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Band Structure of Semiconductor Nanowires with Embeded Quantum Dots

[1]Rahul Kumar Paswan* and [2]Ashok Kumar

Author's Affiliations: [1]Research Scholar, University Department of Physics, B.N. Mandal University, Madhepura, North Campus, Singheshwar, 852128, Bihar, India
[2]University Department of Physics, B.N. Mandal University, Madhepura, North Campus, Singheshwar, 852128, Bihar, India
[1]rahulkumarpaswan926@gmail.com and [2]ashokabnu@yahoo.co.in

***Corresponding author:** **Rahul Kumar Paswan**
Research Scholar, University Department of Physics, B.N. Mandal University, Madhepura, North Campus, Singheshwar, 852128, Bihar, India
E-mail: rahulkumarpaswan926@gmail.com

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ABSTRACT

The structure of nanowire bands by quantum dots or applying external electrostatic potentials have been studied. The nanostructure gave rise to bound states associated with energy levels within the gap between the valence and conduction bands and to resonances for metastable states and did not exist in the unstructured nanowire. When constant external magnetic fields were applied to the nanostructure the transformation of resonances into bound states were found. The resonance binding presented the transition from resonance to bound states. This type of nanostructure was due to using the effective mass approximation. The energy of the conduction band states behaved like Landau states. The behavior was linear. This was done in the case of one and two electron systems. The binding of resonances was effectively applied in semiconductor nanostructures embedded in nanowires in both cases and electronic quantum dots and material quantum dots. The expressions included played dealing with matching conditions at the interfaces between materials and the proper conversion of operators involved in the calculations to their co-ordinate representation. We have considered a quantum dot embedded on a nanowire. The matching conditions at the interfaces of the materials was taken into account in the p and z ordinates. The inclusion of the spin presented novel scenarios where some states made the transition from bound to resonance states depending on spin. The results found were in good agreement with previously obtained results.

KEYWORDS

Nanowire Bands, Quantum Dot, Nanostructure, Resonance, Effective Mass Approximation, Landau States, Interfaces, Transition.

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INTRODUCTION

Avron et al. [1] analysed the stabilization of meta stable states due to the presence of magnetic fields in atom like systems. It was presented the existence of negative Helium ions was numerically studied by Salas et al. [2]. Ho [3] studied the case of atomic like systems, the field strengths were essential to presented the width of a resonance was zero. Sikorski and

Mertt [4] presented that the energies of electronic states in Indium antimonide quantum dots effectively depended on the strength of magnetic field and was restricted for low energy states of very deep quantum dots. Reed et al. [5] demonstrated the evidence for discrete electronic states in semiconductor nanostructures. Buzcko et al. [6] analysed the bound state and resonance state of spherical GaAs/$Ga_{1-x}Al_xAs$ quantum dots and found their characteristics for binding of resonances and physical traits and it was supported by Bylicki et al. [7]. Bylicki and Jaskolski [8] studied and found that the width of shape resonances were noninteracting functions of the magnetic field strength and that for large enough values the width became null. The resonances states of two electron systems without magnetic fields were analysed in quantum dot and atomic systems [9]. Kuros et al. [10] studied that two electron quasi-one dimensional system using entanglement quantities. Sanjeev and Moiseyev [11] studied that the lifetime of resonance states of two electron spherical quantum dots were controlled by varying the confinement strength. Ravi et al. [12] studied the optical and electronic properties of nanowires of zinc blende structure. It was found that the energy of the lowest state of the conduction band had a strongly nonlinear dependence with the intensity of an external magnetic field. The oscillations were also observed in energy states of valence band. Kishore et al. [13] studied that when the null field band was taken for study then it was found that camel backs appeared in the band structure. In camel back the maximum value of the energy of the valence band was not found at the centre of the Brillouinon zone but for non-trivial values of the Bloch wave vector. A similar behavior was found in conduction band. All these phenomenon strongly depend on the radius of the nanowire and occurred in simple nanowires or with core shell structures. Genkin and Lindroth [14] studied the control of the lifetime states compromised by coulomb impurities. The resonance states of one electron cylindrical quantum dots with an external magnetic field using two probabilities were studied by Ramos and Osenda [15]. It was found that the probability of electron inside the potential well characterized the binding phenomenon. Garagiole et al. [16] presented that resonance state was detected using the localization probability and showed the presence of a magnetic field affected degenerate states. The defection procedure was advantageous that did not deepened on complex algebra calculations [17] or the complex absorbing potential methods [18]. Krishtopenko and Teppe [19] studied the band structure of free standing nanowires and resonance staes to band structure properties of quantum well. Durnev and Tarasenko [20] studied the spin-independent Hamiltonian in simplest effective mass approximation or from a spin-dependent Hamiltonian without external magnetic fields. The application of a magnetic field to a given system added to the Hamiltonian the Zeeman term was proportional to the strength of the field and terms came from the canonical momentum which included vector potential. Denning et al. [21] presented coupling between electromagnetic nanoresonators and pristine sheets of two dimensional semiconductors and speculated these systems entered the quantum regime operating at the few polariton levels. It was presented that a microscopic quantum theory for the interaction between excitons in a sheet of two dimensional material and a localized electromagnetic resonator. It was found that interaction broke the symmetry of the translation invariant system and effectively generated a localized exciton mode which was coupled to and environment of residual exciton modes. This dissipative coupling increased with tighter lateral confinement and revealed a potential in realizing nonlinear exciton-exciton interaction. Wen et al. [22] and Zheng [23] studied electromagnetic resonator with pristine sheet of two dimensional semiconductor for splitting of Rabi waves [24]. Delteil et al. [25] studied that polariton blockade and found that if enabled the construction of single photon sources. Tserkezis et al. [26] studied that quantum well and two dimensional materials and presented a microscopic model based on exciton momentum states to measurable properties. Kyriinko et al. [27] analysed theoretically the possibility of polariton blockade in two dimensional semiconductors without dephasing mechanism. Denning et al. [28] presented a formalism for possibility of exciton mode as degenerate in transition metal dichalcogenides.

METHOD

We have presented the model for quantum dots embedded in semiconductor nanowires and numerical methods were used to obtain band structure and calculated expression for matrix elements involved in the Rayleigh-Ritz method. We have used theoretical framework to detect the presence of resonance states in numerically calculated spectra. The results for the model with a quantum dot induced by an electrostatic confining potential were presented and the results corresponding to the model with a semiconductor quantum dot. We have applied Rayleigh-Ritz variational method to obtain the eigen states of the systems. This method was used in a range of situation that from band structure of free standing nanowires and resonance states to band structure properties of quantum wells. For a given Hamiltonian H and test function ϕ^1 and given as $\phi^1 = \sum_v c_i \varphi_v^+$, where $(\varphi_v)^Q$ is a basis bet with Q elements. The Rayleigh-Ritz method minimized the normalized expectation value of Hamiltonian

$$E = \frac{\left(\phi^1, H\phi^1\right)}{\left(\phi^1, \phi^1\right)}$$

With respect to the coefficients c_v, this minimization produced results in a eigen value. The basis set functions were dependent on a set of parameters which had different values termed as nonlinear parameters. For the model, we have considered the basis set depended on radial, angular and longitudinal along the axis of the nanowire co-ordinates and bounding conditions. We have variational eigen value

$$H = E^v \psi^v$$

Where H is the matrix of the Hamiltonian in function basis set ψ^v provided a discrete spectrum for energy subbands around the semiconductor gap and for discrete states inside the gap. The states in the different energy bands were extended like bulk material and those inside the gap were localized. The property was used in localized. This property was used in localized approximation states. The test functions were employed in the Rayleigh-Ritz method were obtained as a linear combination of basis functions.

$$\psi_{nml}(\rho,\varphi,z) = \frac{e^{2m\phi}}{\sqrt{2\pi}} \cdot \frac{\sqrt{2}}{RJ_{m+1}(\alpha_{ml})} \times J_m\left(\alpha_{ml}\frac{\rho}{R}\right)\sqrt{\frac{2}{L}}\cos\left(n\pi\frac{2z}{L}\right)$$

Where J_m are the Bessel functions of the first kind, $\alpha_m e$ is the *l*th zero of the function $J_m(\rho) m = 0, \pm, \pm 2, \ldots\ldots \pm M, l = 1, 2, \ldots, N_z$ and $n = 1, 2, N$. To obtain the band structure we have considered different sets of values of M, N_z and N. We have calculated the result using $N_z = 10$ and $M = 4$ for the study of energy values of a core shell nanowire using the 8 band Kohn Luttinger Hamiltonian. The obtained results were compared with previously obtained results of theoretical and experimental works.

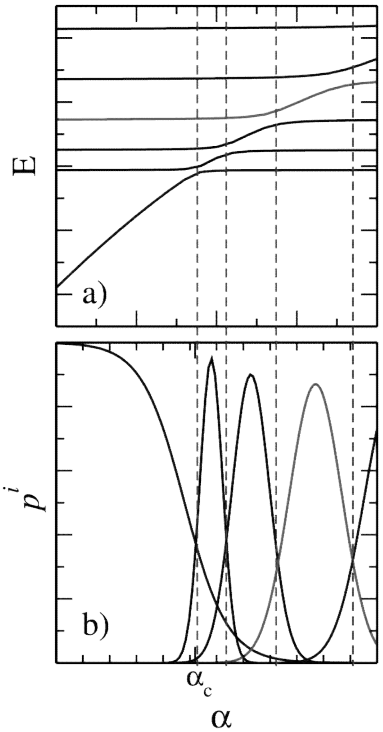
RESULTS AND DISCUSSION

We have studied band structure of semiconductor nanowires with embedded quantum dots. Graph (1) (a) shows the plot fo spectrum of a system near localization versus the function parameter α. It shows the typical behavior of the energy levels versus α in the neighborhood of a localization threshold. It indicates that eigenvalues are repelled by the state that entered into the band and a number of avoided crossings appeared in the spectrum. The resonance dependence with α was signaled by these successive avoided crossings. A complete characterization of resonance states were found by analyzing information stored in the eigen functions. The calculation of probability of localized states were made by the relation

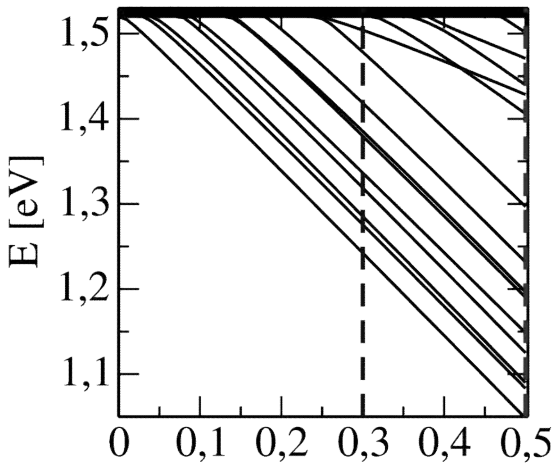
$$p^i(\alpha) = \int_{V_L} \left|\phi_\alpha^i(x)\right|^2 d\mathrm{x}.$$

Where V_L is the region where the potential well is located. ϕ_α^1 is a variational eigen function calculated for a given value of the parameter α with an energy $E_{(\alpha)}^i$ close to the resonance energy. Graph (1) (b) shows the qualitatively

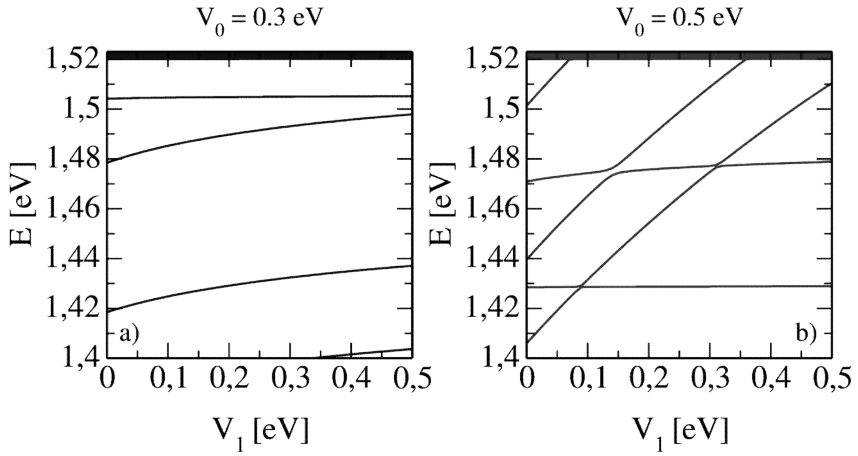
behavior of $p^i(\alpha)$ for the eigen functions corresponding to the eigen values shown in graph (1) (a). Graph (2) shows the plot of energy spectrum as a function of the depth of the well. Which shows the discrete spectrum when $V_1 = 0$ that entered into conduction band for some value of V_1. These eigen values are the origin of resonance states. So the neighborhood of particular values of V_0 and V_1 is an appropriate for binding of resonances when external magnetic field is applied. The eigen values of discrete varied linearly as a function of V_1 but there are groups with very different slopes. This is due to the different symmetries of the corresponding states which made some of them susceptible to the change in the height of the barrier of potential than the other. Graph (3) shows the plot of energy spectrum of the height of barriers versus nanowire radius. It shows that the number of discrete eigen values below the conduction band bottom were reduced for smaller radius of the well keeping the values of V_0 and V_1 in the same range. We have obtained the results for a potential and calculations were made for many other sets of lengths. We have analysed different radius of the potential well. These other cases the binding of resonances were also present. Graph (4) shows the plot of energy spectrum as a function of external magnetic field for gallium arsenide radius. Graph (4) shows the behavior of the variational spectrum near the bottom of the conduction band as function of the field strength B for potential parameters V_0, V_1, Z_1, Z_2 and R_w. It is clear from graph (3) that a state in the gap enters into conduction band for V_1, so larger values of V_1 resonance was found very close to the bottom of the conduction band. All eigen values were doubly degenerate for $B = 0$ and this degeneracy was broken when magnetic field was applied. The two curves emerged from each of the doubly degenerate eigen values at $B = 0$ one was increased and the other was decreased as functions of field intensity. The results found were compared with previously obtained results of theoretical and experimental works and were found in good agreement.



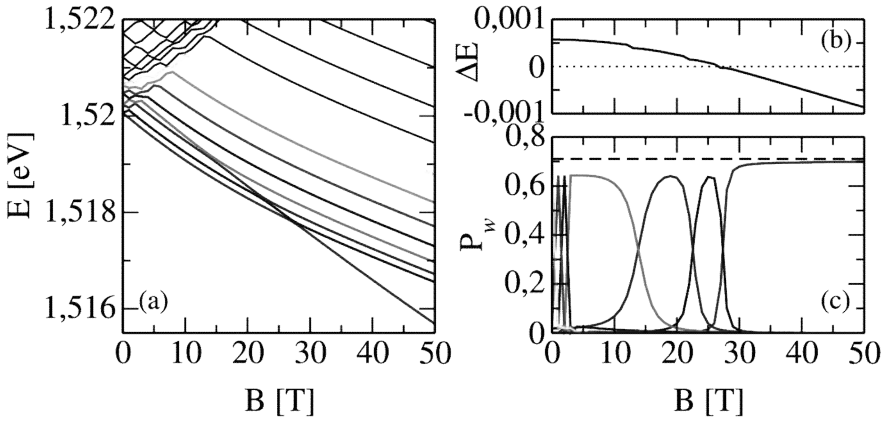
Graph 1: Plot of Spectrum of a system near localization threshold vs the function parameter α.



Graph 2: Plot of energy spectrum as a function of the depth of the well V_0.



Graph 3: Plot of energy spectrum of the height of barriers vs nanowire radius.



Graph 4: Plot of energy spectrum as a function of external magnetic field for gallium arsenide radius.

CONCLUSION

We have studied the structure of semiconductor nanowires with quantum dots. We have found that the spectral properties of systems with potential well and barriers were generated through the application of electrostatic potentials and results differed for systems with wall and barriers constructed with different semiconductor materials. The band structure was calculated using the Rayleigh-Ritz variational method. We have considered quantum dots of two different kinds. The appearance of discrete energy levels in the gap between the conduction band the valence band of nanostructure were found depended on the energy of these levels with the intensity of a magnetic field applied along the wire. It was found that the possibility of binding of resonances in this type of nanostructure was studied using the effective mass approximation. The number of localized states inside the gap is low of resulting the variational method were accurate as value of the gap energy and the values of the lowest energy of the conduction band. These elements were used for indentify the transition from bound to resonance state and back. The precise longitudinal dimensions values of the barriers and wells were close to single out and separated the resonance staes present in the system. The results found in both kinds of models showed that the binding phenomenon was found for an ample sets of materials and dimensions. It was found that the results presented the physics near the bottom of the conduction band the top of the valence band. The obtained results were found in good agreement with previously obtained results.

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