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Research Article

# A Theoretical Estimation of Binding Energy of Hydrogenic Impurities in Quantum Well in the Presence of Titled Magnetic Field

Tajinder Kaur<sup>1</sup>, A. K. Sinha<sup>2</sup> and L. K. Mishra<sup>3</sup>

<sup>1</sup>c/o Dr Hari Sumiran Singh, Salimpure Ahara, Baulia, Gali no 3, Patna-800003, Bihar, India.

<sup>2</sup>Department of Physics, B. D. College, Patna, Bihar, India.

<sup>3</sup>Department of Physics, Magadh University, Bodh-Gaya-824234, Bihar, India.

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**Abstract:** Using the theoretical formalism of E. Kasapoglu et al (Solid State Communication, 2003), we have theoretically evaluated the variation of binding energy of the ground state for a donor at the centre of GaAs quantum well as a function of well width keeping title angle constant and also as a function of title angle keeping well width constant. We have taken four different magnetic fields in this evaluation. We observe that title angle is good tunable parameter providing a change on the impurity binding energy for small width. Our evaluated results are in good agreement with the experimental data and also with the other theoretical workers. This study will help to understand the experimental data of the donor impurities in GaAs quantum well under the applied external titled magnetic field.

**Keywords:** Semiconductor heterostructure, Quantum well, Quantum wires, Quantum dots, confinement effects, Shallow donor impurity, titled magnetic field, hydrogenic donor impurity, effective-mass approximation, confinement potential, coordinate transformation

## INTRODUCTION

With the advancement of technology and improved experimental facilities like molecular beam epitaxy (MBE) and organic chemical –vapor deposition (CVD), a large number of works have been performed to know the hydrogenic impurity states in low dimensional semiconductor heterostructure. These includes quantum wells<sup>1-4</sup>, quantum wires<sup>5-8</sup> and quantum dots<sup>9-12</sup>. In the studies of semiconductor multilayer quasi-two dimensional systems as well as single quantum wells of GaAs/GaAlAs crystal type, it has been observed that the carriers caught by impurity centers effect essentially on the electronic properties of these systems. Magnetic and electric field plays an effective role (or tool) in the studies of these properties. There are number of papers<sup>13-15</sup> on the theoretical studies of the impurity states in the quantum well when the external fields are applied. The use of the titled magnetic field gives confinement effects. If the magnetic field is tilted with respect to the interface the variables in Schrodinger equation cannot be separated. Then, one uses Variational<sup>16,17</sup> or perturbation<sup>18,19</sup> methods. Using a parabolic potential<sup>20</sup>, the eigen energies of the two-dimensional electrons in the presence of titled magnetic fields have been solved analytically. E. Kasapoglu et al<sup>21,22</sup> have solved Schrödinger equation for square well potential as confining potential and obtained analytical solution without making any approximation for two-dimensional semiconductor heterostructures under the titled magnetic field.

In this paper, taking the theoretical formalism of E. Kasapoglu et al<sup>23</sup>, we have presented a method of evaluation of ground state binding energy of a hydrogenic donor impurity at the center of a GaAs quantum well in the presence of magnetic field titled in the growth direction. We have used the variational approximation. To solve the Schrodinger equation, one applies an orthogonal transformation and then using tricky substitution in the potential the Hamiltonian is made separable in terms of the new coordinate. The general solutions give the results in the two limits when the magnetic field is either parallel or perpendicular to the layers. We have theoretically evaluated the variation of binding energy of the ground state for a donor at the center of quantum well GaAs. The variation has been performed in two ways; one as a function of well width  $L_0(A^0)$  keeping title angle  $\Theta$  constant and second as a function of title angle  $\Theta$  keeping well width  $L_0(A^0)$  constant. We have taken four different values of the magnetic field  $B=1T, 10T, 15T$  and  $20T$ . We observe that for  $\Theta=15^0$ , binding energy increases with well width for all the four values of the magnetic field. On the other hand for  $\Theta=30^0, 60^0$  and  $75^0$ , binding energy decreases with increase of well width and is smallest at  $\Theta=75^0$ . On the Other hand keeping  $L_0(A^0)$  constant and varying  $\Theta$  binding energy increases with  $\Theta$  and reaches maximum value at  $\Theta=45^0$  and in the range of  $45^0 < \Theta < 90^0$ , the binding energy decreases up to  $\Theta=75^0$  and for the further tilt angle it converges to a constant value. Our obtained theoretical results are in good agreement with the other theoretical workers<sup>24,25</sup>.

**Mathematical formulae used in the evaluation:** One defines the z-axis to be along the growth axis and the magnetic field is applied in the x-z plane. One chooses the gauge for the magnetic field such that vector potential  $\mathbf{A}$  is written as  $\mathbf{A}=(oxB\sin\Theta-zB\cos\Theta, 0)$  with the help of gauge  $\nabla \cdot \mathbf{A}=0$ . Here  $\mathbf{B}=(B\cos\Theta, 0, B\sin\Theta)$   $\Theta$  is the angle between the direction of the magnetic field and x-axis. Using the effective mass approximation, the Hamiltonian of the hydrogenic donor in a GaAs quantum well in the presence of applied magnetic field is written as

$$H = \frac{1}{2m_e^*} [\vec{p} + \frac{e}{c} \vec{A}]^2 - \frac{e^2}{\epsilon_0 |(\vec{r}_e - \vec{r}_i)|} + V(z_e) \quad (1)$$

Here  $m_e^*$  is the effective mass,  $e$  is the elementary charge,  $P$  is the momentum,  $\epsilon_0$  is the dielectric constant and  $V(z_e)$  is the confinement potential for the electron in the  $z$ -direction. The functional form of the confinement potential is given by

$$V(z_e) = V_0[S(z_L - z_e) + S(z_e - z_R)] \quad (2)$$

Where  $S$  is the step function and left and right hand boundaries of the well is located at  $z=z_L=-L_0/2$  and  $z=z_R=L_0/2$  respectively. Now one uses the following transformation

$$\begin{pmatrix} z' \\ x' \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} z \\ x \end{pmatrix} \quad (3)$$

The Hamiltonian can be written as

$$H = \frac{1}{2m_e^*} (p_x'^2 + p_z'^2) + \frac{1}{2m_e^*} p_y'^2 + \frac{e^2 B^2}{2m_e^* c} z'^2 + V(x'_e, z'_e) - \frac{e^2}{\epsilon_0 \sqrt{[(x'_e - x'_i)^2 + (y - y_i)^2 + (z'_e - z'_i)^2]}} \quad (4)$$

In equation (4), there is no term like  $(\frac{eB}{mc}) z' p_y'$  because the expectation value of this term vanishes for the chosen trial function given by

$$\phi(y, \alpha) = \frac{1}{\sqrt{\alpha}} \left( \frac{2}{\pi} \right)^{\frac{1}{4}} e^{-\frac{y^2}{\alpha^2}} \quad (5)$$

Where  $\alpha$  is a variational parameter. Now, one does coordinate transformation to the left and right boundaries of well on the  $x'$  and  $z'$  axis as

$$x'_{LR} = z_{LR} \cos\theta + x \cos\theta \quad 6(a)$$

$$z'_{LR} = z_{LR} \cos\theta - x \sin\theta \quad 6(b)$$

Now after coordinate transformation the potential energy of the electron in the well  $V(x'_e, z'_e)$  couples with  $x'$  and  $z'$  variables. In order to decompose the potential energy of the electron, one writes the step function of the equation (2) as follows:

$$S(z_L - z_e) = \cos^2 \theta S(z'_L - z'_e) + \sin^2 \theta S(x'_L - x'_e) \quad 7(a)$$

$$S(z_e - z_R) = \cos^2 \theta S(z'_e - z'_R) + \sin^2 \theta S(x'_e - x'_R) \quad 7(b)$$

In order to decompose the potential energy  $V(x'_e, z'_e)$ , one introduces the function

$$f(x', z') = \cos^2 \theta S(z'_L - z') + \sin^2 \theta S(x'_L - x') \quad 8(a)$$

By using the variable  $x'$  and  $z'$  in terms of  $x$  and  $z$ , one can write down the step function  $S(z_L' - z')$  as follows

$$S(z_L' - z') = S(z_L - z) \cos \theta \quad 8(b)$$

Since  $\cos \theta > 0$  then we have

$$S(z_L - z) \cos \theta = S(z_L - z) \quad 8(c)$$

Similarly we have

$$S(x_L' - x') = S(z_L - z) \quad 8(d)$$

Then equation 8(a) takes the form

$$f(x', z') = S(z_L - z) \quad 8(e)$$

With the help of above procedure, one can decompose the potential  $V(x_e', z_e')$

Where

$$V(x_e', z_e') = V(x_e') + V(z_e') \quad 9(a)$$

$$V(x_e') = V_0 \sin^2 \theta [S(x_L' - x_e') + S(x_e' - x_R')] \quad 9(b)$$

$$V(z_e') = V_0 \sin^2 \theta [S(z_L' - z_e') + S(z_e' - z_R')] \quad 9(c)$$

At  $\Theta=90^\circ$ , the applied field is parallel to the growth direction and the electron becomes free in the  $z'$  direction and the eigen value do not depend on  $z'$ . When  $\Theta=0^\circ$ , applied magnetic field is perpendicular to the growth direction and the electron becomes free in the  $x'$  direction and the eigen value do not depend on  $x'$ . For these values of  $\Theta$ , Schrodinger equation can be solved exactly and one does not need such

transformation to solve the problem. Now scaling all length in effective Bohr radius  $a_B = \frac{\epsilon_0 \hbar^2}{m_e^* e^2}$  energies

in effective Rydberg  $R_y = \frac{m_e^* e^4}{2\epsilon_0^2 \hbar^2}$ , one can write down the Hamiltonian of the system (4) in the dimensionless form

$$H = \frac{-d^2}{d\bar{x}'^2} + \tilde{V}(\bar{x}_e') - \frac{d^2}{d\bar{z}'^2} + \tilde{V}(\bar{z}_e') + \frac{e^2 B^2 \hbar^2 \bar{z}'^2}{4m_e^* c^2 R_y^2} - \frac{d^2}{d\bar{y}'^2} - \frac{2}{[\bar{x}_e'^2 + \bar{y}'^2 + \bar{z}_e'^2]^{\frac{1}{2}}} \quad (10)$$

Where  $\bar{x}_e'$ ,  $\bar{y}_e'$  and  $\bar{z}_e'$  is equal to zero as donor impurity is located on the centre of the wall. Now, one takes the variational trial wave function for the electron bound to impurity as

$$\psi = \psi(\bar{x}') \psi(\bar{z}') \phi(y, \alpha) \quad (11)$$

Where the wave function in the y- direction  $\phi(y, \alpha)$  is chosen to be Gaussian type orbital function given in equation (5),  $\psi(\vec{x})$  is the wave function of the electron in the x' directly which is exactly obtained from the Schrodinger equation in the x' direction.  $\Psi(z')$  is the wave function of the electron in the z' direction. To solve the Schrodinger equation in z' direction, one chooses as the base the eigen function of the infinite potential well with the  $L_0$  width. Then, one applies the techniques in calculating the wave function  $\psi(z')$  and ensured that the eigen function are independent of the choice of the infinite potential width  $L_0$ . The wave functions are localized in the well regions.

The total energy of the system is calculated by minimizing the expectation value of the Hamiltonian in equation (10) with respect to the variational parameter  $\alpha$

$$\bar{E} = \min_{\alpha} \langle \psi | H | \psi \rangle \quad (12)$$

The binding energy of the donor impurity ground state is given by

$$E_B = \bar{E}_0 - \bar{E} \quad (13)$$

Where  $\bar{E}_0$  is the lowest electron total sub band energy in the x' and z' direction respectively. Now, substituting the expectation value of the Hamiltonian in equation (12) one gets the ground state energy of the donor impurity. In the numerical evaluation, we take the following parameters

$$M_e^* = 0.0665m_0 \text{ (} m_0 \text{ is the free electron mass)}$$

$$\epsilon_0 = 12.58 \text{ (static dielectric constant.)}$$

The dielectric constant is assumed to be the same for GaAs and GaAlAs. In GaAs/Ga<sub>1-x</sub>Al<sub>x</sub>As heterostructure well Al concentration of x= 0.3. the boundary of the well is chosen as

$$\begin{aligned} x'_{L(R)} &= \pm \frac{L_0}{2} \sin \theta \\ z'_{L(R)} &= \pm \frac{L_0}{2} \cos \theta \end{aligned} \quad (14)$$

Then one does the coordinate transformation which satisfies the following equation

$$\begin{aligned} z'_R - z'_L &= L_0 \cos \theta \\ x'_R - x'_L &= L_0 \sin \theta \end{aligned} \quad (15)$$

## DISCUSSION OF RESULTS

In this paper, we have studied the variation of binding energy for a donor at the centre of GaAs quantum well as a function of well width  $L_0(A^0)$  and also as a function of title angle  $\Theta$  for four different magnetic field values. The evaluation has been performed by a theoretical formalism of E. Kaspoglu et al<sup>23</sup>. In Table T1, we have shown the variation of binding energy of the ground state for the donor at the centre

of GaAs quantum well as a function of well width  $L_0(\text{A}^0)$  for four magnetic field values with  $\Theta=15^\circ$ . Now from our theoretical results, it appears that impurity binding energy increases as well size increases independent of the magnetic field values ( $100 < L_0 < 300$ ).

**Table-T1:** An evaluated results of variation of binding energy of the ground state for a donor at the center of GaAs quantum well as a function of well width for  $\Theta=15^\circ$  at four different magnetic field values

Well width $L_0(\text{A}^0)$	Binding Energy $E_B(\text{RY}) (\square=15^\circ)$			
	B=1T	B=10T	B=15T	B=20T
100	1.526	1.542	1.568	1.576
150	1.625	1.643	1.673	1.692
200	1.738	1.758	1.789	1.805
250	1.756	1.795	1.829	1.853
300	1.829	1.832	1.846	1.872
350	1.702	1.867	1.882	1.899
400	1.607	1.889	1.906	1.925
450	1.538	1.902	1.932	1.946
500	1.427	1.925	1.979	1.995
550	1.365	1.938	2.102	2.132
600	1.314	1.947	2.126	2.158
650	1.276	1.959	2.148	2.247
700	1.228	1.967	2.227	2.306
750	1.186	1.978	2.256	2.418

This is because the geometrical confinement predominates at small  $L_0$ . For  $B=1\text{T}$  the binding energy increases as  $L_0$  increases and reaches a maximum value at  $L_0=300\text{A}^0$ . When the binding energy becomes maximum the system has quasi-two-dimensional character. After  $L_0=300\text{A}^0$ , the impurity binding energy decreases as  $L_0$  increases, since the confinement of the electron in  $z'$  direction decreases. This is because the influence of the Coulomb field of the impurity center on the electron weakens. As the magnetic field increases as  $10\text{T}$ ,  $15\text{T}$  and  $20\text{T}$  the binding energy reaches a constant value for large well width. When these results were compared with the results of the hydrogen atom level<sup>26</sup> it was found very satisfactory. In **Table T2**, we have repeated the calculation for title angle  $\Theta=30^\circ$  with same four magnetic field values. Here we observe that the impurity binding energy decreases as  $L_0$  increases for all four magnetic field values. In **Table T3**, we repeated the calculations for  $\Theta=45^\circ$  and we observe that the impurity binding energy decreases as well width increases. In this case the binding energy becomes maximum since the effective well width and potential heights of the electron in both  $x'$  and  $z'$  direction are equal. Electron is under the effect of the same geometrical confinement in both directions. If one compares the results of the binding energy for  $\Theta=45^\circ$  with  $\Theta=15^\circ$  one observes that the binding energy changes from 1.526(Ry) to 3.895(Ry) for  $L_0=100\text{A}^0$  and for almost all magnetic values. So, it appears that title angle is a good tunable parameter provided that a change on impurity binding energy is for small  $L_0$  values. In **Table T4 and T5**, we repeated the calculations for title angle  $\Theta=60^\circ$  and  $75^\circ$  with the same four magnetic values.

**Table-T2:** An evaluated results of variation of binding energy of the ground state for a donor at the center of GaAs quantum well as a function of well width for  $\Theta=30^0$  at four different magnetic field values

Well width $L_0(A^0)$	Binding Energy $E_B(RY)$ ( $\square=30^0$ )			
	B=1T	B=10T	B=15T	B=20T
100	3.526	3.598	3.621	3.642
150	3.468	3.546	3.524	3.565
200	3.439	3.515	3.386	3.414
250	3.246	3.367	3.224	3.325
300	2.865	2.886	3.105	3.209
350	2.753	2.775	2.958	3.086
400	2.629	2.659	2.864	2.899
450	2.543	2.564	2.765	2.700
500	2.367	2.398	2.687	2.653
550	2.315	2.332	2.597	2.605
600	2.247	2.309	2.534	2.558
650	2.168	2.275	2.458	2.507
700	2.095	2.124	2.365	2.386
750	1.896	1.865	2.295	2.305
800	1.628	1.735	2.106	2.226

**Table-T3:** An evaluated results of variation of binding energy of the ground state for a donor at the center of GaAs quantum well as a function of well width for  $\Theta=45^0$  at four different magnetic field values

Well width $L_0(A^0)$	Binding Energy $E_B(RY)$ ( $\square=45^0$ )			
	B=1T	B=10T	B=15T	B=20T
100	3.985	1.542	1.568	1.576
150	3.872	1.643	1.673	1.692
200	3.765	1.758	1.789	1.805
250	3.629	1.795	1.829	1.853
300	3.448	1.832	1.846	1.872
350	3.329	1.867	1.882	1.899
400	3.167	1.889	1.906	1.925
450	2.786	1.902	1.932	1.946
500	2.653	1.925	1.979	1.995
550	2.509	1.938	2.102	2.132
600	2.365	1.947	2.126	2.158
650	2.232	1.959	2.148	2.247
700	2.106	1.967	2.227	2.306
750	1.753	1.978	2.256	2.418
800	1.679	1.726	1.737	1.805

**Table-T4:** An evaluated results of variation of binding energy of the ground state for a donor at the center of GaAs quantum well as a function of well width for  $\Theta=60^0$  at four different magnetic field values

Well width $L_0(A^0)$	Binding Energy $E_B(RY)$ ( $\square=60^0$ )			
	B=1T	B=10T	B=15T	B=20T
100	3.627	3.638	3.656	3.673
150	3.548	3.567	3.572	3.584
200	3.439	3.455	3.478	3.486
250	3.346	3.367	3.393	3.422
300	3.102	3.133	3.232	3.259
350	2.896	2.925	2.946	2.962
400	2.735	2.746	2.758	2.774
450	2.678	2.697	2.716	2.735
500	2.526	2.566	2.577	2.596
550	2.367	2.384	2392	2.422
600	2.228	2.256	2.261	2.292
650	2.116	2.148	2.158	2.173
700	2.106	1.967	1.847	1.872
750	1.785	1.803	1.764	1.721
800	1.568	1.605	1.642	1.675

**Table-T5:** An evaluated results of variation of binding energy of the ground state for a donor at the center of GaAs quantum well as a function of well width for  $\Theta=75^0$  at four different magnetic field values

Well width $L_0(A^0)$	Binding Energy $E_B(RY)$ ( $\square=75^0$ )			
	B=1T	B=10T	B=15T	B=20T
100	3.372	3.422	3.458	3.468
150	3.328	3.395	3.400	3.422
200	3.205	3.216	3.239	3.254
250	3.107	3.112	3.144	3.173
300	2.986	2.997	3.006	3.086
350	2.825	2.833	2.897	2.922
400	2.708	2.722	2.742	2.764
450	2.615	2.626	2.637	2.652
500	2.527	2.532	2.556	2.573
550	2.438	2.446	2.478	2.497
600	2.296	2.304	2.339	2.356
650	2.196	2.124	2.147	2.168
700	1.867	1.896	1.906	1.922
750	1.586	1.626	1.647	1.662
800	1.386	1.425	1.458	1.506

In all these angles the binding energy decreases as  $L_0$  increases. In case of  $\Theta=75^0$ , we observe the smaller binding energy at  $L_0=100\text{A}^0$  in comparison to previous values for  $\Theta=15^0, 30^0, 45^0$  and  $60^0$ . In the title angle  $60^0$  and  $75^0$ , the well width in which the electron is confined in the z' direction become so small that the electron is delocalized in all  $L_0$  values. The interaction of the electron with the impurity centre is completely provided with the magnetic confinement. In **Table T6 and T7**, we repeated the calculation of variation of binding energy as a function of title angle  $\Theta$  for four different magnetic fields and keeping  $L_0=100\text{A}^0$  and  $200\text{A}^0$  fixed. In these calculations, we observe that in the range  $0<\Theta<45^0$ , impurity binding energy increases as the title angle increases and reaches a maximum value at  $\Theta=45^0$ . In the range of  $45^0 < \Theta < 90^0$  the binding energy decreases up to  $75^0$  and for further title angle, it converges to a constant value. It shows that in the range of  $0<\Theta<45^0$ , as the localization of the donor electron in the z' direction and Coulomb interaction increases the binding energy increases. On the other hand in the range of  $45^0 < \Theta < 90^0$  the well width becomes smaller in the z' direction and interaction decreases between donor electrons and ions and delocalization begins the binding energy decreases. This type of behavior is obtained in the ground state exciton binding energy in quantum well<sup>22</sup>. It also suggests that the direction of the magnetic field plays an essential role in the determination of the binding energy. It is seen that the direction of the magnetic field causes important change in the binding energy. For  $L_0=100\text{A}^0$ , the change in binding energy between  $\Theta=15^0$  and  $45^0$  is approximately equal to  $2.602\text{Ry}$ . It shows that quantum well structure is reduced to quantum wire from the results obtained at  $\Theta=45^0$ . In this case the system is under the effect of same geometrical confinement in both x' and z' directions. There is some recent calculations<sup>27-35</sup> which also reveals the similar behavior.

**Table-T6:** An evaluated results of variation of binding energy of the ground state for a donor at the center of GaAs quantum well as a function of title angle  $\Theta$  at four different magnetic field values and well width  $L_0=100\text{A}^0$

□(degree)	Binding Energy $E_B(\text{RY})$ ( $L_0=100\text{A}^0$ )			
	B=1T	B=10T	B=15T	B=20T
0	1.276	1.324	1.406	1.422
10	1.628	1.633	1.678	1.699
15	2.509	2.523	2.596	2.608
20	2.538	2.546	2.604	2.622
25	2.546	2.558	2.622	2.643
30	2.553	2.564	2.646	2.658
35	2.567	2.576	2.688	2.704
40	2.584	2.593	2.708	2.722
45	2.602	2.618	2.732	2.758
50	2.513	2.604	2.708	2.706
55	2.504	2.550	2.667	2.689
60	2.458	2.464	2.602	2.612
65	2.428	2.439	2.548	2.566
70	2.296	2.344	2.486	2.504
80	2.167	2.232	2.254	2.297

**Table-T7:** An evaluated results of variation of binding energy of the ground state for a donor at the center of GaAs quantum well as a function of title angle  $\Theta$  at four different magnetic field values and well width  $L_0=200\text{A}^0$

$\square$ (degree)	Binding Energy $E_B(\text{RY})$ ( $L_0=200\text{A}^0$ )			
	B=1T	B=10T	B=15T	B=20T
0	1.324	1.355	1.366	1.386
10	1.362	1.405	1.412	1.422
15	1.398	1.424	1.438	1.459
20	2.539	2.803	2.835	2.846
25	2.568	2.784	2.817	2.828
30	2.576	2.778	2.800	2.816
35	2.588	2.756	2.786	2.795
40	2.607	2.743	2.762	2.778
45	2.622	2.722	2.755	2.765
50	2.643	2.708	2.743	2.755
55	2.608	2.697	2.712	2.733
60	2.502	2.653	2.704	2.729
65	2.428	2.629	2.686	2.705
70	2.368	2.467	2.654	2.673
80	2.346	2.425	2.455	2.466

## CONCLUSION

In this study, solution of the Schrodinger equation for square well potential under the influence of externally applied titled magnetic field is obtained by using a variational approximation. The variation of the binding energy of ground state for a donor at the centre of GaAs quantum well were studied as a function of the well width keeping the title angle constant and also as a function of title angle keeping well width constant for four magnetic field values. It is seen that the direction of the magnetic field causes important change in the binding energy. These results will be of important use in the understanding of experimental results related to the donor impurities in GaAs quantum well under the external titled magnetic field.

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**Corresponding author: Tajinder Kaur;** c/o Dr Hari Sumiran Singh, Salimpure Ahara, Baulia, Gali no 3, Patna-800003, Bihar, India.