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A Theoretical Study on Shallow Donor Impurity in Triple Quantum Well Structures Under External Fields

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Abstract: Using theoretical formalism of A. Large etal [Semicond. Sci. Technol. 2002], we have studied the shallow donor impurity in triple quantum well structures. Our theoretically evaluated result for intra-donor transition energy (cm^{-1}) and intra-donor magneto-absorption coefficients (arb. U) are in good agreement with the experimental data.

Keywords: Shallow donor impurity, triple quantum well structure, Intra-donor transition energy, Intra-donor magneto absorption coefficients, coupled homogeneous linear equations, geometrical and induced field confinement, Quantum dots and super lattices, photon polarization vector

INTRODUCATION

Due to large variety of technological applications, single and multiple semiconductors quantum well structures have been extensively studied. Studies have been made in different situations including external perturbations, such as magnetic and electric fields and distinct doping processes. Nowadays, semiconducting devices are designed based on photo detector properties and magneto-optical properties of quantum- well systems. This includes the design of optical modulators based on the quantum-well

confined Stark effects. There is some devices made by double-barrier and double-well systems. In this advancement, one has Triple quantum well (TQW) heterostructures. This has shown to provide interesting change in many physical properties. In particular, these TQW systems have been proven to be superior in resonant tunneling properties, as compared to double quantum wells. Apart from this, asymmetric TQW systems have been found to exhibit nonlinear behavior in the electronic transmission. This is essentially due to the internal electric field induced by photo-excited electrons and holes within the heterostructures[1,2] .There is also possibilities of having different kinds of electromagnetic emission emerging from asymmetric TQW heterostructures. Another interesting application is the fabrication of a three-colour infrared photodetector which operates at a fixed bias composed of TQW structure[3]. Large Stark Shifts have been observed in strongly coupled (Ga,Al) As-GaAs systems[4].

This has been designed for modulator applications at 810nm. The rate at which the excitonic transitions change in energy with the applied electric field is a relevant parameter for the device performance. Impurities in semiconducting heterostructures are known to promote a number of qualitative changes in electronics and optical properties. Therefore, they have been largely studied for different quantum systems such as quantum wires, quantum Dots and superlattices[5-10].M. Pacheco etal.[11] have analyzed the influence of the geometric and induced- field confinements on the binding energy of donor impurities in TQW systems. By changing the intensity of external magnetic and electrical fields, one can obtain binding energies of particular structure. It has also been observed that the spatial distribution of the electronic wave functions within these TQW structures plays a fundamental role on the characteristic features of the impurity binding energy. In fact, the binding energy may be considered as a map of the ground-state wave function associated with an electron confined in the system[12,13]. Due to the interesting impurity –related properties under external fields exhibited by TQW, one is interested to study the optical transitions between states of impurities confined in TQW heterostructures.

Mathematical formula used in the study: The effective mass Hamiltonian of a donor impurity in TQW structure, in the presence of magnetic field **B**=Bz and electric field **F**=Fz is written as

$$H = \frac{1}{2m^*}(p + \frac{|e|}{c}A_0)^2 + V_{conf}(z) + |e|Fz + \frac{e^2}{\varepsilon_0 |r - r_i|} \quad (1)$$

In which m^* is the electronic effective mass, $\mathbf{A_0}$ is the vector potential which is taken in the symmetric gauge, ε_0 is the GaAs dielectric function. The TQW structures are modeled by the potential V_{conf} (z) and impurity is located at $r_i=z_i\mathbf{z}$. The eigen value problem for the given Hamiltonian is solved by adopting a particular variational scheme[14]. In this variational scheme both the ground state and excited states can be simultaneously obtained. The envelope wave functions are expanded in terms of the z-dependent quantum-well eigen functions $f_n(z)$ and a set of Gaussian function with fixed length parameter λ_j

$$\psi(\rho,\phi,z) = \Sigma_n \Sigma_{j,m} D_{j,m}{}^n e^{-\frac{\rho^2}{\lambda_j}} \rho^{|m|} e^{im\phi} f_n(z) \quad (2)$$

In which m denotes the quantum number associated with the z-component of the orbital angular momentum operator. The set of parameters covers the physical range of relevant radii associated with the potential confinement[15,16]. The impurity energies are obtained by solving a set of coupled homogeneous linear equations for the coefficients of the expansion $D_{j,m}{}^n$. In the limit of Zero magnetic field, the on

centre donor spectrum shows the well-known hydrogen like feature of confined impurity in quantum well. For increasing fields, the spectrum clearly exhibits the Zeeman splitting of the m=±1, ±2….excited states. In the high magnetic field regime (for Landau radii smaller than the effective Bohr radius) the energy spectrum resembles a set of Landau-like levels associated with each one of the quantum-well states in the absence of the impurity potential. The intra-donor absorption coefficient is calculated by using Fermi rule. Both circular and linear configurations are derived within the dipolar approximation in which the oscillator strength of the transition is

$$\left|(\psi_f{}^{m'}\left|\varepsilon.(p+\frac{|e|}{c}A_0)\right|\psi_i{}^{m})\right|^2 \tag{3}$$

Here, **ε** denotes the photon polarization vector. For linear photon radiation, the only allowed transitions are those between impurity states with the same angular momentum quantum numbers (m=m') and for quantum well states with n-n' being equal to an odd numbers.

For the case of in-plane circular photon polarization configuration, one obtains

$$\alpha(\omega)=\frac{\alpha_0}{\omega}\Sigma_{n,n',j,j'}\delta_{n,n'}\delta_{m'+1,m}D^{n}{}_{j,m}D_{j',m'}{}^{n'}C_{j,j'}{}^{m,m'}[\frac{M\lambda_j}{\lambda_j+\lambda_{j'}}-\frac{|m|\pm m'}{2}\pm\frac{\lambda_j\lambda_{j'}\pi M}{2l^2{}_B(\lambda_j+\lambda_{j'})}]$$

$$\delta(E_{j,j'}-\hbar\omega) \tag{4}$$

Where

$$C^{m,m'}{}_{j,j'}=\frac{(M-1)!2^{M+1}\lambda^{\frac{|m'|}{2}}{}_j\lambda_j^{\frac{|m|}{2}}}{\sqrt{|m|}!\sqrt{|m'|}!(\lambda_j+\lambda_{j'})^M} \tag{5}$$

Where l_B denotes Landau radius $\sqrt{\frac{\hbar c}{eB}}$. α_0 Is a constant. $M=\frac{(|m|+|m'|+1)}{2}$.$E_{j,j'}$ is the energy difference between the final and initial donor states and δ function is replaced by a Lorentzian function in the calculation of the absorption coefficients.

DISCUSSION OF RESULTS

In this paper, we have theoretically studied the shallow donor-impurity in triple quantum well structures under external magnetic fields. The theoretical estimation has been performed by the help of the work performed by A Large etal[17]. The results are shown from table T1 to T8. In **Table T1**, we have shown the energy spectrum as a function of magnetic field. The impurity energies are obtained by solving a set of coupled homogeneous linear equation for the coefficients of expansion $D^{n}_{j,m}$ .We have evaluated the energy of TQW1 structure(100mev) as a function of magnetic field for different values of z-component angular momentum m. We have taken the values of m=-2, -1, 0 and +1. Our theoretical results were compared with experimental data[18]. Our theoretically evaluated results are in good agreement with the experimental data[18]. For increasing magnetic field, the energy value exhibits the Zeeman splitting of the m=±1, ±2……..excited states. In the high magnetic field regime (Landau radii smaller than the effective

Bohr radius) the energy values resemble with Landau like levels associated with each one of the quantum-well states in the absence of impurity potential. In **Table T2,** we have shown the evaluated values of intra-donor magneto-absorption coefficient (arb.U) of the TQW1 (100mev) structure as a function of photon energy for linear polarization radiation for central-well impurity position. The intra-donor absorption coefficient is calculated by using the Fermi rule. Both circular and linear coefficients are determined with the dipolar approximations in which the oscillator strength of the transition is proportional to $\left|<\psi^{m'}{}_{f}\left|\varepsilon.(p+\frac{|e|}{c}A_0)\right|\psi_i^{m}>\right|^2$. Here ε denotes the photon polarization vector.

Table-1: An evaluated result of energy of TQW1 structure as a function of the magnetic field for different values of z-component angular momentum m. Results were compared with the experimental data[18].

Magnetic field (T)	Energy (cm^{-1})							
	m=-2		m=-1		m=0		m=+1	
	Theo	Expt	Theo	Expt	Theo	Expt	Theo	Expt
2	962	970	874	882	762	770	812	822
4	997	1002	917	924	773	782	824	829
6	1022	1025	968	972	789	795	836	844
8	1154	1160	1010	1016	799	810	888	893
10	1230	1236	1032	1040	810	823	922	934
12	1244	1250	1067	1072	823	840	939	953
14	1267	1270	1096	1107	834	845	956	965
16	1288	1290	1122	1130	855	860	972	987
18	1292	1302	1148	1154	868	875	989	996
19	1299	1308	1156	1163	872	887	998	1005
20	1310	1315	1173	1174	882	893	1010	1018

For linear photon radiation, the only transitions allowed are those between impurity states with the same angular momentum quantum number (m=m') and quantum well states with n-n' being equal to an odd integer. We have evaluated the absorption coefficients for different magnetic field starting from 22T to 0T. Our theoretically evaluated results in **Table T2** indicate that absorption coefficient increases attains a maximum value (peak value) and then decreases for all values of magnetic field. The peak is higher for 22T and lower for 0T. This indicates that the impurity donor energy depends upon the intensity of the magnetic field. In **Table T3**, we have shown the intra-donor transitions energies as a function of magnetic field for central well and lateral well impurity position for TQW1 (100mev) structure. The obtained results were compared with experimental data[19]. Our theoretical results are in good agreement with the experimental data.

Table-2: evaluated results of intra-donor magneto-absorption coefficients as a function of photon energy (cm^{-1}) at fixed magnetic field for TQW1 structure for linear polarization radiation for central-well impurity position.

Photon energy (cm^{-1})	← Absorption coefficient(arb.U) →						
	22T	20T	18T	16T	14T	2T	0T
100	18.72	16.52	15.40	14.88	12.59	6.66	4.52
150	19.61	17.48	16.68	15.45	13.68	7.86	5.68
200	26.32	24.37	23.59	22.50	21.54	10.54	6.59
250	21.30	22.48	21.45	21.87	20.86	0.89	5.86
300	20.54	21.59	20.89	21.37	20.48	9.55	5.29
350	19.86	20.62	20.35	20.89	20.12	9.22	4.86
400	19.50	20.19	20.07	20.48	19.87	8.72	4.53
450	18.89	19.59	19.86	20.13	19.53	8.49	4.22
500	18.35	19.17	19.43	19.79	19.19	8.17	4.07
550	18.07	18.87	19.12	19.27	18.88	7.97	3.98
600	17.97	18.33	18.88	19.04	18.69	7.76	3.67
700	17.62	18.05	18.40	18.87	18.37	7.43	3.42
800	17.48	17.85	18.12	18.43	18.14	7.16	3.28

Table-3: An evaluated results for intra-donor transition energies as a function of magnetic field for central-well and lateral-well impurity position for TQW1 (100mev) results were compared with experimental data[18]

Magnetic field (T)	← Transition energy (cm^{-1}) →			
	Central-well impurity position		Lateral-well impurity position	
	Theo.	Expt	Theo.	Expt.
2	60.6	58.2	48.5	50.9
4	82.5	80.6	55.6	61.8
6	140.2	137.3	84.5	89.5
8	155.6	151.9	110.8	115.2
10	168.8	160.6	127.2	130.8
12	178.2	172.6	138.5	142.6
14	198.6	190.8	150.6	155.9
15	222.5	220.3	168.7	172.6
16	246.8	241.7	172.8	180.4
17	252.5	250.4	187.5	192.3
18	267.8	262.7	200.6	210.4
20	288.9	282.2	210.5	215.3

In **Table T4**, we have repeated the calculation for TQW2 (50mev) structures and obtained results were compared with experimental data[19]. In both two structures, the intra-donor transitions associated with a lateral impurity are shifted to higher energy with respect to the central-well impurity results. In **Table T5**, we have shown the intra-donor absorption coefficients (arb. U) For different electric field and fixed magnetic field B=5T for TQW1 structure as a function of photon energy for lateral well position and central-well position. In this case the absorption coefficients for lateral well position are larger than central-well position. This also shows that the lateral impurity results exhibit a strong dependence on the electric field intensity for low values of photon energy in contrast with the central-well donor results. In **Table T6,** we have repeated the calculation of intra-donor transition energy as a function of electric field intensity (KV/cm) for TQW1 structure. Our theoretical results were compared with the experimental data[19] and are found very satisfactory. In **Table T7,** we have repeated our calculation for intra-donor magneto-absorption coefficients for TQW2 structure as a function of photon energy for both lateral-well position and central-well position for different values of electric field intensity and fixed magnetic field B=5T.

Table-4: An evaluated result for intra-donor transition energies as a function of magnetic field for central-well impurity position and lateral-well impurity position for TQW2 (50mev) structure. Results were compared with the experimental data[18].

Magnetic field (T)	← Transition energy (cm^{-1}) →			
	Central-well impurity Position		Lateral-well impurity position	
	Theo.	Expt.	Theo.	Expt.
2	10.2	9.8	20.6	22.8
4	25.6	22.6	52.8	55.3
5	39.2	42.2	69.2	72.6
6	56.8	57.9	88.8	90.8
8	112.6	115.6	120.9	124.3
10	132.9	135.9	140.2	142.2
12	150.6	155.4	162.4	170.6
14	167.5	168.3	188.9	190.8
15	175.4	178.6	200.4	205.5
16	182.3	184.2	205.8	209.8
17	188.9	190.4	210.7	212.6
18	200.8	202.6	232.4	240.3
20	210.6	212.8	250.6	255.4

Table-5: evaluated results of absorption coefficient (arb. U) of TQW1(100mev) structure as a function of photon energy (cm^{-1}) for lateral-well impurity position and central-well impurity position for fixed magnetic field B=5T and different electric field intensities

Photon energy (cm^{-1})	← Absorption coefficient)(arb.u) →							
	Lateral well impurity position				Central-well impurity position			
	35kv/cm	30kv/cm	20kv/cm	10kv/cm	35kv/cm	30kv/cm	20kv/cm	10kv/cm
40	7.47	6.98	5.87	4.89	6.21	5.33	4.86	4.0
50	7.85	7.29	6.29	5.56	7.38	6.31	5.27	4.6
60	8.32	7.86	7.46	6.42	8.47	7.86	6.84	5.7
70	9.16	8.12	8.88	7.82	9.32	8.43	7.35	6.2
80	14.59	10.57	11.29	10.58	10.46	9.26	8.52	7.8
90	12.32	12.29	10.58	9.29	11.29	10.48	9.76	8.9
100	10.87	11.07	9.86	8.78	10.45	9.22	8.48	7.5
110	9.48	10.58	8.42	8.32	9.39	8.27	7.26	6.8
120	8.40	9.27	8.10	7.72	8.12	7.86	6.86	6.5
130	7.89	8.36	7.38	7.43	7.76	6.95	6.42	6.1
140	7.56	7.43	6.86	6.46	6.39	6.29	6.50	5.8
150	7.42	6.70	5.49	5.30	6.12	6.05	5.86	5.5

Table-6: An evaluated results of transition energy (cm^{-1}) as a function of electric field intensity (kv/cm) for central-well and lateral well impurity position for TQW1 (100mev) structure Results were compared with the experimental data[19].

Electric field Intensity (kv/cm)	← Transition energy (cm^{-1}) →			
	Central-well position		Lateral –well position	
	Theo.	Expt.	Theo.	Expt.
5	95.8	99.2	75.3	78.6
10	92.3	95.6	74.6	77.2
15	87.5	90.3	73.3	76.5
20	84.4	89.5	72.5	75.8
22	82,6	85.6	70.0	74.3
24	79.8	80.9	71.2	74.0
25	77.5	79.5	72.8	75.2
30	76.4	78.2	73.4	76.4
32	72.2	76.5	74.5	76.8
34	70.8	74.3	75.2	77.3
35	69.6	72.2	76.7	77.6
40	65.8	70.5	77.5	78.0

Table-7: An evaluated results of absorption coefficient (abr.u) of TQW2(50mev) structure as a function of photon energy (cm^{-1}) for central well and lateral well impurity position for fixed magnetic field and different electric field intensities.

Photon Energy (cm^{-1})	← Absorption coefficient (arb. U) →					
	Central well position			Lateral well position		
	20kv/cm	18kv/cm	16kv/cm	20kv/cm	18kv/cm	16kv/cm
40	8.29	7.25	6.69	7.48	6.26	5.86
50	9.37	8.47	7.28	6.29	7.43	6.48
60	10.52	9.72	8.56	9.47	8.85	7.72
70	12.89	11.85	10.74	11.58	9.96	8,84
80	11.46	10.59	9.27	10.23	8.58	7.55
90	10.58	9.86	8.96	9.87	8.16	6.63
100	10.12	9.22	8.48	9.52	7.87	6.47
110	9.87	8.95	8.15	9.15	7.52	6.23
120	9.52	8.72	7.92	8.86	7.32	6.06
130	9.14	8.37	7.62	8.53	7.13	5.89
140	9.05	8.14	7.47	8.29	6.94	5.67
150	8.78	7.89	7.31	7.88	6.45	5.42

Table-8: An evaluated results of transition energy (cm^{-1}) as a function of electric field intensities (kv/cm) for central well and lateral well impurity position forTQW2 (50mev) structure Results were compared with the experimental data[19].

Electric field (kv/cm)	← Transition energy (cm^{-1}) →			
	Lateral well position		Central well position	
	Theo.	Expt.	Theo.	Expt.
2	92.6	94.8	76.2	78.6
4	94.7	90.2	75.6	77.5
5	95.6	93.5	74.5	76.2
6	93.4	90.7	73.2	76.8
7	90.0	89.5	72.9	74.9
8	86.3	88.4	70.5	73.5
9	84.6	87.6	69.4	70.6
10	82.2	85.2	68.8	69.6
11	80.7	84.5	67.7	68.4
12	79.6	82.3	66.6	67.2
14	78.2	80.2	65.2	66.5
15	77.3	76.3	64.6	63.9
16	75.8	74.3	63.8	63.2
18	74.4	70.5	63.2	62.8

In this case opposite results were obtained in contrast to TQW1. The absorption coefficients for central-well position are larger than lateral well position. In **Table T8,** we repeated the calculation of intra-donor transition energy as a function of electric field intensity for TQW2 structure. In this case, the transition energy for lateral well position is larger than central-well impurity position. On comparing our theoretical results are in god agreement with the experimental data[19]. There are some recent[20-30] results which also reveal the same findings.

CONCLUSION

From above theoretical analysis and evaluation, we came across the following conclusions.

- In this evaluation, other intra-donor transitions allowed by the quantum angular momentum selection rules of simple quantum well systems are not visible in the intra-donor magneto-absorption coefficients due to quite small values of the calculated oscillator strength.
- In this evaluation, impurity related optical absorption for TQW2 structure exhibit a different dependence on the electric field for low intensities. The results indicate the importance of the electronic confining regime which depends on the geometrical characterization of the multi-well systems, intensity of the applied fields and also the doping profile.
- We have used effective-mass approximation in the analysis of impurity related optical spectra. We have obtained the results for an isolated impurity but this can be extended for a low concentration of weakly interacting impurities.

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