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Quantum Pseudodot Systems in One-Dimension, Two-Dimensions and Three-Dimensions

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Abstract

The energy eigenvalues and wave functions of the quantum pseudodot systems formed at pseudo-harmonic potential containing both quantum dot potential and quantum antidot potential are calculated in one, two and three dimensions. For the present case, all three systems form an exactly solvable system and we found exact solutions of the energy eigenvalues and normalized wave functions for the three systems. Ground states of energy eigenvalues and wave functions are found and the results are analyzed for some special cases.

Keywords: Pseudodot, Quantum Pseudodot Systems, Quantum Dots

INTRODUCTION

Since the discovery of nanotubes [1] and nanoballs [2], studies on nanostructures have been increasingly continued. In parallel with nanofabrication technology, both experimental and theoretical studies on new nanostructures such as dots, antidots, pseudodots, wells, wellwires and antiwells have been carried out continuously by researchers for a few decades.

Over the past few years, there has been an abundance of research on two-dimensional (2D) quantum pseudodot systems (QPS's) constructed by a pseudo harmonic potential (PHP) that includes both harmonic quantum dot and antidot potential. Researches on 2D QPSs have been intensified on optical properties [3-9], polaron efects [13-18], impurity states [6, 10, 14], magnetic effects [4, 5, 11, 19] and Aharonov-Bohm (AB) flux field effects [4, 11, 19]. In one of these, Cetin investigates the energy spectrums and the corresponding wave functions of an electron confined by a PHP both including harmonic dot and antidot potentials in the presence of a strong magnetic field together with an AB flux field [19]. Rezaei et al. theoretically investigated the optical absorption coefficient changes and refractive index changes associated with intersubband transitions in a 2D QPS under the influence of a uniform magnetic field. In this regard, they examined the electronic structure of the pseudodot system using the one-band effective mass theory, and calculated linear and nonlinear optical absorption coefficient and refractive index changes by means of the compact density matrix approach [4]. Khordad studied the direct interband transitions in QPS under the influence of an external magnetic field. He obtained an analytical expression for the light interband absorption coefficient and threshold frequency of absorption as the functions of applied magnetic field and geometrical size of QPS. Besides, he studied the absorption threshold frequency at small and high applied magnetic field and also as a function of size of QPS [5]. Ikhdair and Hamzavi calculated the energy levels and the wave functions of an electron confined in a 2D pseudoharmonic quantum dot potential under the influence of temperature and an external magnetic field inside dot and AB field inside a pseudodot by using the Nikiforov-Uvarov method. They computed the exact solutions for energy eigenvalues and wave functions as functions of the chemical potential parameters, applied magnetic field strength,

AB flux field, magnetic quantum number and temperature [11]. Rani and Chand studied the energy spectrum of a quantum dot system consisting of an electron confined by a three dimensional parabolic confinement potential which is a combination of harmonic, coulomb, linear and an-harmonic potential terms [12]. Liu et al. [20] theoretically investigated linear and nonlinear optical absorption coefficients and refractive index changing with the 3D ring-shaped PHP.

While many works have been done on 2D QPS, there has been dearth of studies on 1D and 3D QPSs. 3D QPSs are especially important for optical transitions, polaron effects, impurity effects and magnetic effects in bulk materials and they need further investigation.

The paper is organized as follows. In Sect. 2, we first describe a one-dimensional quantum pseudodot structure and solve exactly the related Schrödinger equation and calculate the energy spectrum and wave functions. In Sect. 3, we solve the Schrödinger equation which corresponds to the 2D QPS and find the energy eigenvalues and the wave functions analytically. In the fourth section, the radial Schrödinger equation which determines the 3D QPS is solved and the energy eigenvalues and the wave functions are found. In the last section, energy eigenvalues and wave functions associated with 1D, 2D and 3D QPS are analyzed for the ground states and some special cases.

QUANTUM PSEUDODOT SYSTEM IN 1D

Within the effective-mass approximation, we write the one-dimensional Schrödinger Equation for a particle mass and energy trapped in a 1D pseudoharmonic potential,

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(x)\psi = E\psi \tag{1}$$

where $V(x)$ potential is 1D PHP that includes both harmonic quantum dot potential and antidot potential and given by $V(x)=V_0\left(\frac{x}{x_0}-\frac{x_0}{x}\right)^2$ with V_0 chemical potential of electron gas and x_0 zero point of the pseudoharmonic potential in 1D as illustrated in Figure 1 as a function of $\frac{x}{x_0}$

for a special value $V_0 = 0.5\,meV$. Substituting $V(x)$ into the Eq. (1), we obtain

$$\left[\frac{d^2}{dx^2} + \frac{2m^*(E+2V_0)}{\hbar^2} - \frac{2m^*V_0}{\hbar^2 x_0^2}x^2 - \frac{2m^*V_0 x_0^2}{\hbar^2}\frac{1}{x^2}\right]\psi = 0 \tag{2}$$

by replacing x with $\rho = \alpha_{1D}x^2$ where $\alpha_{1D} = \sqrt{\frac{2m^*V_0}{\hbar^2 x_0^2}}$, we obtain

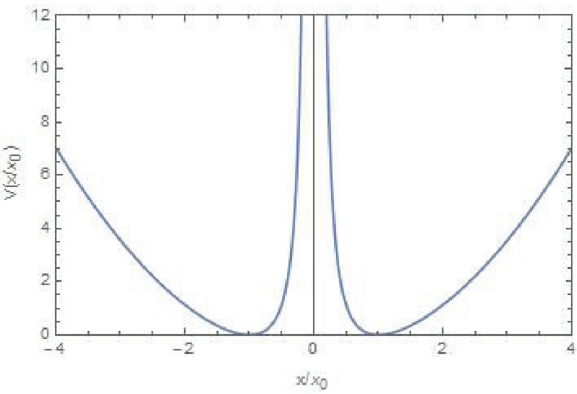


Figure 1. Pseudo harmonic potential in one dimension as a function for a special value $V_0 = 0.5\,meV$

$$\left[\rho\frac{d^2}{d\rho^2} + \frac{1}{2}\frac{d}{d\rho} + \frac{\lambda_{1D}}{4} - \frac{\rho}{4} - \frac{\beta_{1D}(\beta_{1D}-1)}{4\rho}\right]\psi = 0 \tag{3}$$

where in Eq. (3), we use abbreviations $\lambda_{1D} = \left(\frac{2m^*x_0^2}{\hbar^2 V_0}\right)^{1/2}(E+2V_0)$ and $\beta_{1D}(\beta_{1D}-1) = \frac{2m^*V_0x_0^2}{\hbar^2}$. In order to find suitable solution for the differential equation in Eq. (3), it is useful to utilize the limits of $\rho \to 0$ and $\rho \to \infty$. For $\rho \to \infty$, the term $\rho/4$ is dominant and one gets the equation

$$\left[\rho\frac{d^2}{d\rho^2} - \frac{\rho}{4}\right]\psi = 0 \tag{4}$$

In this case, the solution the Eq. (4) is $\psi(\rho) = A\,e^{-\rho/2} + B\,e^{\rho/2}$. Here we can ignore the second term because it becomes infinite as $\rho \to \infty$.

In the other asymptotic limit ($\rho \to 0$), one gets the equation

$$\left[\rho\frac{d^2}{d\rho^2} + \frac{1}{2}\frac{d}{d\rho} - \frac{\beta_{1D}(\beta_{1D}-1)}{4\rho}\right]\psi = 0 \tag{5}$$

Hence, the solution of the Eq. (5) is $\psi(\rho) = C\,\rho^{\frac{1}{2}\beta_{1D}} + D\,\rho^{-\frac{1}{2}(\beta_{1D}-1)}$. Here, we can disregard the second term, since it becomes infinite as $\rho \to 0$.

With the solution of the asymptotic cases, we try the substitution

$$\psi(\rho) = e^{-\frac{\rho}{2}}\rho^{\frac{1}{2}\beta_{1D}}u(\rho) \tag{6}$$

After inserting Eq. (6) into Eq. (3)

$$\rho\frac{d^2u(\rho)}{d\rho^2} + \left[(\beta_D - \frac{1}{2}) + 1 - \rho\right]\frac{du(\rho)}{d\rho} + nu(\rho) = 0 \tag{7}$$

where $n = \frac{\lambda_{1D}-1}{4} - \frac{\beta_{1D}}{2}$ is an integer. To find the energy eigenvalue of the 1D pseudodot, one can use abbreviations used in Eq. (3) and Eq. (7)

$$\lambda_{1D} = 2(2n + \beta_{1D} + \frac{1}{2}) = \left(\frac{2m^*x_0^2}{\hbar^2 V_0}\right)^{1/2}(E+2V_0)$$

$$E_n = \hbar\omega_{1D}(2n + \beta_{1D} + \frac{1}{2}) - 2V_0 \tag{8}$$

where $\omega_{1D} = \left(\frac{2V_0}{m^*x_0^2}\right)^{1/2}$ and $\beta_{1D} = \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{2m^*V_0x_0^2}{\hbar^2}}$

are used. Differential equation in Eq. (7) is known as Associated Laguerre differential equation and its solution is Associated Laguerre Polynomials $L_n^{\beta_{1D}-\frac{1}{2}}(\rho)$.

The normalized wave functions of the pseudodot system in 1D are

$$\psi_n(\rho) = (\alpha_{1D})^{\frac{1}{4}}\left(\frac{n!}{\Gamma(n+\beta_{1D}+1/2)}\right)^{1/2} e^{-\frac{\rho}{2}}\rho^{\frac{1}{2}\beta_{1D}}L_n^{\beta_{1D}-\frac{1}{2}}(\rho) \tag{9}$$

where $\rho = \alpha_{1D}x^2$ with $\alpha_{1D} = \sqrt{\frac{2m^*V_0}{\hbar^2 x_0^2}}$, $\Gamma(n)$ is the Gamma function and n is the quantum number which must be an integer ($n = 0,1,2,3,...$).

QUANTUM PSEUDODOT SYSTEM IN 2D

The 2D Schrödinger equation for a particle mass and energy trapped in a 2D PHP is

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(r)\psi = E\psi \tag{10}$$

where $V(r) = V_0\left(\frac{r}{r_0} - \frac{r_0}{r}\right)^2$ is 2D PHP that includes quantum dot and antidot potential. A 2D PHP potential is illustrated in Figure 2 at an arbitrary unit. Substituting this potential into the Eq. (10) and let us consider the wave function in the form of $\psi(r,\phi) = \frac{1}{\sqrt{2\pi}}R(r)e^{-im\phi}$

$$\left[\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} + \frac{2m^*(E+2V_0)}{\hbar^2} - \left(m^2 + \frac{2m^*V_0r_0^2}{\hbar^2}\right)\frac{1}{r^2} - \frac{2m^*V_0}{\hbar^2 r_0^2}r^2\right]R(r) = 0 \tag{11}$$

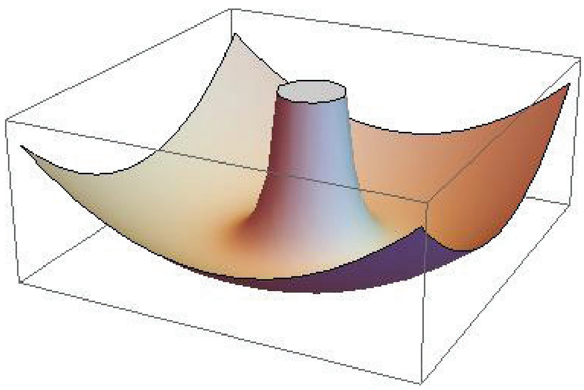


Figure 2. Pseudo harmonic potential in two-dimensions at an arbitrary unit

where m is the magnetic quantum number. If we change the variable r to $\rho=\alpha_{2D}r^2$ with $\alpha_{2D}=\sqrt{\frac{2m^*V_0}{\hbar^2 r_0^2}}$, we obtain

$$\left[\rho\frac{d^2}{d\rho^2}+\frac{d}{d\rho}+\frac{\lambda_{2D}}{4}-\frac{\rho}{4}-\frac{(\beta_{2D})^2}{4\rho}\right]R(\rho)=0 \quad (12)$$

where $\lambda_{2D}=\sqrt{\frac{2m^*r_0^2}{\hbar^2 V_0}}(E+2V_0)$ and $\beta_{2D}=\sqrt{m^2+\frac{2m^*V_0r_0^2}{\hbar^2}}$ are used. To find suitable substitution for Eq. (12), it is convenient to use the limits of $\rho\to 0$ and $\rho\to\infty$. For $\rho\to\infty$, the term $\rho/4$ is dominant and one gets the equation

$$\left[\rho\frac{d^2}{d\rho^2}-\frac{\rho}{4}\right]R(\rho)=0 \quad (13)$$

in which case the solution of Eq. (13) is $\psi(\rho)=A\,e^{-\rho/2}+B\,e^{\rho/2}$. We have to exclude the second term, because it becomes infinite as $\rho\to\infty$.

For $\rho\to 0$, the dominant terms in Eq. (12)

$$\left[\rho\frac{d^2}{d\rho^2}+\frac{d}{d\rho}-\frac{(\beta_{2D})^2}{4\rho}\right]R(\rho)=0 \quad (14)$$

Solution of Eq. (14) is $R(\rho)=C\,\rho^{\frac{1}{2}\beta_{2D}}+D\,\rho^{-\frac{1}{2}\beta_{2D}}$. We have to exclude the second term, because it becomes infinite as $\rho\to 0$.

As in our treatment of the 1D case, a solution which covers the whole region

$$R(\rho)=e^{-\rho/2}\rho^{\frac{1}{2}\beta_{2D}}u(\rho) \quad (15)$$

Substituting Eq. (15) into Eq. (12), we have

$$\rho\frac{d^2u(\rho)}{d\rho^2}+(\beta_{2D}+1-\rho)\frac{du(\rho)}{d\rho}+n\,u(\rho)=0 \quad (16)$$

where $n=\frac{\lambda_{2D}-2}{4}-\frac{\beta_{2D}}{2}$ must be an integer ($n=0,1,2,\ldots$). Differential equation in Eq. (16) is Associated Laguerre Differential Equation and its solution is Associated Laguerre Polynomials $L_n^{\beta_{2D}}(\rho)$.

To find the energy eigenvalue of the 2D pseudodot system, we must use the constant

$$\lambda_{2D}=\sqrt{\frac{2m^*r_0^2}{\hbar^2V_0}}(E+2V_0)=2(2n+\beta_{2D}+1)$$

$$E_{n,m}=\hbar\omega_{2D}(2n+\beta_{2D}+1)-2V_0 \quad (17)$$

where $\omega_{2D}=\left(\frac{2V_0}{m^*r_0^2}\right)^{1/2}$ is used. The wave functions of the pseudodot system in 2D are

$$\psi_{n,m}(\rho,\phi)=\left(\frac{\alpha_{2D}}{\pi}\right)^{1/2}\left(\frac{n!}{\Gamma(n+\beta_{2D}+1)}\right)^{1/2}e^{-\rho/2}\rho^{\frac{1}{2}\beta_{2D}}L_n^{\beta_{2D}}(\rho)e^{-im\phi} \quad (18)$$

where $\rho=\alpha_{2D}r^2$ with $\alpha_{2D}=\sqrt{\frac{2m^*V_0}{\hbar^2r_0^2}}$ and $\beta_{2D}=\sqrt{m^2+\frac{2m^*V_0r_0^2}{\hbar^2}}$ are used. In Eq. (18) $\Gamma(n+\beta_{2D}+1)$ is the Gamma Function.

QUANTUM PSEUDODOT SYSTEM IN 3D

Radial part of the Schrödinger equation for a particle mass m^* and energy E trapped in a 3D PHP is given by

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right)+\frac{2m^*}{\hbar^2}\left[E-V_0\left(\frac{r}{r_0}-\frac{r_0}{r}\right)^2-\frac{\ell(\ell+1)\hbar^2}{2m^*r^2}\right]R(r)=0 \quad (19)$$

It is convenient to make a change of variable $\rho=\alpha_{3D}r^2$ with $\alpha_{3D}=\sqrt{\frac{2m^*V_0}{\hbar^2r_0^2}}$, the equation then reads

$$\rho\frac{d^2R}{d\rho^2}+\frac{3}{2}\frac{dR}{d\rho}+\left[\frac{\lambda_{3D}}{4}-\frac{\rho}{4}-\frac{\beta_{3D}(\beta_{3D}+1)}{4\rho}\right]R=0 \quad (20)$$

where we have introduced parameters $\lambda_{3D}=\sqrt{\frac{2m^*r_0^2}{\hbar^2V_0}}(E+2V_0)$ and $\beta_{3D}(\beta_{3D}+1)=\ell(\ell+1)+\frac{2m^*V_0r_0^2}{\hbar^2}$ where ℓ is the angular momentum quantum number. One can solve Eq. (20) in such a familiar way that we consider first the behavior the equation for the large ρ. In this case, the only terms that remains in the equation

$$\rho\frac{d^2R(\rho)}{d\rho^2}-\frac{\rho}{4}R(\rho)=0 \quad (21)$$

and the solution, which behaves properly at infinity, is $R(\rho)\approx e^{-\rho/2}$. Secondly, for small ρ, the dominant terms in Eq. (20)

$$\rho\frac{d^2R(\rho)}{d\rho^2}+\frac{3}{2}\frac{dR(\rho)}{d\rho}-\frac{\beta_{3D}(\beta_{3D}+1)}{4\rho}R(\rho)=0 \quad (22)$$

And the solution of Eq. (22) is $R(\rho)=A\,\rho^{\frac{1}{2}\beta_{3D}}+B\,\rho^{-\frac{1}{2}(\beta_{3D}+1)}$. The solution, which behaves properly at $\rho\to 0$, is $R\approx\rho^{\frac{1}{2}\beta_{3D}}$. We may propose a solution to Eq. (20)

$$R(\rho)=e^{-\rho/2}\rho^{\frac{1}{2}\beta_{3D}}u(\rho) \quad (23)$$

which covers the whole region. After substituting this solution into the Eq. (20), we have

$$\rho\frac{d^2u(\rho)}{d\rho^2}+\left[(\beta_{3D}+\frac{1}{2})+1-\rho\right]\frac{du(\rho)}{d\rho}+n\,u(\rho)=0 \quad (24)$$

where $n=\frac{\lambda_{3D}-3}{4}-\frac{\beta_{3D}}{2}$ must be an integer and Eq. (24) is Associated Laguerre differential equation which solutions are Associated Laguerre Polynomials $L_n^{\beta_{3D}+\frac{1}{2}}(\rho)$.

To find the energy eigenvalue of the 3D QPS, we may use abbreviations used in Eq. (20) and Eq. (24)

$$E_{n,\ell}=\hbar\omega_{3D}\left(2n+\beta_{3D}+\frac{3}{2}\right)-2V_0 \tag{25}$$

where $\omega_{3D}=\left(\frac{2V_0}{m^* r_0^2}\right)^{1/2}$ and $\beta_{3D}=-\frac{1}{2}+\sqrt{\left(\ell+\frac{1}{2}\right)^2+\frac{2m^*V_0r_0^2}{\hbar^2}}$ are used. Normalized wave functions of the 3D QPS are

$$\psi_{n,\ell,m}(r,\theta,\phi)=(\alpha_{3D})^{\frac{3}{4}}\left(\frac{2n!}{\Gamma(n+\beta_{3D}+\frac{3}{2})}\right)^{\frac{1}{2}}e^{-\frac{\rho}{2}}\rho^{\frac{1}{2}\beta_{3D}}L_n^{\beta_{3D}+\frac{1}{2}}(\rho)Y_\ell^m(\theta,\phi)$$

(26)

where $Y_\ell^m(\theta,\phi)$ are spherical harmonics, $\Gamma(n+\beta_{3D}+\frac{3}{2})$ is the Gamma function and $\rho=\alpha_{3D}r^2$ with $\alpha_{3D}=\sqrt{\frac{2m^*V_0}{\hbar^2 r_0^2}}$ are used.

DISCUSSION

In this paper, we calculated exact solutions for the energy spectrums and the normalized wave functions of QPSs in 1D, 2D and 3D. Energy spectrum of the 1D QPS is equidistant with the spacing $2\hbar\omega_{1D}$ and has a value in the ground state ($n=0$), the zero point energy $E_0=\hbar\omega_{1D}(\beta_{1D}+\frac{1}{2})-2V_0$ with $\beta_{1D}=\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{2m^*V_0x_0^2}{\hbar^2}}$. To find the ground state wave function of 1D quantum pseudodot system one can put $n=0$ in Eq. (9)

$$\psi_0(\rho)=\left(\frac{(\alpha_{1D})^{\frac{2\beta_{1D}+1}{2}}}{\Gamma(\beta_{1D}+1/2)}\right)^{\frac{1}{2}}e^{-\alpha_{1D}x^2/2}x^{\beta_{1D}} \tag{27}$$

Energy spectrum of the 2D QPS depends on principal quantum number n and magnetic quantum number m. The ground state energy of the 2D QPS has a value of ($n=0$ and $m=0$) $E_{0,0}=\hbar\omega_{2D}(\beta_{2D}+1)-2V_0$ (the zero point energy) with $\beta_{2D}=\sqrt{\frac{2m^*V_0r_0^2}{\hbar^2}}$. In order to obtain the ground state wave function of 2D QPS one can take $n=0$ and $m=0$ in Eq. (18)

$$\psi_{0,0}(r,\phi)=\left(\frac{(\alpha_{2D})^{\beta_{2D}+1}}{\pi\,\Gamma(\beta_{2D}+1)}\right)^{1/2}e^{-\alpha_{2D}r^2/2}r^{\beta_{2D}} \tag{28}$$

This results for energy eigenvalues and wave functions agrees with other 2D QPS in the literature [5, 19].

In 3D case, energy spectrum of the 3D QPS depends on principal quantum number n and angular momentum quantum number ℓ. There are $2\ell+1$ times degeneracy on magnetic quantum number m because the energy spectrum does not depend on the magnetic quantum number m. When the magnetic field is applied, the degeneracy of the energy eigenvalues is removed. The ground state energy of the 3D QPS is $E_{0,0}=\hbar\omega_{3D}\left(\beta_{3D}+\frac{3}{2}\right)-2V_0$ with $\beta_{3D}=-\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{2m^*V_0r_0^2}{\hbar^2}}$. In the case of 3D, the ground state wave function for QPS is

$$\psi_{0,0,0}(r,\theta,\phi)=\left(\frac{(\alpha_{3D})^{\frac{2\beta_{3D}+3}{2}}}{2\pi\,\Gamma(\beta_{3D}+3/2)}\right)^{\frac{1}{2}}e^{-\frac{\alpha_{3D}r^2}{2}}r^{\beta_{3D}} \tag{29}$$

The ground state energies of 1D, 2D and 3D QPS are plotted in Figure 3 as a function of the zero point r_0 of the PHP. In Figure 3, the ground state energy of the 1D QPS is represented by a solid line, the ground state energy of 2D QPS is indicated by dashed line, and the ground state energy of the 3D QPS is represented by dash dotted line. Figure 3 is drawn using some special values ($V_0=0.5\,meV$ and $m^*=0.067m_e$ where m_e is rest mass of the electron). As shown in Figure 3, as the dot size increases, the ground state energies decrease for all three systems. The ground state energy of the 2D QPS is close to the ground state energy of the 3D QPS where the zero point of the PHP is small, while it is closer to the ground state energy of the 1D QPS where the zero point of the PHP is large. For the zero value of the principal quantum number n, energies of the three-dimensional quantum pseudodot system and energies of the three-dimensional harmonic oscillator with the same frequency $\left(E_{n,\ell}=\hbar\omega_{3D}\left(2n+\beta_{3D}+\frac{3}{2}\right)\right)$ are shown in Figure 4 as the function of the angular momentum quantum number ℓ for special values $V_0=0.5\,meV$, $m^*=0.067m_e$ and $r_0=100\,nm$. In Figure 4, the 3D QPS energies and 3D harmonic oscillator energies are denoted by dots and diamonds, respectively. For all values of the angular momentum quantum number ℓ, the energy of the 3D QPS is lower than the energy of the 3D harmonic oscillator. The intervals between the energies increases with increasing value of angular momentum quantum number ℓ.

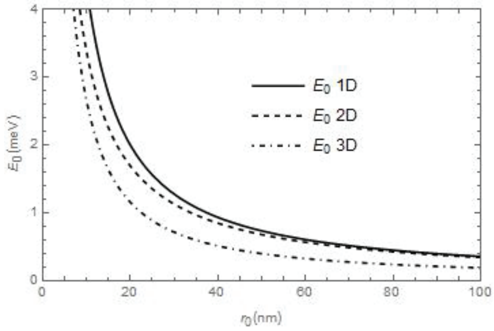
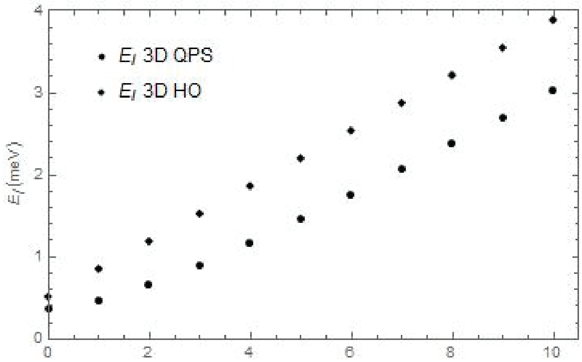


Figure 3. The ground state energies of 1D, 2D and 3D quantum pseudodot systems as a function of the zero point of the pseudo harmonic potential for special values $V_0 = 0.5\,meV$ and $m^* = 0.067\,m_e$ where m_e is the rest mass of the electron.



Angular momentum quantum number (l)

Figure 4. Energies of the 3D quantum pseudodot system and energies of the 3D harmonic oscillator with the same frequency as the function of the angular momentum quantum number *l* for special values $V_0 = 0.5\,meV$, $m^* = 0.067\,m_e$ and $r_0 = 100\,nm$ where is the rest mass of the electron.

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