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EFFECTS OF ELECTRIC FIELD AND IMAGE CHARGES ON THE IMPURITY-RELATED OPTICAL ABSORPTION COEFFICIENTS IN A SPHERICAL QUANTUM DOT

A. L. VARTANIAN *, A. L. ASATRYAN, A. A. MKHITARYAN, S. S. AVETISYAN, A. A. KIRAKOSYAN

Chair of Solid State Physics YSU, Armenia

The influence of an image charge effect on the impurity-related energies, the oscillator strengths of transitions from the $1s$-like state to $2p_x$ and $2p_z$ states as well as the optical absorption coefficients in a spherical quantum dot in the presence of an external electric field have been studied. The results show that the image charges lead to significant changes in the optical coefficients of the system.

Keywords: quantum dot, hydrogen-like impurity, image charge effect, absorption coefficient.

Introduction. Electronic and optical properties related to impurities in semiconductor nanostructures can be changed effectively by engineering the size and the shape of the system, the position of the impurity in the structure and the strength and direction of applied fields [1]. In order to modulate the properties of devices, effect of applied electric field on the impurity states in semiconductor nanostructures has been studied extensively in the past few years (see [2] and references therein). The dielectric mismatch often turns into a key factor in the understanding of the physical properties of various nanostructures [3,4]. In the article a study of the Image Charge Effect (ICE) on the impurity-related optical properties in a spherical quantum dot in the presence of an electric field is presented.

Theory. The Hamiltonian of the system can be written as

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega_0^2 r^2 + |e|Fr\cos\theta + V_c(r), \tag{1}$$

where m is the electron effective band mass, ω_0 is the parabolic confinement strength and can be chosen as $\omega_0 = \hbar/2mR^2$, R is the nominal value of the dot radius, F is the intensity of the electric field, θ is the angle between $\mathbf{r}$ and $\mathbf{F}$, $V_c(r)$ is the electrostatic energy for the electron inside the quantum dot interacting with impurity and image charges arising in the QD due to the difference in dielectric constants inside and outside the dot [3,4]:

$$\begin{gathered} V_c(r) = \frac{e^2}{\varepsilon_\infty|\mathbf{r}-\mathbf{r}_i|} + \sum_{l=0}^{\infty}\left(\frac{1}{\varepsilon_d} - \frac{1}{\varepsilon_\infty}\right)\frac{\varepsilon_d(l+1)}{\varepsilon_\infty l + \varepsilon_d(l+1)}\left(\frac{r}{R}\right)^{2l}\frac{e^2}{2R} - \\ -\sum_{l=0}^{\infty}\left(\frac{1}{\varepsilon_d} - \frac{1}{\varepsilon_\infty}\right)\frac{\varepsilon_d(l+1)}{\varepsilon_\infty l + \varepsilon_d(l+1)}\cdot\frac{e^2}{R}\cdot\left(\frac{rr_i}{R^2}\right)^{l}P_l(\cos\vartheta), \end{gathered} \tag{2}$$

where ε_∞ is the high-frequency dielectric constant, ε_d is the dielectric constant of the embedding medium, $\mathbf{r}_i = (r_i, \theta_i, \varphi_i)$ is the radius-vector of the impurity, $P_l(x)$ is a Legendre

* E-mail: vardan@ysu.am

polynomial, ϑ is the angle between $\mathbf{r}$ and $\mathbf{r}_i$. The first term in Eq. (2) is conditioned by the electron interaction with the impurity, the second and the third terms constitute the image charge potential energies.

The wave function $\phi_0(r,\theta)$ and the energy E_0 of the ground state in the absence of the impurity are given in [2]:

$$\phi_0(r,\theta) = \left(\frac{m\omega_0}{\pi\hbar}\right)^{3/4} \exp\left\{-\frac{m\omega_0}{2\hbar}\left[r^2 + 2\frac{eFr}{m\omega_0^2}\cos\theta + \left(\frac{eF}{m\omega_0^2}\right)^2\right]\right\}, \tag{3}$$

$$E_0 = \frac{3}{2}\hbar\omega_0 - \frac{e^2F^2}{2m\omega_0^2}.$$

The variational envelope wave functions $\psi_{nlm}(r,\theta,\varphi)$ associated with the different impurity ground and excited states in the QD can be labeled for convenience by their bulk hydrogenic limits, namely, $1s, 2s, 2p_x$, etc., and taken as the product of the electron ground state wave function ϕ_0 in the dot without impurity, and the hydrogen-like wave functions Γ_{nlm} that correspond to different impurity ground and excited (nlm) states, i.e.

$$\psi_{nlm}(r,\theta,\varphi) = N_{nlm}\phi_0(r,\theta)\Gamma_{nlm}\left(r,\theta,\varphi\{\lambda_{nl}\}\right), \tag{4}$$

where N_{nlm} are the normalization constants and

$$\Gamma_{1s} = \exp(-\lambda_{1s}r),\ \Gamma_{2p_x} = r\sin\theta\cos\varphi\exp(-\lambda_{2p_x}r),\ \Gamma_{2p_z} = r\cos\theta\exp(-\lambda_{2p_z}r). \tag{5}$$

The variational parameters λ_{nl} are determined after minimization of the energy E_{imp}^{ep}.

The linear and the third-order optical absorption coefficients can be derived by using the compact-density-matrix approach and iterative procedure. Within a two-level system approach they are given as [5]:

$$\alpha^{(1)}(\Omega) = \frac{4\pi e^2\sigma_s\Omega}{n_r c}\cdot\frac{|M_{21}|^2\hbar\eta}{(E_{21}-\hbar\Omega)^2 + (\hbar\eta)^2}, \tag{6}$$

$$\alpha^{(3)}(\Omega,I) = -\frac{32\pi^2e^4\sigma_s\Omega I}{(n_r c)^2}\cdot\frac{|M_{21}|^4\hbar\eta}{[(E_{21}-\hbar\Omega)^2+(\hbar\eta)^2]^2}\times$$
$$\times\left\{1 - \frac{|M_{22}-M_{11}|^2}{4|M_{21}|^2}\cdot\frac{\left[(E_{21}-\hbar\Omega)^2-(\hbar\eta)^2\right)+2E_{21}(E_{21}-\hbar\Omega)\right]}{E_{21}^2+(\hbar\eta)^2}\right\}, \tag{7}$$

where σ_s is the electron density in the quantum dot, $E_{21} = E_2 - E_1$, $E_1(E_2)$ is the initial (final) state energy, M_{ij} is the matrix element of the dipole operator, n_r is the refractive index, c is the speed of light in vacuum, Ω is the photon frequency, I is the incident optical intensity, η is the relaxation rate for states 1 and 2.

Results and Discussion. We have calculated the impurity ground and excited states energies, the oscillator strength, and the optical absorption coefficients of the $1s \to 2p_x$ and $1s \to 2p_z$ transitions. The parameters used in calculations are: $\varepsilon_\infty = 10.89$, $\varepsilon_0 = 13.18$, $\varepsilon_d = 2.25$, $m = 0.067m_0$, $\sigma_s = 5\cdot 10^{16}\ cm^{-3}$, $n_r = 3.2$, $I = 3\cdot 10^3\ W/cm^2$, $\eta = 10^{12}\ s^{-1}$.

Image charge effect leads to the red shift of the ground $(1s)$ as well as excited $(2p_x$ and $2p_z)$ impurity states (Fig. 1). As we can see, the impurity ground-state energy without ICE are not changed, meanwhile it increases when ICE is taken into account. The changes in the energies of the excited $2p_x$ and $2p_z$ impurity states with ICE are smaller compared to those without ICE. The oscillator strength as an important physical characteristic of the optical properties is related to the electric dipole-allowed transitions. Fig. 2 shows the numerical results obtained for oscillator strength as a function of the electric field strength. These plots exhibit the following general features: (i) the oscillator strength of transition $1s \to p_z$ with and without ICE dominates over the one of transition $1s \to 2p_x$; (ii) ICE leads to the significant enhancement of the oscillator strengths of transitions between the impurity states (about 50% for transition $1s \to 2p_z$ and 40% for transition $1s \to 2p_x$ at $F = 3\ kV/cm$ and at $\hbar\omega_0 = 5.65\ meV$); (iii) the oscillator strength of transition $1s \to 2p_z$ increases with electric field strength both with and without ICE. Meanwhile, one can see that with and without ICE the oscillator strength of transition $1s \to 2p_x$ slowly decreases with electric field. The linear, nonlinear and total absorption coefficients for transitions $1s \to 2p_x$ and $1s \to 2p_z$ with and without image charge effect are shown as a function of the photon energy at $F = 3\ kV/cm$ and at $\hbar\omega_0 = 5.65\ meV$ in Fig. 3.

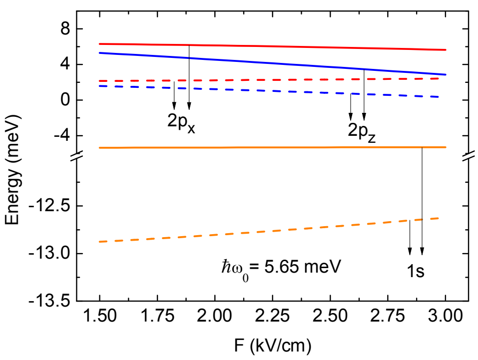

Fig. 1. Hydrogen-like impurity energies of the $1s$-, $2p_x$- and $2p_z$-like states as a function of the strength of the electric field with (dashed lines) and without (solid lines) ICE.

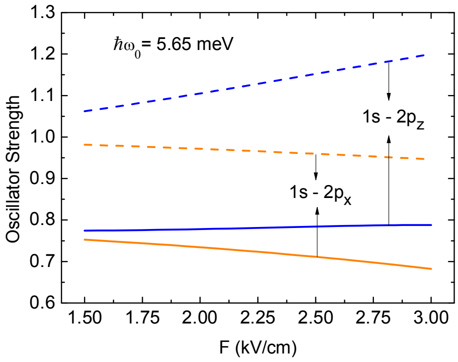

Fig. 2. The oscillator strengths of the $1s{\to}p_x$ and $s{\to}p_z$ transitions as a function of the strength of the electric field with (dashed lines) and without (solid lines) ICE.

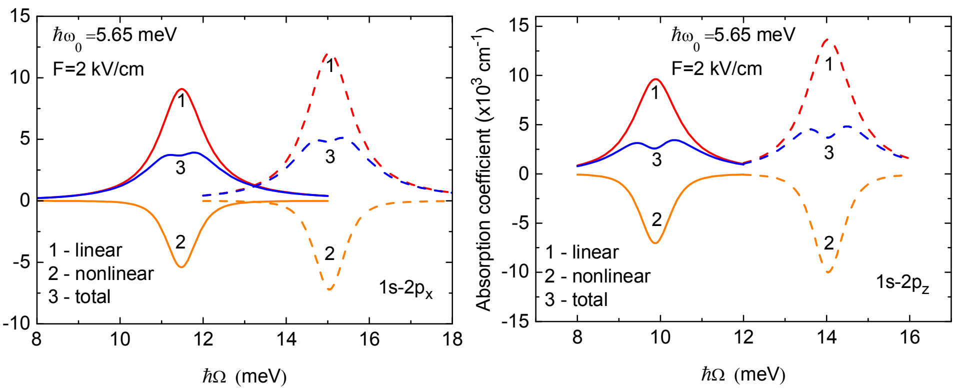

Fig. 3. The linear (1), the nonlinear (2), and the total (3) absorption coefficients as a function of photon energy without (solid lines) and with (dashed lines) ICE for transitions: (a) $1s{\to}2p_x$ and (b) $1s{\to}2p_z$.

Comparatively large blue shifts in linear, nonlinear and total absorption coefficients, connected to the image charge effect, are observed. Particularly, at $F = 3\ kV/cm$ and at $\hbar\omega_0 = 5.65\ meV$ the shifts are about $3.56\ meV$ and $4.16\ meV$ for transitions $1s \to 2p_x$ and $1s \to 2p_z$ respectively. The resonance peaks of linear and nonlinear absorption coefficients are increasing, taking into account the ICE. Despite the negative sign of the nonlinear absorption coefficient, the total absorption coefficient increases with ICE, because the linear absorption coefficient enhancement with ICE is larger than the nonlinear absorption coefficient enhancement.

Conclusion. The influence of the image charges on the ground-state and the first excited state energies, as well as oscillator strength of a hydrogen-like donor in a spherical QD in the presence of an external electric field has been investigated. Also, the effects of both electric field and image charges on the linear, third-order nonlinear and total absorbtion coefficients for $1s \to 2p_x$ and $1s \to 2p_z$ transitions have been studied.

Our results indicate that the image charges lead to significant changes in the optical absorbtion coefficients of the system.

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