J Math Chem (2013) 51:1815–1821
DOI 10.1007/s10910-013-0183-2

ORIGINAL PAPER

The possibility of semiconductor–metal transition in a spherical quantum dot

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Received: 15 January 2013 / Accepted: 18 April 2013 / Published online: 27 April 2013

Abstract We observe an abrupt change in diamagnetic susceptibility at critical donor concentration for an $Al_xGa_{1-x}As/GaAs$ quantum dot system in the effective mass approximation indicating a possible semiconductor metal transition. The effect of confining potential and the laser intensity on the abrupt change in diamagnetic susceptibility has also been studied. The effect of nonparabolicity of the conduction band has been included in our calculations. Results are presented and discussed.

Keywords Square well potential · Parabolic potential · Hydrogenic donor · Diamagnetic susceptibility · Spherical quantum dot · Semiconductor metal transition

1 Introduction

Metal-Insulator transition (MIT) is one of the current topics of research in condensed matter physics. Abrahams et al. [1] developed the scaling theory of localization and applying to non interacting electron predicted that no MIT could occur in low dimensional systems. But MIT has been observed in low dimensional systems experimentally and hence needs refocusing in the understanding of MIT. Anderson [2] has shown that

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a three dimensional electron gas could undergo MIT in the presence of strong disorder. Thouless [3] argued that MIT could be regarded as a quantum phase transition. Since electron–electron interaction was not considered in the scaling theory of localization, there are reasons to believe that such MIT may be driven by interactions and there is no consensus yet for the correct theory for the occurrence of MIT in low dimensional systems. According to Mott and Hubbard [4], Semiconductor–Metal transition is usually achieved due to the increase of overlap of impurity wave functions and correlation among electrons at critical concentration. In these scenario, Arora and Spector [5] predicted Semimetal–Semiconductor transition to occur at critical thickness of the quantum well wire (QWW) due to the carrier freeze out because of the increase in effective bandgap from the size quantization. Merwyn et al. [6] had shown the possibility of SMT to occur in a QWW in the effective mass approximation, using Anderson localization and Hartree Fock dielectric function with exchange and correlation of electrons. They have computed the critical concentration for the SMT by the abrupt change in diamagnetic susceptibility. Extending the work of the Merwyn et al. [6] to quantum dot (QD) and using the Anderson localization and Hartree Fock dielectric function with exchange and correlation of electrons in the effective mass approximations the possibility of SMT in a QD is demonstrated. The Schrodinger equation is solved variationally. As there is no evidence to the nature of confining potential in a spherical quantum dot (SQD) we have discussed the SMT for SQD with square well confinement and SQD with Parabolic confinement. Merwyn et al. [7] had shown that SMT could be controlled by applying a laser field in a quantum well. Extending this approach,the influence of the laser field on the SMT in SQD has been discussed. We present the theory in the next section and result and discussions in the subsequent section.

2 Theory

The Hamiltonian of the hydrogenic donor in a GaAs/$Al_xGa_{1-x}As$ SQD with square well confinement (in the finite barrier model) in the effective mass approximation is given by

$$H = \begin{cases} \dfrac{-\hbar^2\nabla^2}{2m_1} - \dfrac{e^2}{\varepsilon_1\left(r^2+a^2\right)^{1/2}} & r \leq R \\ \dfrac{-\hbar^2\nabla^2}{2m_2} - \dfrac{e^2}{\varepsilon_2\left(r^2+a^2\right)^{1/2}} + V(r,a) & r \geq R \end{cases} \tag{1}$$

where R is the radius of the SQD and m_1, ε_1 and m_2, ε_2 are the effective masses of electron and dielectric constant for the GaAs well and $Al_xGa_{1-x}As$ barrier material respectively and a is the amplitude of electron oscillation in laser field.

The Hamiltonian for a hydrogenic donor in a SQD with parabolic confinement is given by

$$H = \begin{cases} \dfrac{-\hbar^2\nabla^2}{2m_1} - \dfrac{e^2}{\varepsilon_1\left(r^2+a^2\right)^{1/2}} + \dfrac{1}{2}m_1\overset{2}{\omega}r^2 & r \le R \\ \dfrac{-\hbar^2\nabla^2}{2m_2} - \dfrac{e^2}{\varepsilon_2\left(r^2+a^2\right)^{1/2}} + V(r,a) & r > R \end{cases} \tag{2}$$

where ω is the parabolic oscillator frequency given by (2) $\frac{V(r,a)}{m_1R^2}$

As disorder was attributed as the key ingredient in explaining experimental results on SMT [8,9], we have considered Anderson localization which arises due to the randomness in the potential seen by the electron because of the random distribution of impurities [10] which is given by

$$\frac{1}{\varepsilon(r)\,r_a} = -\frac{e^{-\lambda r}}{\varepsilon(\vec{r})\,r_a} + \left[\frac{e^2}{\varepsilon(\vec{r})\,r_a} + \frac{\tau}{\varepsilon(\vec{r})} - \frac{\tau^3}{2\,\varepsilon(\vec{r})\,\rho^2} + \frac{\tau^2\,r_a}{2\,\varepsilon(\vec{r})} - \frac{\tau^3\,r_a}{2\,\varepsilon(\vec{r})\,\rho}\right]e^{-\rho r} \tag{3}$$

where $r_a = \sqrt{r^2+a^2}$, $\rho = \tau + \kappa$ where $\kappa^2 = 4\pi e^2 n(\xi)$, wherein $n(\xi)$ is the density of states at the Fermi energy.

The exchange and correlation of electrons is considered through the Hartree Fock (HF) dielectric function in the second term of the Hamiltonian and is given by [11]

$$\frac{1}{\varepsilon(\vec{r})} = \frac{1}{2\pi^2}\int\frac{e^{-i\vec{k}.\vec{r}}}{k^2\,\varepsilon(k)}d^3k \tag{4}$$

$$\varepsilon(k) = 1 - \left(\frac{4\pi e^2}{k^2} + 2E_k\right)\chi(\eta) \tag{4a}$$

where

$$\chi(\eta) = -\frac{\eta(\xi)}{2}\left(\frac{1-\eta^2}{2\,\eta}\ln\left|\frac{1+\eta}{1-\eta}\right| + 1\right) \tag{4b}$$

$\eta = k/2k_f$; $\eta(\xi) = m^*k_f/\pi^2\hbar^2$ is the density of states at the Fermi energy and

$$2E_k = E(k)_{exc} + E(k)_{cor}$$

$$E(k)_{exc} = -\frac{\pi^2e^2}{2k_F^2} - \frac{0.764e^2}{k_F^2}\left(\frac{k}{k_F}\right)^2 + \cdots \tag{4c}$$

$$E(k)_{cor} = \frac{-0.154m^*e^4}{\hbar^2k_F^3} + \frac{0.338e^2}{k_F^2}\left(\frac{k}{k_F}\right)^2 + \cdots \tag{4d}$$

where $e = \hbar = 1$ in atomic unit.

The trial wavefunction of the ground state in a confined square well potential is chosen as [12]

$$\psi = \begin{cases} N_1 \frac{Sin(\alpha r)}{\alpha r} e^{-\lambda r} & r \le R \\ N_2 \frac{e^{i\beta r}}{\beta r} e^{-\lambda r} & r > R \end{cases} \tag{5}$$

where $\alpha = \sqrt{2m_1 E}$, $\beta = \sqrt{2m_2(V(r,a) - E)}$ in atomic units, N_1 and N_2 are the Normalisation constants, E is the subband energy and λ is the variational parameter. The ground state trial wave function for the donor confined in a parabolic potential is given by [13]

$$\psi = \begin{cases} N_3 e^{-\frac{\gamma^2 r^2}{2}} F\left[\frac{1}{2}\left(\frac{3}{2}\right) - \frac{\delta}{4}, \frac{3}{2}; \gamma^2 r^2\right] e^{-\varsigma r} & r \le R \\ N_4 \frac{e^{i\xi r}}{\xi r} e^{-\varsigma r} & r > R \end{cases} \tag{6}$$

where $\gamma = \sqrt{2m_1 V(r,a)}/R$, $\delta = E\sqrt{2m_1 R^2}/V(r,a)$, $\xi = \sqrt{2m_2 (V(r,a) - E)}$, N_3 and N_4 are the Normalisation constants and F[u,v; ρ] is the confluent hypergeometric function and ς is the variational parameter.

In the presence of laser field the electron—impurity ion interaction is screened and is given by [14] $\frac{-e^2}{\varepsilon(r)(r^2+a^2)^{1/2}}$ with amplitude of electron oscillation in the radiation field a=eA/mc ω which is proportional to $I^{1/2}\omega^{-1/2}$, I being the intensity of laser radiation, ω is the frequency of laser radiation and V(r,a) is the laser dressed confining potential which is given by $V(r,a) = \frac{1}{2} V_B \Theta\left(r^2 - R_{EW}^2\right)$ where Θ(z) is the step function, $R_{EW} = R/2$—a is the effective Radius for a laser dressed QD.

V_B is the barrier potential of the carrier and is given by

$$V_B(R) = \begin{cases} 0 & r \le R_{EW} \\ 0.6\Delta E_g & r > R_{EW} \end{cases} \tag{7}$$

where $\Delta E_g = 1.155\,x + 0.37\,x^2$ and x is the Al composition.

The effect of non parabolicity of the conduction band has been considered through the effective mass m* Chaudhuri and Bajaj model [11] as

$$\frac{m^*}{m_0} = m\left[1 + \frac{\gamma\left(E_{n,l}\right)}{m/m_0}\right] \tag{8}$$

where $\gamma(E) = 0.0436\,E + 0.236\,E^2 - 0.147\,E^3$ with E taken in eV.

The ⟨H⟩ is minimized with respect to λ for the square well and ς for parabolic potential confinement to fix the wave function ψ for both the cases.

The diamagnetic susceptibility of a donor in a ground state is calculated from [11]

$$\chi_{dia} = -\frac{e^2}{6m_1\,\varepsilon_1\,c^2}\langle r^2 + a^2\rangle \tag{9}$$

where $e = 1, c = 137$ in atomic units and $\langle r^2 \rangle$ is the mean square distance of the electron from the nucleus. The results and discussions are presented in the next section.

3 The results and discussions

In Fig. (1) we present the variation of χ_{dia} against donor concentration (n_d) for laser amplitude $a = 150$ Å and without laser field ($a = 0$Å) for x=0.4. The figure shows a drastic drop in χ_{dia} indicating metallization at a donor concentration of $\sim 3 \times 10^{21}$ cm^{-3} for the SQD with parabolic confinement and at $\sim 1 \times 10^{21}$ cm^{-3} for SQD with square well confinement when no laser field is applied. Thus the SMT occurs at a higher n_d for SQD with parabolic confinement than for SQD with square well confinement. When the laser field is applied the SMT occurs at a lower n_d and for a laser field of amplitude $a = 150$ Å the SMT occurs at a n_d of $\sim 2 \times 10^{20}$ cm^{-3} for the SQD with parabolic confinement and at a n_d of $\sim 1 \times 10^{20}$ cm^{-3} for SQD with square well confinement. When an increasing laser field of amplitude 'a' is applied, the effective Radius R_{EW}, and hence the radius of the QD, is decreased which in turn decreases the donor binding leading to an abrupt change in χ_{dia} at a lower donor concentration 'n_d' [7]. The difference in the value of n_d for SMT between the SQD with parabolic confinement and SQD with square well confinement is reduced when a laser field is applied.

Similar result are observed for $x = 0.1$ as shown in Fig 2. The SMT occurs at a lower donor concentration for $x = 0.1$ compared to $x = 0.4$ and is appreciable when there is no laser field compared to the case when a laser field of amplitude of $a = 150$ Å is applied. The nonparabolicity of conduction band has no significant effect on SMT for both $x = 0.4$ and $x = 0.1$. Since we were unable to minimize the Hamiltonian for

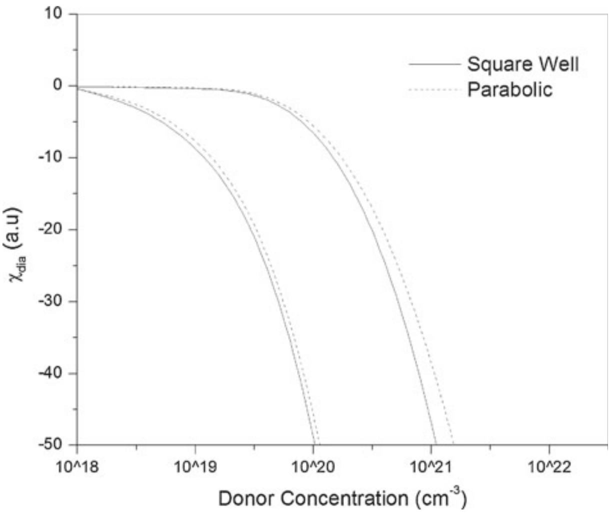

Fig. 1 Variation of χ_{dia} against donor concentration (n_d) for laser amplitude $a = 150$ Å and without laser field ($a = 0$Å) for $x = 0.4$

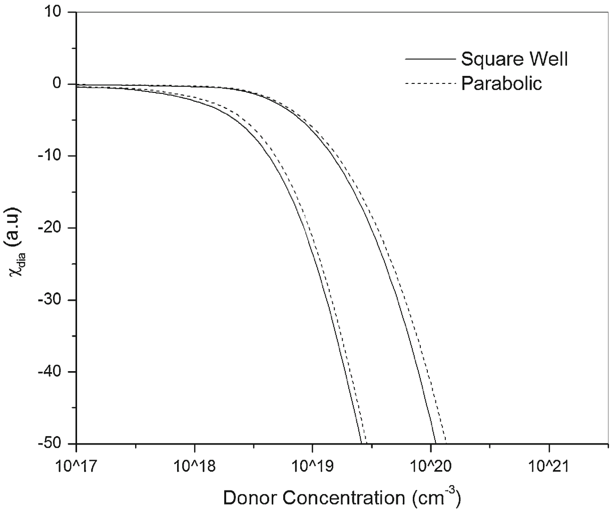

Fig. 2 Variation of χ_{dia} against donor concentration (n_d) for laser amplitude a = 150 Å and without laser field (a = 0Å) for x = 0.1

well widths less than 80 Å (a situation of almost strictly 0D system), which indicates that for a strictly zero dimensional system SMT may not be possible as per the scaling theory.

To conclude, there is a possibility of occurrence of SMT in quasi zero dimensional electron system like QD at critical concentration and if so it can be triggered and controlled by the amplitude of laser field. As mentioned earlier, as there is no concrete theory or experiment to understand SMT in 2D systems or lower than that, perhaps, some newer theory to explain its mechanism like traps etc as suggested by Alfshuler et al. [15] and general lowering of effective barrier height due to the formation of impurity bands in highly doped systems and diminishing of effective barrier thickness in both regimes of above and below SMT by individual impurities as proposed by Rakoczy et al. [16] have to be considered which may throw more light on this.

4 Conclusions

This study can be used as novel direction towards tuning of Fermi level and gap energy which may provide an important step towards the band gap engineering in Nanostructure and tunable devices.

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