Binding energy of a confined hydrogenic impurity in a semiconductor quantum well

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We have variationally calculated the binding energy of a hydrogenic atom in an infinite semiconductor quantum well with and without an applied electric field along the growth axis. The hydrogenic ground states associated with even-parity excited quantized levels are considered. The binding-energy variation with well width is different for hydrogenic impurity ground state associated with different excited states of the well. The variation of electron energy with applied electric field is also different for different excited quantized levels. The electric-field-induced polarization is quite different for the excited quantized levels. Unlike exciton ground states, the hydrogenic ground states do not appear to be pinned when an electric field is applied.

I. INTRODUCTION

There have been several theoretical studies on shallow donors in a quantum well formed by a layer of GaAs between $Ga_{1-x}Al_xAs$ barriers.[1] Experimental results on the binding energy of donors in a quantum well based on far-infrared magnetospectroscopy have been reported by Jarosik *et al.*[2] Bastard *et al.*[3] have performed variational calculations on an infinite quantum well in an electric field and obtained the Stark shift and the electric-field-induced spatial shift of the single-particle wave function. Exact calculations on a finite-well case have been done by Ahn and Chuang.[4] Experimental results on the quantum-well energy states in an electric field using electroreflectance have been reported by Alibert *et al.*[5] and Klipstein *et al.*[6] Brum and Bastard[7] have reported their results on the electric-field-induced dissociation of excitons. They observed that the reduction in the binding energy of an exciton due to an applied electric field was due to the shifting of the quantized energy level of the well and not due to the shifting of the ground-state energy of the exciton. Brum, Priester, and Allen[8] have calculated the binding energy of shallow donors in a quantum well subject to an electric field. Ilaiwi and Tomak[9] in their work on polarizability of shallow donors in a quantum well have reported the electric-field-dependent donor binding energy of an on-center impurity in a wide quantum well. Experimental exciton binding energies have been reported by Koteles and Chi.[10] All the above studies relate to the hydrogenic state associated with the lowest quantized level of the well.

Matsuura and Kamizato,[11] in their work on the effects of electric fields on the subbands and excitons in a quantum well, find that the energy-level shift is different for different quantized levels when an electric field is applied. They find an upward shift of the excited quantized levels with increased electric field. For fields they consider the exciton ground state is nearly pinned and the change in the exciton binding energy is due to the shift in the well states. Zhu, Tang, and Xiang[12] also notice a similar behavior in the case of excited heavy-hole states in a semiconductor quantum well. On the other hand, the estimates reported in Ref. 6 show a monotonic lowering of the energy of the first excited state in a quantum well. Also, experimental estimates made from the work of Yamanaka *et al.*[13] as reported in Ref. 11 show only a downward shift of the quantized states with higher quantum numbers in an electric field. The photoluminescence measurements in $GaAs/Ga_{1-x}Al_xAs$ quantum wells associated with excited confinement subbands reported by Petrou *et al.*[14] have brought out the importance of higher-lying quantized states in a well. These studies, however, relate to the hole subbands. To our knowledge there has just been one previous report on the hydrogenic states associated with higher subbands in a semiconductor quantum well.[15]

We report in the present work our results on the binding energy of the ground state of a hydrogen atom associated with the quantized levels of the infinite-potential well. Calculations have been done for different well widths. The presence of an applied electric field is also considered and the results on the variation of the hydrogen ground-state energy with applied field, associated with several quantized levels of the well are reported. In Sec. II we outline the theory and in Sec. III the results and discussions are presented.

II. THEORETICAL CONSIDERATIONS

For simplicity we consider a hydrogenlike atom placed in an infinite quantum well of width l in the presence of an applied electric field which is uniform and is parallel to the growth axis (z axis). Choosing the unit of length as the effective Bohr radius a_B^* $(=K\hbar^2/m^*e^2)$ and the unit of energy as the effective atomic unit $(=m^*e^4/K^2\hbar^2)$ where e is the magnitude of the electronic charge, m^* is the electron effective mass in the well region, K is the static dielectric constant of the well region, the Hamiltonian for the electron in the effective-mass approximation is

$$H=-\tfrac{1}{2}\nabla^2-Z/r+V_w(z)+\phi z \ , \qquad (1)$$

where Z is the nuclear charge (=1 for hydrogen and 2 for He^+, etc.) and ϕ is a measure of the electric field E, given by $\phi = eEa_B^*/(\hbar^2/m^*a_B^{*2})$. $V_w(z)$ is the well potential taken to be

$$V_w(z) = \begin{cases} 0 & |z| < l/2 \\ \infty & |z| > l/2 \end{cases} . \quad (2)$$

The impurity atom is taken to be at the center of the well. We use a trial function of the form

$$\psi(\rho,\phi,z) = Nf_n(z)\exp(-ar)\exp(-bz) , \quad (3)$$

where $f_n(z)$ is the energy eigenfunction with quantum number n for an electron in the potential $V_w(z)$, N is the normalization constant, and a and b are variational parameters. With $b=0$ and when the applied electric field is zero, the trial function is suitable for obtaining the hydrogenlike ground-state energy in the quantum well. With $a=0$ and with the Coulomb field absent, the trial function is suitable for obtaining the effect of an applied electric field on the quantized energy states in the well. Though this part of the problem is exactly solvable through Airy functions, we prefer the variational procedure so as to be consistent throughout our work. We prefer this form of the trial function over a separable trial function used by Priester, Brum, and Allan.[8] The expectation value of the Hamiltonian H can be worked out analytically, and the expression so obtained is lengthy and hence is not presented here.

III. RESULTS AND DISCUSSION

As is customary, we have fixed the variational parameter b by minimizing numerically the expectation value of H with the Coulomb term absent. For convenience of comparison with results of Ref. 3, we have chosen for this part the electric field parameter as ϕ' ($=eEl/E_1^{(0)}$ where $E_1^{(0)}$ is the energy of the lowest quantized level in the infinite-potential well with zero applied electric field). Calculations are repeated for various values of ϕ' and odd integral values of n corresponding to even-parity states. In Fig. 1 we have given the reduced energy of an electron ($\langle H \rangle_{\min}/E_1^{(0)}$) in an infinite potential well as a function of ϕ'. The reduced energy monotonically decreases with increasing ϕ'. For $n=1$, our results agree with the results presented in Ref. 3. Our results show that the nature of the shift in the quantized level due to electric field is different for higher n values when compared to the ground state. This reflects that the polarization of the electrons associated with the higher quantized levels is different when compared to the polarization in the ground state. The monotonic variation for $n=3$ is different from that reported in Ref. 11. As was mentioned in the Introduction, earlier estimates based on experimental results give indications of monotonic variation.

We have also performed calculations for getting the minimum expectation value of H with the electric-field term absent and with $b=0$ in the trial function. The ground-state energy of the confined hydrogen atom associated with several even-parity quantized levels of the infinite-potential well are obtained for different well widths and the results are presented in Figs. 2 and 3. From the figures the following observations are made. The binding energy monotonically increases with decrease of well width and approaches the two-dimensional limit of 2 a.u. (4 effective rydbergs) at $l=0$. These are in agreement with earlier published results. The hydrogenic ground state associated with excited quantized levels of the well show a similar variation except the rate of decrease of energy with increase of well width is slower for higher n values as we approach large l values. The magnitude of the binding energy decreases with n for a given l. From Fig. 3, which shows the variation of a with l, it is seen that the a value decreases with increase of l initially rapidly and then vary slowly stabilizing around $1a_B^{*-1}$. For small l values the large a indicates the highly localized character of the wave function. For higher n values the binding energies are nearly the same within the scales chosen and thus in Fig. 2 the curves for $n=5$ and 7 are not resolved separately.

In order to see the effect of increasing the nuclear charge we have repeated the calculations with $Z=2$, which corresponds to a singly ionized He-like center.

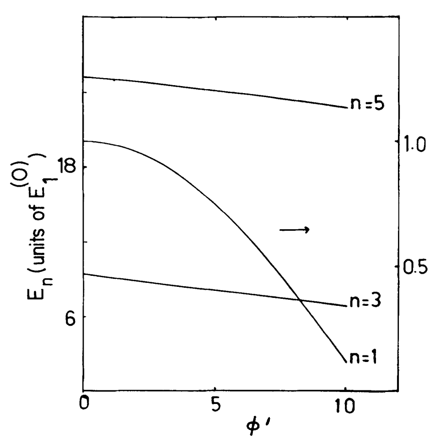

FIG. 1. Variation of energy of an electron in an infinite quantum well as a function of electric-field parameter ϕ'; the energy is in units of $E_1^{(0)}$, the energy of the lowest quantized level and $\phi'=eEl/E_1^{(0)}$, chosen as the electric-field parameter so as to compare results with Ref. 3.

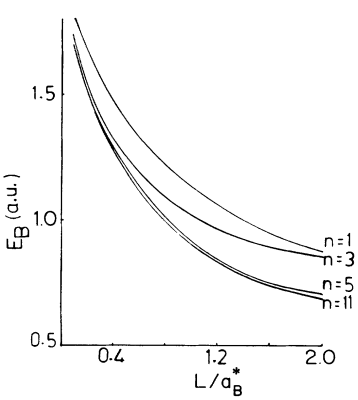

FIG. 2. Variation of binding energy (in effective atomic units) of a hydrogenlike ground state associated with different quantized levels of an infinite quantum well as a function of well width l (in units of an effective Bohr radius).

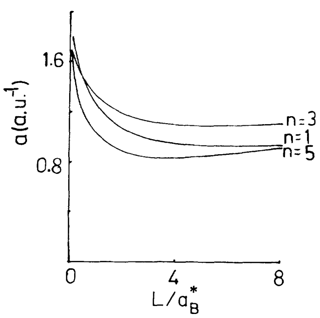

FIG. 3. Variation of the variational parameter a in units of $a_B^{*\,-1}$ and well width l in units of a_B^*.

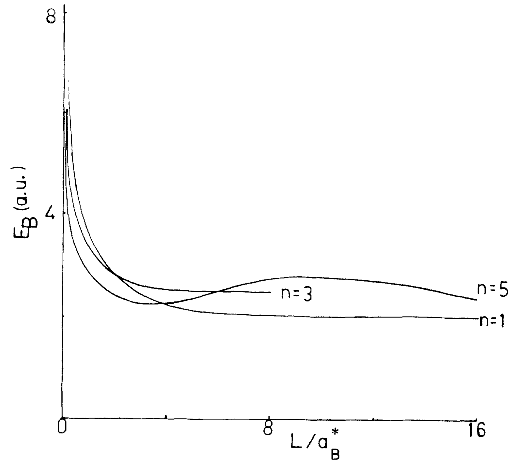

FIG. 4. Variation of binding energy (in effective atomic units) of a He^+-like ground state associated with different quantized levels of an infinite quantum well as a function of well width l (in units of a_B^*).

The binding energy variation with l is presented in Fig. 4. The monotonic decrease of binding energy with increase of l is seen in the range $0<l<2$ (with the two-dimensional limit of 8 a.u.). For $l>2$ the monotonic decrease is seen only for $n=1$ and 3; for higher n values there is a slight increase of binding energy with increase of l and then again a decrease. This seems to suggest that for these cases the competition between the Coulomb potential-energy term and the kinetic energy is more delicate.

Our calculations of binding energy of a confined hydrogenlike atom as a function of electric field for various values of n obtained by minimizing the expectation value of H with respect to a (with both Coulomb term and the electric-field term present) with b fixed with Coulomb term absent show the following results: For $n=1$ and for a well width of $1a_B^*$ the binding energy goes to zero for $\phi=5.5$, which corresponds to an electric field of about 67 kV/cm. For larger l values the binding energy goes to zero at much smaller value of ϕ. For higher n values the ϕ values at which the binding energy goes to zero are also higher. We also find that for higher n values the binding energy remains nearly constant for a range of ϕ values, thereby indicating that the electric field in this range does not alter the energy eigenstate. We have plotted the wave function with $\rho=0$ for $n=7$ as a function of z for the range of ϕ from 1 to 3. The wave function remained the same. This curious result for higher n values is interpreted as zero polarization in the sense that as the electric field increases the binding energy remains constant. We have also seen that the shift in the binding energy of a confined hydrogenlike atom in an electric field is much more than the shift in the quantized level due to the electric field. This shows that unlike the exciton ground state, the hydrogenlike ground state is not pinned.

In summary, we have calculated variationally the binding energy of the ground state of a hydrogenlike atom associated with several even-parity quantized levels of an infinite-potential well subjected to an applied electric field for various l values and for various electric field values. The behavior of the hydrogenic state associated with higher quantized levels appear somewhat different when compared to the state associated with the lowest quantized level.

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