Physica E 11 (2001) 186–189

PHYSICA E

www.elsevier.com/locate/physe

A method of measuring the contribution of the image potential energy of the shallow impurity ground state in a quantum well ☆

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Abstract

We show that the binding energy of the shallow impurity (at the center of the quantum well) ground state is strongly reduced by the presence of a metallic mirror at a few effective Bohr radii from the quantum well. For a given depth of the quantum well, we find that the absolute value of the image potential energy without the metallic mirror is equal to that with a fixed metallic mirror while a certain width of the quantum well is met. Hence, it is proposed that the binding energy of the shallow impurity ground state in the quantum well with and without the metallic mirror can be separately measured by the variation of the width of quantum well. The contribution of the image potential energy to the binding energy of the shallow impurity ground state may then be deduced.

PACS: 73.40.L

Keywords: Metallic mirror; Image potential energy; Shallow impurity; Quantum well

1. Introduction

The role of image charge effect on the binding energy of hydrogenic shallow impurity in a quantum well and the properties of exciton in quantum barrier has attracted much attention [1–4] in recent years. In a very recent work, Benoit á la Guillaume et al. [4] studied the quantum well exciton changes induced by the presence of a metal located at a distance from it. They find that the exciton binding energy is strongly reduced by the presence of a metallic mirror at a few exciton Bohr radii from the quantum well. Their idea enables rise to us to ask about the effect of the metallic mirror on the binding energy of hydrogenic shallow impurity in the quantum well. The result would be similiar to the case of exciton. But when we investigate the issue deeply, we find a new result which can be used to determine the contribution of binding energy due to image potential. This is what we want to present in this short paper.

☆ This work is partially supported by National Science Council of Republic of China.

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1386-9477/01/$ - see front matter
PII: S1386-9477(01)00200-4

In this paper, we calculate the binding energy of the ground state of hydrogenic impurity seated at the center of quantum well GaAs–$Ga_{1-x}Al_xAs$ with the inclusion of the effect due to the image charges (excluding the self-energy image potential). In Section 2, the calculational method is presented. In Section 3, results and discussion are presented. Finally, we give our conclusion.

2. Formalism

The energy level of the ground state for on-center shallow donor in GaAs–$Ga_{1-x}Al_xAs$ quantum well with and without a metallic mirror at a few effective Bohr radius from the quantum well is studied within the framework of the effective mass approximation. The variational method is used to calculate the ground state energy of on-center shallow impurity (image potential not included) in a single quantum well. Then, we treat image potential (excluded self-energy image potential) to be a perturbed potential and use the perturbation method to calculate the correction energy for both cases, without and with the metallic mirror on one side of the potential barrier.

The hydrogenic impurity is seated at the center of the quantum well with width L. The barrier height of the well is V_o. The Hamiltonian of this system is

$$H_1 = \frac{-\hbar^2}{2m_1^*}\nabla^2 + V_1(r), \quad |z| < \frac{L}{2},$$

$$H_2 = \frac{-\hbar^2}{2m_2^*}\nabla^2 + V_2(r) + V_0, \quad z < -\frac{L}{2},$$

$$H_3 = \frac{-\hbar^2}{2m_2^*}\nabla^2 + V_3(r) + V_0, \quad z > \frac{L}{2},$$

where m_1^*, m_2^* is the effective mass of, respectively, quantum well (say GaAs) and barrier (say $Ga_{1-x}Al_xAs$). The image charge potential arises from the difference of the dielectric constant between GaAs(ε_1) and $Ga_{1-x}Al_xAs(\varepsilon_2)$. $V_1(r)$, $V_2(r)$ and $V_3(r)$ represent the sum of the Coulomb interaction due to electron-impurity ion, electron-image ion. Let us define the dielectric mismatch between GaAs and $Ga_{1-x}Al_xAs$ as $p=(\varepsilon_1-\varepsilon_2)/(\varepsilon_1+\varepsilon_2)$ and $p'=2\varepsilon_1/(\varepsilon_1+\varepsilon_2)$. The position of the image of the impurity ion on the z-axis is

$$z_0^+(n) = 2\left\{\left(n - \left[\frac{n+1}{2}\right]\right)\left(\frac{L}{2}+z_i\right) + \left[\frac{n+1}{2}\right]\left(\frac{L}{2}-z_i\right)\right\} + z_i,$$

$$z_0^-(n) = -2\left\{\left[\frac{n+1}{2}\right]\left(\frac{L}{2}+z_i\right) + \left(n - \left[\frac{n+1}{2}\right]\right)\left(\frac{L}{2}-z_i\right)\right\} + z_i,$$

where z_i is the position of the hydrogenic impurity in the quantum well, $[x]$ is the integer part of x and n is the index of the nth image charge of the impurity ion. Let $\rho=\sqrt{x^2+y^2}$, $r=\sqrt{\rho^2+(z-z_i)^2}$. Then

$$V_1(r) = \frac{-e^2}{\varepsilon_1}\frac{1}{r} + V_1^+ + V_1^-,$$

where

$$V_1^+(r') = \frac{e^2}{\varepsilon_1}\sum_{n=1} p^n \left\{\rho_+^2[z - z_0^+(n)]^2\right\}^{-1/2}$$

and V_1^- is the same expression as V_1^+ except z_0^+ is replaced by $z_0^-(n)$; $V_2(r)=\varepsilon_1/\varepsilon_2\, p' V_1^+(r)$ and $V_3(r)=\varepsilon_1/\varepsilon_2\, p' V_1^-(r)$.

The contribution from the image potential to the ground state energy of the hydrogenic impurity is expected to be small because $p \ll 1$ if $x \le 0.4$ in $Ga_{1-x}Al_xAs$. Hence, the Hamiltonian can be rewritten as

$$H = H_0 + H',$$

where

$$H_0 = \frac{-\hbar^2}{2m}\nabla^2 - \frac{e^2}{\varepsilon_1[\rho^2+(z-z_i)^2]^{1/2}} + V(z)$$

and

$$V(z) = \begin{cases} 0 & \text{for } |z| < \dfrac{L}{2}, \\ V_0 & \text{for } |z| > \dfrac{L}{2}, \end{cases}$$

$$H' = \begin{cases} V_1^+(r) + V_1^-(r) & \text{for } |z| < \dfrac{L}{2}, \\ V_2(r) & \text{for } z < -\dfrac{L}{2}, \\ V_3(r) & \text{for } z > \dfrac{L}{2}. \end{cases}$$

Since the wave function of the electron is mostly confined in the quantum well, the electron's effective mass and dielectric constant in the quantum well may be used in the expression of H_0. The ground state wave function of H_0 cannot be obtained analytically. Here, we use the variational method to get the ground state energy of H_0. The tried wave function is

$$\psi_0 = f(z)\exp\left[-\frac{1}{\lambda}\sqrt{\rho^2+(z-z_i)^2}\right],$$

where $f(z)$ is equal to $A\cos(k_1 z)$ for $|z| < L/2$ and $B\mathrm{e}^{-k_2|z|}$ for $|z| > L/2$.

$f(z)$ is the ground state wave function in one-dimensional potential well without impurity and k_1 and k_2 are defined separately as $k_1 = \sqrt{2m^* E_0'}/\hbar$ and $k_2 = \sqrt{2m^*(V_0 - E_0')}/\hbar$.

E_0' is the ground state energy in this one-dimensional potential well and f and $\mathrm{d}f/\mathrm{d}z$ are forced to be continuous at the boundary $z = \pm L/2$. Then, two equations containing E_0' are obtained and E_0' is determined.

The ground state energy of the hydrogenic impurity at the center of the quantum well, excluding the image potential contribution, can be determined by the variation of $\langle\psi_0|H_0|\psi_0\rangle = E_0$ with respect to λ to have a minimum value E_0. Also, the binding energy of electron in the quantum well is equal to $U = E_0' - E_0$. Now the correction due to the image potential ΔE is determined by the perturbation method and the corrected binding energy is $U' = U - \Delta E$.

Next, let us consider a metallic mirror located away from the quantum well at a distance d. Between the metallic mirror and the quantum well, there is a quantum barrier (here it is $Ga_{1-x}Al_xAs$) (see Fig. 1). Now, the image potential will be changed due to the presence of the metallic mirror. Then, the correction of the binding energy due to this new image potential $\Delta E'$ would be different from ΔE. It is interesting to make a comparison between $\Delta E'$ and ΔE over the variation of the width of quantum well L (in effective Bohr radius a^*) for the impurity seated at the center of the well.

3. Results and discussion

The quantum well is GaAs. The effective Bohr radius $a^* = 103.4$ Å and the effective Rydberg $Ry^* = 5.29$ meV. In the case of no metallic mirror, the correction ΔE due to the image potential is negative because p is positive. ΔE becomes smaller while the width of the quantum well increases. The barrier height V_0 increases, the dielectric mismatch also becomes bigger, which will give rise to an increase in ΔE. Now, in the presence of the metallic mirror, the correction energy $\Delta E'$ is positive, because the metallic mirror will give rise to a stronger Coulomb interaction between the negative image charge and electron. But $\Delta E'$ will become smaller as V_0 increases for a given width of the quantum well. This is due to the electron wave function being more localized in the quantum well; the effect of the metallic mirror will be less. For a given V_0, $\Delta E'$ will become larger as the width of the quantum well decreases from 10a* until a certain width. Now, how about the effect on $\Delta E'$ while we change the position of the metallic mirror for a given V_0 and the width of the quantum well? We have carried out the calculation of $\Delta E'$ over the range of d from $5a^*$ to $800a^*$ for a given width $L = a^*$ and $V_0 = 10Ry^*$. $\Delta E'$ would approach the value of ΔE as $d \to \infty$. We find the value of $\Delta E'$ at $d = 800a^*$ to be quite consistent with ΔE as expected. Here, we specially attach Fig. 2 to show the results of the absolute value of the correction due to image potential with and without the metallic mirror for a given $V_0 = 50R_y^*$ over the range of $L = 0.9a^*$ to $1.3a^*$. We find that $|\Delta E| = |\Delta E'| = 1.57\times10^{-2}Ry^*$ at $L = 1.1665a^*$. The binding energy of the ground state of the donor shallow impurity (including image potential) is $U' = U - \Delta E$. Thus, $U'_{\mathrm{wm}} = U + |\Delta E|$ without

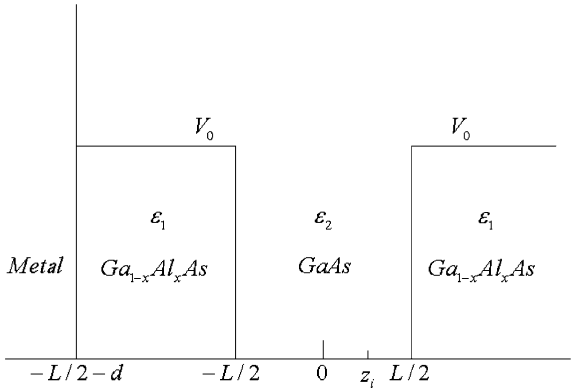

Fig. 1. Schematic diagram of metal $|Ga_{1-x}Al_xAs|GaAs|Ga_{1-x}Al_xAs$.

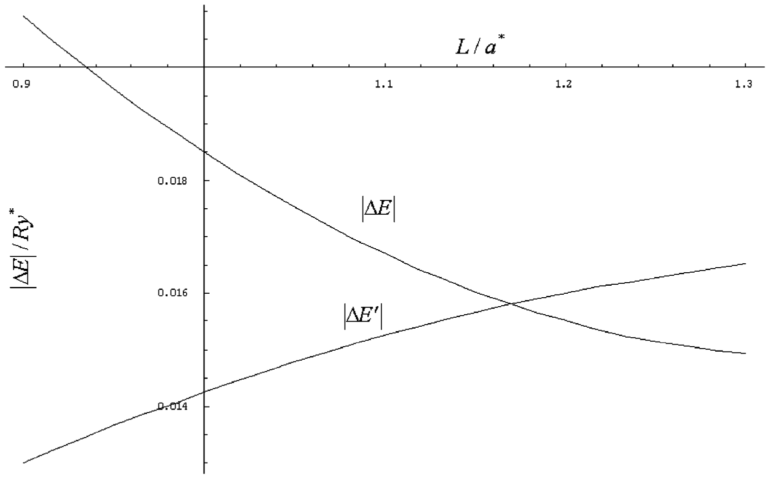

Fig. 2. The absolute value of the contribution of the image potential to the binding energy of the impurity at the center of the quantum well with ($|\Delta E|$) and without ($|\Delta E'|$) the metallic mirror varies with the width of quantum well for $V_0 = 50Ry^*$.

the metallic mirror. $U'_{\mathrm{m}} = U - |\Delta E|$ with the metallic mirror, therefore $U'_{\mathrm{wm}} - U'_{\mathrm{m}} = 2|\Delta E| \simeq 0.166\,\mathrm{meV}$.

Hence, the binding energy of the ground state of the impurity with and without the metallic mirror can be measured seperately. Then, the image potential contribution to the binding energy can be determined at a certain width of the quantum well.

4. Conclusion

We have demonstrated how to get the contribution of the image potential to the binding energy of the shallow impurity at the center of a quantum well. The method we propose here is a general one which may be applied to the case of the shallow impurity center not only at the center of the quantum well, but also the dielectric constant of the barriers on the sides of quantum well may be set to different values. The self-energy of the image potential can be easily incorporated into our future work. We do believe that our idea to obtain the contribution of the ground state binding energy due to image potential cannot be changed without self-energy of the image potential.

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