Binding energy of a hydrogenic donor and of a Wannier exciton in the $|z|^{2/3}$ quantum well

M. Arulmozhi and S. Balasubramanian*
Department of Theoretical Physics, School of Physics, Madurai Kamaraj University, Madurai-625 021, India
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We have calculated variationally the binding energy of a hydrogenic donor and a Wannier exciton in a quantum well with a potential shape proportional to $|z|^{2/3}$ as a function of well width and barrier height. The exciton binding energy compares favorably with the experimental result of Sputz and Gossard. A comparison of the results relating to a rectangular well and those of the $|z|^{2/3}$ well is also presented.

I. INTRODUCTION

Low-dimensional semiconductor systems have been of considerable interest both from the basic physics point of view and due to the many possible applications. With molecular-beam epitaxy, quantum wells with varied potential profiles have become possible. Quantum wells with rectangular potential wells formed by the GaAs/$Ga_{1-x}Al_xAs$ system have been extensively studied.[1,2] Quantum wells with potential shapes with a parabolic function have also been grown by several workers since these offer a three-dimensional electron gas to be realized for high-mobility devices in practice.[3-5] Sputz and Gossard have reported their studies on the photoluminescence and excitation spectra in a quantum well formed by GaAs/$Ga_{1-x}Al_xAs$ where the potential profile is given by a function proportional to $|z|^{2/3}$, where the growth axis is taken to be the Z axis.[6] Their experimental results on the electron and hole state energies are consistently smaller than their theoretical estimates. The average difference is attributed to the binding energy of an exciton. Their results also show nearly the same binding energy for both light-hole and heavy-hole excitons attached to the lowest quantized states.

Binding energies of hydrogenic donors in rectangular quantum wells have been measured experimentally and calculated theoretically by many authors.[7-9] Energy levels of Wannier excitons in such rectangular wells have also been reported in the literature.[10-12] Similar calculations have not so far been reported for the quantum well with potential profile proportional to $|z|^{2/3}$.

The purpose of the present paper is to report our results on the binding energies of a hydrogenic donor and a Wannier exciton in the $|z|^{2/3}$ quantum well formed by GaAs/$Ga_{1-x}Al_xAs$ with a view to estimating theoretically the exciton binding energy and also to predicting the variation of hydrogenic binding energy and exciton binding energy as a function of well width and barrier height. We also wish to compare the results with those corresponding to the rectangular well.

II. THEORY

The Hamiltonian for a hydrogenic donor and that for a Wannier exciton are given in the effective-mass approximation as

$$\mathcal{H}=-\left[\frac{1\partial}{\rho\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right]-\frac{\partial^2}{\partial z_e^2}+V(z_e)-2/r \quad (1)$$

and

$$\mathcal{H}=-\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right]-\frac{\mu_{hi}^*}{m_e^*}\frac{\partial^2}{\partial z_e^2}-\frac{\mu_{hi}^*}{m_{hi}^*}\frac{\partial^2}{\partial z_h^2}+V(z_e)+V(z_h)-2/r , \quad (2)$$

where $r=|\mathbf{r}_e-\mathbf{r}_h|$. We have used the effective Rydberg as the unit of energy: $R^*=m_e^*e^4/2\hbar^2\epsilon_0^2$ for the hydrogenic donor and $R_i^*=\mu_{hi}^*e^4/2\hbar^2\epsilon_0^2$ for the excitons. The unit of length is the effective Bohr radius $a^*=\hbar^2\epsilon_0/m_e^*e^2$ for the hydrogenic donor and $a_i^*=\hbar^2\epsilon_0/\mu_{hi}^*e^2$ for the excitons. The subscripts e and h stand for the electron and the hole respectively. ϵ_0 is the static dielectric constant of GaAs. μ_{hi}^* is the reduced effective mass of the conduction electron and the heavy hole ($i=h$) or the light hole ($i=l$). We have taken

$$\frac{1}{\mu_{hi}^*}=\frac{1}{m_e^*}+\frac{1}{m_{hi}^*} .$$

For GaAs, we have used $\epsilon_0=13.2$, $m_e^*=0.0665m_0$, $m_{hh}^*=0.340m_0$, and $m_{lh}^*=0.094m_0$, where m_0 is the free-electron mass. The potential profiles for the electron and the hole are taken to be of the form

$$V(z)=\begin{cases}V_0\left|\dfrac{z}{L/2}\right|^{2/3}, & |z|\le L/2\\ V_0, & |z|>L/2 ,\end{cases} \quad (3)$$

where V_0 is the barrier height, which depends on the Al composition x, and $z=z_e$ or z_h.

The trial wave functions used for the ground state of the hydrogenic donor (associated with the lowest quantized state) and the Wannier exciton (associated with the lowest electron and hole states) are, respectively, of the form

$$\psi=\begin{cases}Ne^{-\alpha^2z_e^2}e^{-ar}, & |z_e|<L/2\\ N_ie^{-\beta|z_e|}e^{-ar}, & |z_e|>L/2 ,\end{cases} \quad (4)$$

where α, β, and a are the variational parameters and $r=\sqrt{\rho^2+z_e^2}$,

$$\psi=\begin{cases}Ne^{-\alpha_e^2z_e^2}e^{-\alpha_h^2z_h^2}e^{-ar}, & |z_e|,|z_h|<L/2\\ N_1e^{-\beta_e|z_e|}e^{-\beta_h|z_h|}e^{-ar}, & |z_e|,|z_h|>L/2 ,\end{cases} \quad (5)$$

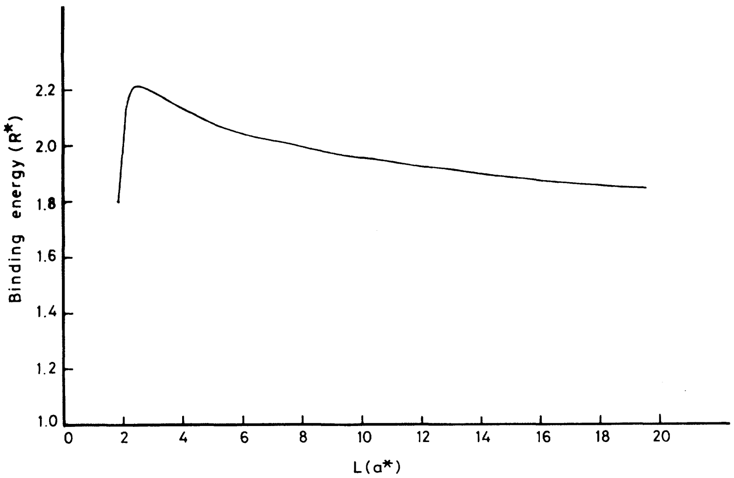

FIG. 1. Variation of the binding energy of a hydrogenic donor at the center of the $|z|^{2/3}$ quantum well as a function of well width L, having a barrier height $V_0=220.23$ meV.

where $r=\sqrt{\rho^2+|z_e-z_h|^2}$. α_e, α_h, β_e, β_h, and a are the variational parameters. N is the normalization constant. N_1 is related to N through the continuity of ψ at $|z|=L/2$ with $a=0$. Using the Hamiltonian in Eqs. (1) and (2) and the appropriate trial functions in (4) and (5), we have evaluated $\langle \mathcal{H} \rangle$ as a function of the variational parameters. The kinetic energy part has been analytically evaluated (expressions involve error functions) for both the donor and the exciton. The potential energy part involves numerical integration for the z variables (z_e for the donor and z_e and z_h for the exciton), while the ρ and ϕ parts have been analytically evaluated. The expressions are given in the Appendix, except for the exciton case where the expressions are too lengthy.

III. RESULTS AND DISCUSSION

We have performed the calculation for different values of L and V_0. In each case the minimization of $\langle \mathcal{H} \rangle$ with respect to the variational parameters is carried out using the International Mathematical and Statistical Libraries Inc. routine UMINF on the CYBER 180 computer. Figure 1 shows the binding energy of a hydrogenic donor as a function of L for a barrier height of $V_0=220.23$ meV which corresponds to the experimental sample used by Sputz and Gossard[6] with Al composition $x=0.27$. The binding energy is obtained as the difference between the ground quantized energy level for the electron in the bare quantum well (without the hydrogenic donor) obtained variationally and $\langle \mathcal{H} \rangle_{\min}$ with the hydrogenic donor present [Eq. (1)].

We have also solved the Schrödinger equation numerically for the quantum well without the impurity. But for consistency we have used the variational method throughout since the cases with an impurity and an exciton are conveniently handled variationally.

We display in Fig. 2 the binding energy vs $1/\sqrt{V_0}$. We see that the donor binding energy increases with decrease of L rather slowly up to a particular value of L $(=2.4a^*)$ and then starts decreasing rapidly. This behavior is qualitatively similar to the case of a hydrogenic donor in a rectangular quantum well. On closer examination, we see the following differences between a hydrogenic donor in the $|z|^{2/3}$ well and that in the rectangular well.

(1) The increase of binding energy with decrease of well width is much slower in the $|z|^{2/3}$ well.

(2) The L value at which the turnover occurs is much larger in the $|z|^{2/3}$ well.

(3) The limiting value of the binding energy as $L\rightarrow\infty$ turns out to be 1 Ry* as in the case of the rectangular well.

However, the way the value approaches 1 Ry* appears

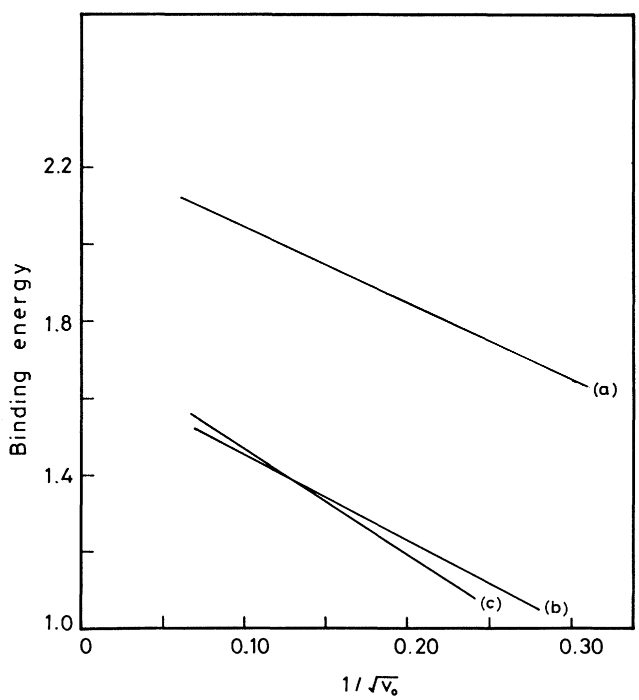

FIG. 2. Variation of the binding energy (in effective Rydbergs) as a function of $1/\sqrt{V_0}$ where V_0 is expressed in effective Rydbergs in the $|z|^{2/3}$ quantum well of width $L=1024$ Å: curve a for a hydrogenic donor at the center of the well, curve b for a heavy-hole exciton, and curve c for a light-hole exciton.

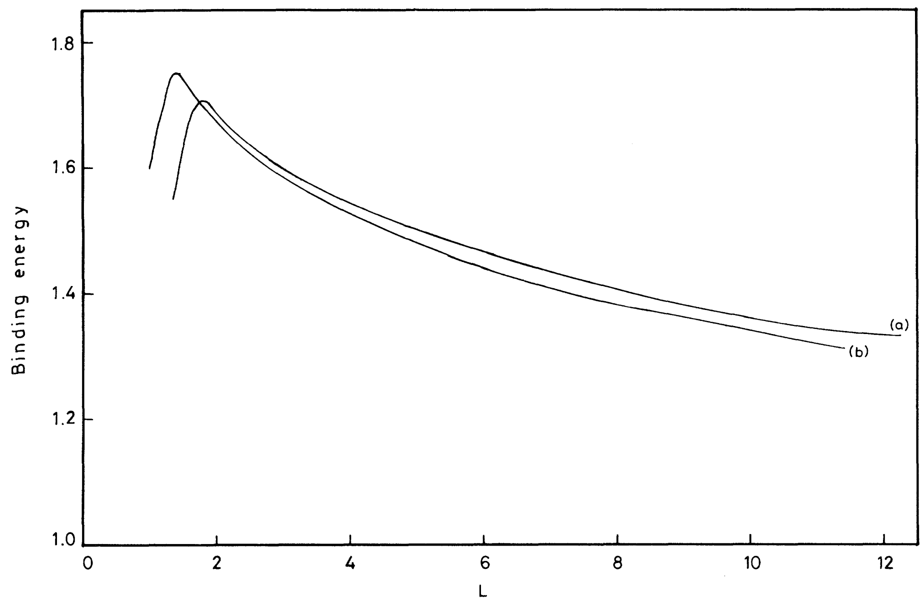

FIG. 3. Variation of the binding energy (in effective Rydbergs) as a function of well width L (in units of the effective Bohr radius) in the $|z|^{2/3}$ quantum well having a barrier height $V_0=220.23$ meV for electrons and $V_0=118.59$ meV for holes: curve b for a heavy-hole exciton and curve b for a light-hole exciton.

different in the two cases.

(4) The limiting value of the binding energy as $L \rightarrow 0$ turns out to be 1 Ry* as in the case of the rectangular well. Again, the way the limiting value approaches 1 Ry* is different in the two cases.

(5) The variation of binding energy with $1/\sqrt{V_0}$ is nearly linear in the case of both the rectangular well and the $|z|^{2/3}$ well.

Figure 3 shows the binding energy of the heavy-hole and the light-hole excitons as a function of the well width L, with barrier heights of 220.23 meV for electrons and 118.59 meV for holes. We have taken the ratio of the potential barrier for electrons and holes as 65:35. The variation is qualitatively similar to the binding energy of excitons in a rectangular quantum well. The L value at which there is a turnover in the binding-energy variation is larger for the light hole when compared to that for the heavy hole. This L is about 224 Å for the heavy holes and about 256 Å for the light holes, and both the values are larger than the respective values for the case of a rectangular well.

Figure 2 also shows the binding-energy variation with $1/\sqrt{V_0}$ for the heavy- and light-hole excitons. The variation is nearly linear especially for small V_0 values. For the experimental sample ($L=1024$ Å and $V_0=220.23$ meV for the electrons and 118.59 meV for the holes), the exciton binding energy is 6.1 meV for the heavy hole and 4.4 meV for the light hole. The estimates made by Sputz and Gossard[6] are 6.6 and 6.4 meV, respectively. As mentioned in the Introduction, their estimate of the binding energy of the light-hole exciton is quite large.

It should be mentioned that in our calculations we have not considered the conduction-band nonparabolicity for GaAs, or the effects due to the dielectric-constant mismatch and the effective-mass mismatch. These effects are expected to be small when we consider the binding energies of a hydrogenic donor and an exciton since these binding energies are obtained as results of differences in the eigenvalues of two Hamiltonians each having to have the above features.

In summary, we have presented the binding energies of a hydrogenic donor associated with the ground quantized level in a $|z|^{2/3}$ well for different well widths and barrier heights. Similarly, binding energies of light-hole and heavy-hole excitons associated with the ground quantized states are presented for different well widths and barrier heights.

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APPENDIX

1. Variational expression for a bare quantum well

The Hamiltonian is

$$\mathcal{H}=-\frac{d^2}{dz^2}+V(z)\ ,$$

where $V(z)$ is as given in Eq. (3). The trial function used is

$$\psi=\begin{cases} Ne^{-\alpha^2 z^2}, & |z|<L/2 \\ N_1 e^{-\beta|z|}, & |z|>L/2\ . \end{cases}$$

One gets (writing $X=\alpha L/\sqrt{2}$)

$$\langle \mathcal{H} \rangle = \frac{\left[\alpha \left[\frac{\pi}{2}\right]^{1/2} \phi(X) + \left[\beta - \alpha^2 L + \frac{V_0}{\beta}\right] e^{-X^2} + \frac{V_0 \gamma(\frac{5}{6}, X^2)}{2^{1/6} \alpha^{5/3} L^{2/3}}\right]}{\left[\frac{1}{\alpha}\left[\frac{\pi}{2}\right]^{1/2} \phi(X) + \frac{e^{-X^2}}{\beta}\right]} ,$$

where $\phi(x)$ is the error function $(2/\sqrt{\pi})\int_0^x e^{-t^2} dt$ and $\gamma(a,b)$ is the incomplete gamma function $\int_0^b t^{a-1} e^{-t} dt$.

2. Variational expressions for a hydrogenic donor at the center of a $|z|^{2/3}$ quantum well

For the Hamiltonian given in (1) with the trial function given in (4), we get the normalization integral as (writing $X = \alpha L/\sqrt{2}$)

$$4\pi \left\{ N^2 e^{a^2/2\alpha^2} \left[\frac{1}{8a\alpha^2}\left(e^{-a^2/2\alpha^2} - e^{-(X+a/\alpha\sqrt{2})^2}\right) + \left[\frac{\pi}{2}\right]^{1/2} \frac{1}{8a\alpha}\left[\frac{1}{a} - \frac{a}{\alpha^2}\right]\phi_1 \right] + \frac{N_i^2 e^{-(\beta+a)L}}{8a^2(\beta+a)^2}[(\beta+a)(aL+1)+a] \right\}$$

with $N_1 = Ne^{-X^2/2+\beta L/2}$ and

$$\phi_1 = \phi\left[X + \frac{a}{\alpha\sqrt{2}}\right] - \phi\left[\frac{a}{\alpha\sqrt{2}}\right] .$$

The kinetic energy expectation turns out to be

$$4\pi N^2 \left\{ e^{a^2/2\alpha^2} \left[\frac{1}{8a} e^{-a^2/2\alpha^2} - \frac{1}{8a^2}(aL+1)(\alpha^2 L + a) e^{-(X+a/\alpha\sqrt{2})^2} + \left[\frac{\pi}{2}\right]^{1/2} \left[\frac{\alpha}{8a^2} - \frac{1}{2a\alpha} + \frac{1}{8\alpha}\right]\phi_1 \right] \right\}$$
$$+ \frac{4\pi N_1^2 e^{-(\beta+a)L}}{4(\beta+a)^2} \left\{ [(\beta+a)L+1]\left[\frac{a}{2} + \frac{\beta^2}{2a} + \beta\right] + 2(\beta+a)\left[\frac{1}{4} + \frac{\beta^2}{4a^2} - \frac{1}{a}\right] \right\} .$$

The potential energy expectation comes out as

$$4\pi N^2 \frac{V_0}{4a^2}\left[\frac{2}{L}\right]^{2/3} \int_0^{L/2} z^{2/3}(2az+1) e^{-2\alpha^2 z^2 - 2az} dz + \frac{4\pi N_1^2 e^{-(\beta+a)L}}{4(\beta+a)^2} \left\{ [(\beta+a)L+1]\frac{V_0}{2a} + 2(\beta+a)\frac{V_0}{4a^2} \right\} .$$

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*Present address: Physics Department, Indian Institute of Science, Bangalore-560 012, India.

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