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Photoionization Cross Section of Hydrogenic Impurities in Spherical Quantum Dots: Infinite Well Model

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We have used a variational wave function for hydrogenic impurities in spherical quantum dots to calculate the dependence of the photoionization cross section of such impurities on the photon energy. The calculation has been performed using the infinite confining well model. The results are presented for various dot radii and for different locations of the impurity in the dot. We find that for hydrogenic impurities at the center of a spherical quantum dot, the transition takes place between the impurity level associated with the ground subband and the free particle state in the second subband, and the cross section is independent of the polarization of the photons. For off-center impurities, the transition takes place between the impurity level associated with the ground subband and the free particle state in the ground subband when the photons are polarized along the direction connecting the impurity with the center of the dot while for photons polarized perpendicular to the direction, we find that the transitions take place between the impurity level associated with the ground subband and the free particle state in the second subband.

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I. INTRODUCTION

With the development of advanced techniques of crystal growth in the recent past, it has become possible to grow semiconductor nanostructures in which the carriers are confined in their motion in one, two, and three dimensions such as quantum wells, quantum wires and quantum dots [1–3]. There has been a great deal of interest in the optical properties of these structures. Of particular interest have been the properties of hydrogenic impurities in such semiconducting nanostructures [4–19]. Calculations have been performed on the binding energy of hydrogenic impurities in such structures as quantum wells, wires and quantum dots, and it has been found that the greater the confinement in such structures, the greater the binding energy of these hydrogenic impurities. Therefore, it is expected that the physical properties, such as the optical characteristics of hydrogenic impurities, will be more pronounced in quantum dots and quantum wires. One property which has been of great interest, both theoretically and experimentally, is the photoionization cross section of these hydrogenic impurities. This cross section should depend strongly on the binding energy of the impurity and its wave function as well as the wave function of the free particle states to which the electron which is bound to the impurity is ionized. Lax [20] first investigated the photoionization cross section of hydrogenic impurities in bulk semiconductors. In recent years, work has been done on the photoionization cross section of hydrogenic impurities in structures of reduced dimensionality such as quantum wells and quantum wires. El-Said and Tomak [21, 22] have investigated the photon energy dependence of the photoionization cross section of hydrogenic impurities using the infinite barrier model. They found that the photoionization cross section depended upon the polarization of the incident light relative to the direction of carrier confinement. llaiwi and El-Said [23] extended these calculations using the finite barrier model. Sali *et al.* [24] took account of the interaction between the electron and the bulk polar optical phonons on the photoionization cross section in quantum wells using the infinite barrier model. More recently, Sali *et al.* [25] have investigated the photon energy dependence of the photoionization cross section in quantum wires. Here we wish to perform similar calculations for the photoionization cross section of hydrogenic impurities in quantum dots. In our calculations, we will treat the quantum dots as spherical for ease of the calculation and consider the infinite confining potential barrier models.

II. CALCULATION

The photoionization cross section of the impurity is given by

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$$\begin{aligned}\sigma = \quad & (\frac{4}{3}\pi^2\alpha)\hbar\omega(\frac{n}{\varepsilon})(\frac{\xi_{eff}}{\zeta_0}) \\ & \times\sum_f | < \varphi_f|\overrightarrow{r}|\varphi_i > |^2\delta(E_f - E_i - \hbar\omega),\end{aligned} \qquad (1)$$

Here, n is the index of refraction of the semiconductor, ε is the dielectric constant of the medium, α =e^2 /$\hbar$c is the fine structure constant, $\hbar\omega$ is the photon energy, ξ_{eff}/ζ_0 is the ratio of the effective electric field of the incoming photon and the average electric field in the medium, and $| < \varphi_f|\overrightarrow{r}|\varphi_i > |$ is the matrix element between the initial and final states of the dipole moment of the impurity. The position vector **r** in a spherical quantum dot system is given by $\mathbf{r} = r\{\cos(\theta)\cos(\phi)\widehat{x} + sin(\theta)\sin(\phi)\widehat{y} + \cos(\phi)\widehat{z}\}$. For quantum dots, the selection rules which determine the final state of the electron when it is ionized from the hydrogenic impurity depend upon the location of the impurity. For impurities located at the center of the dot, the selection rules determine that the final state of the system after the impurity is photoionized is the first excited state of the free particle in the dot. Therefore, the initial and final states of the electron which come into the matrix element $| < \varphi_f|\overrightarrow{r}|\varphi_i > |$are

$$\varphi_{100} = \frac{N}{\sqrt{4\pi}}j_0(k_{10}r)e^{-\beta r}, r < R, \qquad (2)$$

$$\varphi_{210} = \sqrt{\frac{3}{4\pi}}A_1 j_1(k_{11}r)\cos(\theta), r < R, \qquad (3)$$

$$\varphi_{21\mp1} = \pm\sqrt{\frac{3}{8\pi}}A_2 j_1(k_1 1r)\sin(\theta)e^{\pm i\phi}, r < R. \qquad (4)$$

Here, β is a variational parameter. k$_{10}$ and k$_{11}$ are given by $k_{10} = \sqrt{2mE_{10}/\hbar^2}$, and $k_{11} = \sqrt{2mE_{11}/\hbar^2}$. $j_0(x) = \frac{sin(x)}{x}$, and R is the radius of the spherical quantum dot. N is the normalization coefficient and is given by

$$N^{-2} = R^3\int_0^1 dtt^2 J_0^2(\pi t)e^{-2\beta rt}, \qquad (5)$$

A$_1$ and A$_2$ are normalization coefficients, and they are given by $A_1^{-2} = A_2^{-2} = R^3 j_0^2(k_{11}R)/2$. Using the wave functions given by Equations (3) and (4) for on-center impurity, we find that the square of the matrix element $| < \varphi_f|\overrightarrow{r}|\varphi_i > |$ is independent of the direction of polarization of the photon field and is given by

$$| < \varphi_{210}|z|\varphi_{100} > | = \sqrt{\frac{2}{3}}arH_1, \qquad (6)$$

where

$$H_1 = \frac{\int_0^1 dtt^3 j_0(\pi t)j_1(k_{11}Rt)e^{-\beta rt}}{\sqrt{\int_0^1 dtt^2 j_0^2(\pi t)e^{2\beta rt}}j_0(k_{11}R)}. \qquad (7)$$

Here, $\pi = k_{10}R$, and k$_{11}$R=4.49341 for the infinite well model. Using equation (6) in the equation for the photoionization cross section, we have

$$\sigma = (\frac{8\pi^2\alpha}{9})\hbar\omega(\frac{n}{\varepsilon})(\frac{\xi_{eff}}{\zeta_0})^2 a^2r^2H_1^2\delta(E_f - E_i - \hbar\omega).(8)$$

Here, a is the Bohr radius of the hydrogenic impurity. The initial and final state energies in the argument of the delta function are $E_i = \hbar^2k_{10}^2/2m - E_B$ and $E_f = \hbar^2k_{11}^2/2m$ respectively. E$_B$ is the hydrogenic impurity binding energy in a spherical quantum dot in the infinite well model. To obtain numerical values for the photoionization cross section given by equation (8), we arbitrarily take the ratio ξ_{eff}/ζ_0 =1 and replace the energy-conserving delta function by the Lorentzian.

$$\delta(E_f - E_i - \hbar\omega) \to \frac{\Gamma}{\pi\{(E_f - E_i - \hbar\omega)^2 + \Gamma^2\}}. \qquad (9)$$

Therefore, the photoionization cross section can be expressed as

$$\sigma = (\frac{8\pi\alpha}{9})\hbar\omega(\frac{n}{\varepsilon})a^2r^2H_1^2\frac{\Gamma}{\{(E_f - E_i - \hbar\omega)^2 + \Gamma^2\}}(10)$$

where Γ is the linewidth of the hydrogenic impurity, and in our calculation we use a value of Γ=0.1 meV. In Fig. 1, the photoionization cross section is shown as a function of the dot radius.

For off-center impurities, the photoionization cross section depends upon the polarization of the photon field relative to the direction of the location of the impurity relative to the center of the dot. If the photon field is polarized parallel to r$_0$, the selection rules allow a transition to the ground state subband of the electron in the spherical quantum dot. The initial state wave function of the off-center impurity is given by

$$\begin{aligned}\varphi_i \quad & = \varphi_{100}(r) \\ & = \frac{A_4}{\sqrt{4\pi}}j_0(k_{10}r)e^{-\beta\sqrt{r^2+r_0^2-2rr_0cos\theta}}, r < R.\end{aligned} \quad (11)$$

A$_4$ is the normalization coefficient and is given by

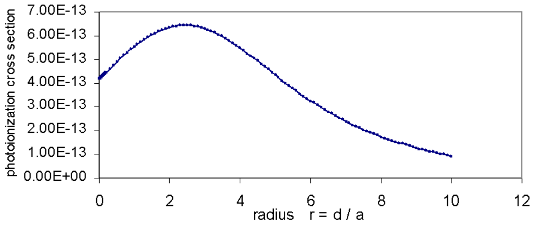

Fig. 1. The peak value of the photoionization cross section is shown as a function of dot radius for on-center impurities using the infinite well model. The unit of the photoionization cross section is cm^2.

$$A_4^{-2} = \frac{1}{2r_0}\int_0^R drrj_0^2(k_{10}r)\Big\{\frac{1}{\alpha}(|r-r_0|e^{-2\alpha|r-r_0|} - |r+r_0|e^{-2\alpha|r+r_0|}) + \frac{1}{4\alpha^2}(e^{-2\alpha|r-r_0|} - e^{-2\alpha|r+r_0|})\Big\}, \tag{12}$$

$$\varphi_f = \varphi_{100}(r) = \frac{A_5}{\sqrt{4\pi}}j_0(k_{10}r), r < R. \tag{13}$$

A_5 is the normalization coefficient and is the same as A_1. Using the matrix element $< \varphi_{100}|\overrightarrow{r}|\varphi_{100} >$ in the equation for the photoionization cross section, we have

$$\sigma = \frac{\pi}{3}\alpha\hbar\omega(\frac{n}{\varepsilon})\frac{a^2}{t_0^3 r^4}H_2^2\frac{\Gamma}{\{(E_f - E_i - \hbar\omega)^2 + \Gamma^2\}}, \tag{14}$$

$$H_2 = \frac{\int_0^1 dttj_0^2(\pi t)H_4}{\sqrt{\int_0^1 dttj_0^2(\pi t)H_3 j_1(k_{10}R)}}, \tag{15}$$

H_3 and H_4 are given by

$$H_3 = \frac{r}{2b}\Big(|t-t_0|e^{-2br|t-t_0|} - |t+t_0|e^{-2br|t+t_0|}\Big) + \frac{1}{4b^2}\Big(e^{-2br|t-t_0|} - e^{-2br|t+t_0|}\Big), \tag{16}$$

$$\begin{aligned} H_4 = \quad & r^2(t^2+t_0^2)\Big\{e^{-br|t-t_0|}(\frac{r|t-t_0|}{b} + \frac{1}{b^2}) - e^{-br|t+t_0|}(\frac{r|t+t_0|}{b} + \frac{1}{b^2})\Big\} \\ & + e^{-br|t+t_0|}\Big(\frac{r^3|t+t_0|^3}{b} + \frac{3r^2|t+t_0|^2}{b^2} + \frac{6r^2|t+t_0|^2}{b^2} + \frac{6}{b^4}\Big) \\ & - e^{-br|t-t_0|}\Big(\frac{r^3|t-t_0|^3}{b} + \frac{3r^2|t-t_0|^2}{b^2} + \frac{6r^2|t-t_0|^2}{b^2} + \frac{6}{b^4}\Big). \end{aligned} \tag{17}$$

Again, we use the value Γ=0.1 meV in our numerical calculations. In Fig. 2, the photoionization cross section is shown as a function of the dot radius. When the photon field is polarized perpendicular to $\overrightarrow{r_0}$ for off-center impurities, the selection rules only allow a transition to the first excited state subband of the electron in the spherical quantum dot, as in the case of on-center impurities. Thus, the initial state wave function of the off-center impurity is φ_{100} which is given by equation (11), and the final state wave function is $\varphi_{21\pm1}$which is given by equation (4).

Using the matrix element $< \varphi_{100}|\overrightarrow{r}|\varphi_{21\pm1} >$ in the equation for the photoionization cross section, we have

$$\sigma = \pi\alpha\hbar\omega(\frac{n}{\varepsilon})\frac{a^2}{t_0}H_5^2\frac{\Gamma}{\{(E_f - E_i - \hbar\omega)^2 + \Gamma^2\}}, \tag{18}$$

$$H_5 = \frac{\int_0^1 dtt^2 j_0(\pi t)j_1(k_{11}Rt)H_6}{\sqrt{\int_0^1 dttj_2(\pi t)H_3 j_1(k_{11}R)}}, \tag{19}$$

$$\begin{aligned} H_6 = \quad & \frac{1}{4t^2t_0^2}\{(t^2-t_0^2)^2(-\frac{e^{-2br|t-t_0|}}{b^2} + \frac{e^{-2br|t+t_0|}}{b^2}) + (t^2-t_0^2)^2(-\frac{r|t-t_0|e^{-2br|t-t_0|}}{b} + \frac{r|t+t_0|e^{-2br|t+t_0|}}{b}) \\ & + 2\frac{(t^2+t_0^2)}{r^2}(\frac{r^3|t+t_0|^3}{b} + \frac{3r^2|t+t_0|^2}{b^2} + \frac{6r^2|t+t_0|^2}{b^3} + \frac{6}{b^4})e^{-br|t+t_0|} \\ & - 2\frac{(t^2+t_0^2)}{r^2}(\frac{r^3|t-t_0|^3}{b} + \frac{3r^2|t-t_0|^2}{b^2} + \frac{6r^2|t-t_0|^2}{b^3} + \frac{6}{b^4})e^{-br|t-t_0|} \\ & + \frac{1}{r^4}(\frac{r^5|t+t_0|^5}{b} + \frac{5r^4|t+t_0|^4}{b^2} + \frac{20r^3|t+t_0|^3}{b^3} + \frac{60|t+t_0|^2}{b^4} + \frac{120r|t+t_0|}{b^5} + \frac{120}{b^6})e^{-br|t+t_0|} \\ & - \frac{1}{r^4}(\frac{r^5|t-t_0|^5}{b} + \frac{5r^4|t-t_0|^4}{b^2} + \frac{20r^3|t-t_0|^3}{b^3} + \frac{60|t-t_0|^2}{b^4} + \frac{120r|t-t_0|}{b^5} + \frac{120}{b^6})e^{-br|t-t_0|}\}, \end{aligned} \tag{20}$$

Again, we use the value Γ=0.1 meV in our numerical calculations. In Fig. 3, the photoionization cross section is shown as a function of the dot radius.

III. RESULTS AND DISCUSSION

In Fig 1, the value of the photoionization cross section is shown as a function of the dot radius for on-center impurities. Here, the photoionization cross section is independent of the polarization of the photon. From the figure, we see that the peak value initially increases with increasing dot size, reaches a maximum value and then decreases with a further increase in dot size. Since both the subband energies and the impurity binding energy increase with decreasing dot radius, the frequency at which the photoionization cross section peaks increases with decreasing dot size.

In Fig 2, we show the peak value of the photoionization cross section as a function of the dot radius for off center impurities when the photon field is polarized along the direction connecting the position of the impurity with the center of the dot. This peak value of the cross section is shown for three values of the location of the impurity. Since for this polarization, the final state is the free electron state associated with the first subband in the dot, $\hbar\omega$=E$_b$. Therefore, the peak value of the cross section occurs at lower photon frequencies for this polarization. In this case, the peak value of the cross section increases with increasing dot radius with the increase being larger, the closer the location of the impurity is to the center of the dot, because the threshold energy for the photoionization cross section is lower for off-center impurities when the photons are polarized along the direction connecting the impurity with the center of the dot than it is for on-center impurities or for off-center impurities for photons polarized perpendicular to this direction.

In Fig 3, we show the peak value of the photoionization cross section as a function of the dot radius for off-center impurities when the photon field is polarized perpendicular to the direction connecting the position of the impurity with the center of the dot for three locations of the impurity in the dot. Here we see that when the impurity is located in the dot, the behavior with increasing dot radius is the same as for on-center impurities. However, the peak value is smaller and occurs at a smaller dot radius, the closer the impurity is to the center of the dot.

IV. SUMMARY

We have calculated the photoionization cross section of the hydrogenic impurities in spherical quantum dots as a function of the dot radii using a variational wave function for hydrogenic impurities in spherical quantum dots, using the infinite confining potential well model. For on-center impurities, the transitions take place between the impurity level associated with the ground subband and the free particle state in the second subband and the cross section is independent of the polarization of the photons. For off-center impurities, the transitions take place between the impurity level associated with the ground subband and the free particle state in the ground subband when the photons are polarized along the direction connecting the impurity with the center of the dot, while for photons polarized perpendicular to this direction, we find that the transitions take place between the impurity level associated with the ground subband and the free particle state in the second subband. Therefore, the threshold energy for the photoionization cross section is lower for off-center impurities when the photons are polarized along the direction connecting the impurity with the center of the dot than it is for on-center impurities or for off-center impurities for photons polarized perpendicular to this direction.

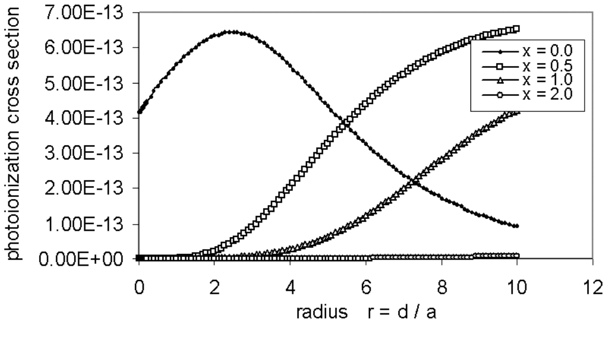

Fig. 2. The peak value of the photoionization cross section is shown as a function of dot radius for off-center impurities when the electromagnetic field is polarized parallel to r$_0$ for three locations of the impurity in the dot using the infinite well model. The unit of the photoionization cross section is cm^2.

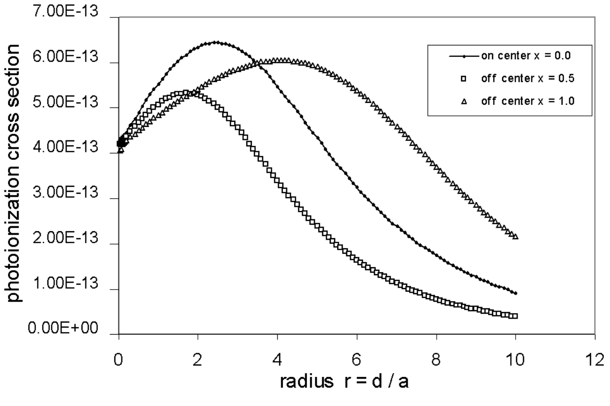

Fig. 3. The peak value of the photoionization cross section is shown as a function of dot radius for off-center impurities when the electromagnetic field is polarized perpendicular to r$_0$ for three locations of the impurity in the dot using the infinite well model. The unit of the photoionization cross section is cm^2.

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