_{r_\perp}^4 - \frac{e^2}{4\pi\epsilon r_\perp}\right]\psi = E\psi \tag{16}$$

where $r_\perp = \sqrt{x^2 + y^2}$ is the electron-hole separation in such 2D case.

Accordingly,

$$\nabla_{r_\perp}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \tag{17}$$

For conversion of Cartesian co-ordinate system into plane polar co-ordinate system, we proceed as follows:

$\frac{\partial\psi}{\partial x} = \frac{x}{r_\perp}\,.\frac{\partial\psi}{\partial r_\perp}$ and $\frac{\partial^2\psi}{\partial x^2} = \frac{1}{r_\perp}\frac{\partial\psi}{\partial r_\perp} - \frac{x^2}{r_\perp^3}\frac{\partial\psi}{\partial r_\perp} + \frac{x^2}{r_\perp^2}\frac{\partial^2\psi}{\partial r_\perp^2}$
which together with similar form of $\frac{\partial^2\psi}{\partial y^2}$ leads to

$$\nabla_r^2\psi = \frac{\partial^2\psi}{\partial {r_\perp}^2} + \frac{1}{r_\perp}\frac{\partial\psi}{\partial r_\perp} \tag{18}$$

From this, we can calculate $\nabla_r^4\psi$ in the same way as done earlier and get the final form as,

$$\nabla_r^4\psi = \frac{\partial^4\psi}{\partial r_\perp^4} + \frac{2}{r_\perp}\frac{\partial^3\psi}{\partial r_\perp^3} - \frac{1}{r_\perp^2}.\frac{\partial^2\psi}{\partial r_\perp^2} + \frac{1}{r_\perp^3}.\frac{\partial\psi}{\partial r_\perp} \tag{19}$$

Use of equations (18), (19) and finally of similar trial wavefunction $\psi \sim \exp\left(\frac{-r_\perp}{\lambda}\right)$ gives the Schrödinger equation (16) modified to the form:

$$\left[\frac{1}{\lambda^2}\psi + \frac{\alpha\hbar^2}{2\mu\lambda^4}\psi + \frac{2\mu}{\hbar^2}\left(E_r - E_g\right)\psi\right] + \frac{1}{r_\perp}\left(\frac{-1}{\lambda} - \frac{\alpha\hbar^2}{\mu\lambda^3} + \frac{\mu e^2}{2\pi\epsilon\hbar^2}\right)\psi + \frac{\alpha\hbar^2}{2\mu}\left[\frac{1}{{r_\perp}^2}\left(\frac{-1}{\lambda^2}\right)\psi + \frac{1}{{r_\perp}^3}\left(\frac{-1}{\lambda}\right)\psi\right] = 0 \tag{20}$$

The above equation is not valid as $r \to 0$. Therefore, both the second and third terms in equation (20) are equated to zero. The second term while equated to zero gives exciton Bohr radius in QW as,

$$\lambda^3 - \frac{2\pi\epsilon\hbar^2}{\mu e^2}\lambda^2 - \frac{\alpha\hbar^2}{\mu}.\frac{2\pi\epsilon\hbar^2}{\mu e^2} = 0 \tag{21}$$

Upon solving equation (21), we get exciton Bohr radius in QW for semiconductors with non-parabolic energy bands.

Use of the Bohr radius (λ_{2D}) in the first term of equation (20) gives the corresponding exciton binding energy in QW as

$$E_B^{(2D)} = \frac{\hbar^2}{2\mu\lambda_{2D}^2} + \alpha\left(\frac{\hbar^2}{2\mu\lambda_{2D}^2}\right)^2 \tag{22}$$

Substitution of $\alpha = 0$ in equations (21) and (22) yields

$$\lambda_{2D} = \frac{2\pi\epsilon\hbar^2}{\mu e^2} \tag{23}$$

and

$$E_B^{(2D)} = \frac{\mu e^4}{8\pi^2\hbar^2\epsilon^2} \tag{24}$$

The above expressions (23) and (24) give the Bohr radius and binding energy for exciton ground state in a QW of semiconductor with parabolic energy bands, while those in presence of band non-parabolicity are given respectively by equations (21) and (22).

RESULTS AND DISCUSSION

Exciton Bohr radii in bulk and QW of different III-V semiconductors are estimated using equations (14) and (23) respectively and presented in Table I. The basic expressions, and thereby, the results in Table I indicate the well-known fact that the exciton Bohr radius in a QW is reduced to half of that in the bulk material.

TABLE 1. Bohr Radius for Ground Excitonic State in Semiconductor Bulk and QW

Semiconductor	Bohr radius λ [Å]	
	Bulk	QW
InSb	675.4	337.7
InAs	355.1	177.6
GaSb	234.0	117.0
InP	97.1	48.5
GaAs	116.1	58.0

Next, we calculate exciton binding energies in bulk and QW from expressions (13) and (22) respectively, where the E-k dispersion relation is assumed to be non-parabolic. Expression (4) and its simplest form (5) are used for the band non-parabolicity factor α. Such results for different III-V semiconductors are presented in Table II, along with those for $\alpha = 0$, calculated from expressions (15) and (24).

TABLE 2. Ground State Binding Energy for Excitons in Bulk and QW in the presence and absence of Band Non-Parabolicity

Semiconductor	Band gap $E_g[eV]$	Binding Energy (meV) for bulk			Binding Energy (meV) for QW		
		Non-parabolic		Parabolic	Non-parabolic		Parabolic
		α from equation (4) $[eV^{-1}]$	$\alpha = \frac{1}{E_g}[eV^{-1}]$		α from equation (4) $[eV^{-1}]$	$\alpha = \frac{1}{E_g}[eV^{-1}]$	
InSb	0.23	0.60	0.600	0.6	2.422	2.425	2.4
InAs	0.42	1.38	1.400	1.4	5.572	5.572	5.5
GaSb	0.81	1.94	1.945	1.94	7.83	7.875	7.8
InP	1.42	5.99	6.025	6	24.2	24.29	23.9
GaAs	1.52	4.74	4.715	4.7	19.13	19.13	18.9

It is evident from Table II that in the case of semiconductors with parabolic energy bands, the exciton binding energy in QW is enhanced four times with respect to that in bulk. The Table further indicates that the influence of band non-parabolicity is almost insignificant on excitons in bulk materials. However, such influence is quite pronounced in case of QW. The tabulated results reveal that exciton binding energy in QW with $\alpha \neq 0$ is even greater than four times of that in bulk with $\alpha = 0$. In presence of band non-parabolicity, carrier energies are lowered, which effectively reduces the electron-hole separation and in turn, increases the exciton binding energy. It may further be noted that the original expression (4) and the approximate one (5) of non-parabolicity factor α do not make any significant change in estimated binding energies. Thus, the simple form of α can safely be used in calculating exciton binding energy.

CONCLUSIONS

In 2D systems, due to quantum size effect ground states electron and hole are lifted with respect to the allowed band edges. Such energy level lifting will increase in Quantum Wires and Quantum Dots due to higher degree of confinement. So, influence of band non-parabolicity is expected to be more and more prominent, and can be further investigated for structures with dimensionality lower than 2D.

REFERENCES

[1] R. Dingle, in *Festkorperprobleme, Advances in Solid State Physics,* edited H. J. Queisser, (Pergamon/ Vieweg, Braunschweig, (1975), vol. XV, p. 21.
[2] R. Dingle, W. Wiegmann and C. H. Henry, Phys. Rev. Lett. 33, 827, (1974).
[3] R. C. Miller, D.A. Kleinman, W. T. Tsang and A. C. Gossard, Phys. Rev. B 24,1134, (1981).
[4] G. Bastard, E. E. Mendez, L. L. Chang and L. Esaki, Phys. Rev. B 26, 1974, (1982).
[5] R. L. Greene, K. K. Bajaj and D. E. Phelps, Phys. Rev. B 29, 1807 ,(1984).
[6] Ronald L. Greene and K. K. Bajaj, Solid State Communications. 88, 955, (1993).
[7] R. P. Leavitt and J. W. Little, Phys. Rev. B 42, 11774 ,(1990).
[8] .V.Ponomarev, L.I.Deych, V.A. Shuvayev, A.A. Lisyansky, Physica E 25, 539, (2005).
[9] Chen- kaikao,Anirban Bhattacharyya, Christos Thomidis, Roberto Paiella and Theodore D. Moustakas, Journal of applied physics 109, 083102, (2011).
[10] E. O. Kane, J. Phys. Chem. Solids I 249, (1957).
[11] Q. H. F. Vrehen, J. Phys. Chem. Solids 29, 129, (1968).
[12] Paul Harrison, *Quantum wells, wires and dots, 2nd edition: Theoretical and computational physics of semiconductor nanostructures,* Wiley, (2005).