

The D-dimensional Analysis of Magnetic Field, Potential Depth and the Screening Parameter Impact on the Energy Spectra of Lead Selenide

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Abstract

An analysis of the impact of the magnetic field, potential depth and the screening parameter on the nature of the energy eigen values of Lead Selenide is done in this study. By using Hulthen-Yukawa Potential Model (HYPM) in an applied magnetic field, the Schrödinger wave equation (SWE) is solved analytically using the Nikiforov-Uvarov (NU) method to get the solution of the SWE in D-dimensions. With the energy equation obtained, the numerical values were generated with the aid of the Maple software. An investigation of how the magnetic field, the potential depth and the screening parameter affect the energy spectra was done. We observed from our graphical plots that as the values of the applied field are increasing, the energy eigenvalues also increased for the different dimensions. The eigen values decreased proportionally with increase in the potential depth. We also observed that as the values of the screening parameter are increasing, the energy eigenvalues increased as well.

Keywords: *Magnetic Field; Potential Depth; Screening Parameter; Hulthen-Yukawa Potential; Nikiforov-Uvarov method.*

1. INTRODUCTION

The energy eigen values of materials particularly semiconductors are important in knowing the electronic, optical and transport properties of such materials. In a crystal lattice, there are energy levels that electrons are allowed to occupy. These allowed energy levels are referred to energy eigen values. For an empirical/periodic potential interacting with electrons in a quantum well, one can

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obtain these energy eigen values by solving the Schrödinger wave equation (SWE). The other methods that can be adopted in determining the energy eigen values include density functional theory (DFT), tight-binding and k.p perturbation theory. Thus, energy bands formed from energy eigen values can give us the behavior of materials whether they are conductors, semiconductors or insulators. Therefore, the current flow, the absorption and emission of photons in materials can be determined by the energy eigen values (Sze and Kwork, 2007; Streetman and Banerjee, 2015; Yu and Cordona, 2010).

In this study, we want to use (HYPM) in the region of magnetic field to solve the radial part of the (SWE) in D-dimensions with the (NU) method. An investigation of how the magnetic field, the screening parameters and depth of the potential of the quantum well affect the nature of the energy eigen values will be done. The Hulthen potential has been instrumental in solving problems in solid state, nuclear, atomic and condensed matter physics. With Hulthen potential, the interaction that exists between the molecular and nuclear structure of an atom can be described. The potential is short-ranged which shows a Coulombic nature for small values of the screening parameter, δ , but when the values of δ becomes large, it shows an exponential decrease. On the other hand, Yukawa potential is a non-relativistic potential used for the description of the interactions between nucleons (Otete, 2023). Here, Lead Selenide (PbSe) is considered for study in our system. Lead Selenide (PbSe) is one of the metal chalcogenide compounds that is semiconducting in nature. Its application in the electronics and opto-electronics industry has made it a research hub for material scientists. It is widely used in solar cell technology (Smu and Nnabuchi, 2010). Lead Selenide is a rock salt. It crystallizes in the cubic form of the Sodium Chloride (NaCl) crystal structure-the fcc structure. It has an octahedral coordination, that is each lead ions is surrounded by six Selenium ions and each Selenium is also surrounded by six Lead ions. It has a space group of Fm-3m with a lattice constant $a=6.12\text{\AA}$. It has a narrow direct band gap of about 0.27eV at room temperature and its effective mass is $0.114m_o$ (Walton et al., 1962). In addition to being used in solar cell technology, Lead Selenides (PbSe) are used in infrared detectors and thermoelectric devices (Shankar and Prabhu, 2023).

This paper is organized as follows; in section 2, the Hamiltonian for a charged particle in the presence of magnetic field will be considered and the radial part of the SWE will be solved analytically for confining potential in D-dimensions to get the eigenvalues and the wave function. In section 3, will contain the numerical values and graphical plots. Our results are discussed in section 4. The last section will take the conclusion and then the references.

2. MATERIALS AND METHOD

The Hamiltonian of our system for a charged particle can be modeled in the presence of magnetic field as:

$$H = \frac{1}{2\mu} (i\hbar\vec{\nabla} - e\vec{A})^2 + V_{(r)} \quad (1)$$

We denoted μ as the effective mass of PbSe. The magnetic field is aligned in the z-direction. The choice of our symmetric gauge is $\nabla \cdot \vec{A} = 0$. The vector potential $A = \left(-\frac{1}{2}y, \frac{1}{2}x, 0\right)$ is used. $V_{(r)}$ is our potential written in Eq. (3) (Behzadi and Hajimirghasemi, 2017; Ikot et al; 2014).

The SWE in D-dimension is written (Otete and Eleje, 2023) as:

$$\frac{d^2 U_{n,l}(r)}{dr^2} + \frac{2\mu}{\hbar^2} [E - V_{(r)}] U_{n,l} - \frac{1}{r^2} \left[\frac{(D-1)(D-3)}{4} + l(l + D - 2) \right] U_{n,l}(r) = 0 \quad (2)$$

$$V_{(r)} = -\frac{A_0 e^{-\delta r}}{(1 - e^{-\delta r})} - A_1 \left(\frac{e^{-\delta r}}{r} \right) \quad (3)$$

Here, A_0 stands for the potential strength, A_1 , δ are the potential depth and the screening parameter.

For one to solve Eq. (3), we use the approximation scheme given in Eq. (4) to handle the centrifugal term of Eq. (2) (Otete et al; 2021).

$$\frac{1}{r^2} \approx \frac{\delta^2}{(1 - e^{-\delta r})^2}, \quad \frac{1}{r} \approx \frac{\delta}{(1 - e^{-\delta r})} \quad (4)$$

After solving little calculation with Eq. (4), and Eqs. (1,2 and 3), one will obtain Eq. (5) written as:

$$\frac{d^2 U_{nl}}{dr^2} + \left[\frac{2\mu}{\hbar^2} \left(E + \frac{A_0 e^{-\delta r}}{(1 - e^{-\delta r})} + A_1 \left(\frac{e^{-\delta r}}{r} \right) \right) - \frac{eB\mu\hbar}{2\mu} - \frac{e^2 B^2}{8\mu} \right] U_{n,l} = 0 \quad (5)$$

where

$$\omega = \frac{eB}{\mu}, \text{ the cyclotron frequency}$$

By using the transformation $z = e^{-\delta r}$, Eq. (5) becomes

$$\frac{d^2 U_{n,l}(z)}{dz^2} + \frac{(1-z)}{z(1-z)} \frac{dU_{n,l}}{dz} + \frac{1}{z^2(1-z)^2} \left[\frac{2\mu E}{\hbar^2 \delta^2} + \frac{2\mu A_0 z}{\hbar^2 \delta^2 (1-z)} - \frac{2\mu V_1}{\hbar^2 \delta (1-z)} - \frac{\omega \hbar \mu}{2\delta^2} - \frac{\omega^2}{8\delta^2} \right] U_{nl} = 0 \quad (6)$$

where,

$$-\varepsilon = \frac{2\mu E}{\hbar^2 \delta^2} \quad (7)$$

$$\beta_1 = \frac{2\mu A_0}{\hbar^2 \delta^2} \quad (8)$$

$$\eta_1 = \frac{2\mu A_1}{\hbar^2 \delta} \quad (9)$$

$$\eta_2 = \frac{\omega \hbar \mu}{2\delta^2} \quad (10)$$

$$\beta_2 = \frac{\omega^2}{8\delta^2} \quad (11)$$

$$\lambda = \left(\frac{(D-1)(D-3)}{4} + l(l+D-2) \right) \quad (12)$$

$$\frac{d^2 U_{n,l}(z)}{dz^2} + \frac{(1-z)}{z(1-z)} \frac{dU_{n,l}}{dz} + \frac{1}{z^2(1-z)^2} [-\varepsilon(1-z)^2 + \beta_1(1-z)z + \eta_1(1-z) - \eta_2(1-z)^2 - \beta_2(1-z)^2 - \lambda] U_{nl} = 0 \quad (13)$$

This gives the hyper-geometric form written in Eq. (14) as:

$$\frac{d^2 U_{n,l}(z)}{dz^2} + \frac{(1-z)}{z(1-z)} \frac{dU_{n,l}}{dz} + \frac{1}{z^2(1-z)^2} [-(\varepsilon + \beta_1 + \eta_2 + \beta_2)z^2 + (2\varepsilon + \beta_1 - \eta_1 + 2\eta_2 + 2\beta_2)z - (\varepsilon - \rho + \delta + \eta + \vartheta + \chi + \lambda)] U_{nl} = 0 \quad (14)$$

Comparing Eq. (14) with the parametric form of the NU Equation (15) written below (Otete et al; 2024) as:

$$\varphi'' + \frac{y_1 - y_2 z}{z((1-y_3 z))} \varphi' + \left[\frac{-\zeta_1 z^2 + \zeta_2 z - \zeta_3}{z^2(1-y_3 z)^2} \right] \varphi_{(s)} = 0 \quad (15)$$

the following parameters can be found:

$$y_1 = y_2 = y_3 = 1, \quad y_4 = \frac{1}{2}(1 - y_1) = 0, \quad \zeta_1 = \varepsilon + \beta_1 + \eta_2 + \beta_2 \quad (16)$$

$$\zeta_2 = 2\varepsilon + \beta_1 - \eta_1 + 2\eta_2 + 2\beta_2 \quad (17)$$

$$\zeta_3 = \varepsilon - \eta_1 + \eta_2 + \beta_2 + \lambda \quad (18)$$

$$y_5 = \frac{1}{2}(y_2 - 2y_3) = -\frac{1}{2} \quad (19)$$

$$y_6 = y_5^2 + \zeta_1 = \frac{1}{4} + \varepsilon + \beta_1 + \eta_2 + \beta_2 \quad (20)$$

$$y_7 = 2y_4 y_5 - \zeta_2 = -(2\varepsilon + \beta_1 - \eta_1 + 2\eta_2 + 2\beta_2) \quad (21)$$

$$y_8 = y_4^2 + \zeta_3 = \varepsilon + \eta_2 + \beta_2 + \lambda \quad (22)$$

$$y_9 = y_3 y_7 + y_3^2 y_8 + y_6 = \frac{1}{4} + \eta_1 + \lambda \quad (23)$$

$$y_{10} = y_1 + 2y_4 + 2\sqrt{y_8} \quad (24)$$

$$y_{11} = y_2 - 2y_5 + 2(\sqrt{y_9} + y_3 \sqrt{y_8}) \quad (25)$$

$$y_{12} = y_4 + \sqrt{y_8} \quad (26)$$

$$y_{13} = y_5 - ((y_9)^{1/2} + y_3(y_8)^{1/2}) \quad (27)$$

The energy equation and the wave function are written as (Tezcan and Server, 2009):

$$y_{2n} - (2n+1) y_5 + (2n+1) [\sqrt{y_9} + y_3 \sqrt{y_8}] + n(n-1) y_3 + y_7 + 2y_3 y_8 + 2\sqrt{y_8 y_9} = 0 \quad (28)$$

$$\varphi_{(z)} = z^{y_{12}} (1 - y_3 z)^{-y_{12} - y_{13}/y_3} p_n^{y_{10}-1, y_{11}/y_3 - (y_{10}-1)} (1 - 2y_3 z) \quad (29)$$

In Eq. (7), $-\varepsilon = \frac{2\mu E}{\hbar^2 \delta^2}$, so by substituting Eq (16-23) into Eq. (28) and one performing little algebra, Eq. (30) is gotten as the eigen values equation:

$$E_{n,l} = -\frac{\hbar^2 \delta^2}{2\mu} \left\{ \left[\frac{(\rho-\alpha)}{2(n+\sqrt{\alpha})} + \frac{(n+\sqrt{\alpha})}{2} \right]^2 - \Lambda \right\} \quad (30)$$

where,

$$\Lambda = \eta_2 + \beta_2 + \lambda \quad (31)$$

$$\alpha = \frac{1}{4} + \eta_1 + \lambda \quad (32)$$

$$\rho = -\beta_1 + \eta_1 + 2\lambda \quad (33)$$

Eq. (24-27) are substituted into Eq. (29), the wave function will be gotten as:

$$\varphi_{(z)} = z^{\sqrt{\varepsilon+\eta_2+\beta_2+\lambda}} (1-z)^{\frac{1}{2}+\sqrt{\frac{1}{4}+\eta_1+\lambda}} p_n^{2\sqrt{\varepsilon+\eta_2+\beta_2+\lambda}, 2\sqrt{\frac{1}{4}+\eta_1+\lambda}} (1-2z) \quad (34)$$

3. RESULT AND DISCUSSION

3.1 Results

We use the Maple software to analyze our results. The eigen values of Eq. (32) are tabulated below.

Table 1. Energy eigenvalues of PbSe (in units of meV) for different values of n, l with $\hbar = 0.1 \mu = 0.114$, $\delta = 0.2$, $A_0 = 0.6$, $A_1 = 0.4$, $B = 0T$ for $D = 2, 3, 4$ and 5

n	l	D=2	D=3	D=4	D=5
0	0	-0.8482918785	-0.8403925850	-0.8172032420	-0.7801697560
1	0	-0.5823580105	-0.5769538475	-0.5610532185	-0.5355468175
2	0	-0.4051764191	-0.4012955524	-0.3898565634	-0.3714429765
	1	-0.3898565634	-0.3714429765	-0.3469431060	-0.3174448204
3	0	-0.2826336734	-0.2797415756	-0.2712047649	-0.2574240826
	1	-0.2712047649	-0.2574240826	-0.2390130726	-0.2167292472
	2	-0.2390130726	-0.2167292472	-0.1913991582	-0.1638498232
4	0	-0.1956961284	-0.1934781410	-0.1869234016	-0.1763176794
	1	-0.1869234016	-0.1763176794	-0.1621003222	-0.1448173606
	2	-0.1621003222	-0.1448173606	-0.1250698362	-0.1034657630

Table 2. Energy eigenvalues of PbSe (in units of meV) for different values of n, l with $\hbar = 0.1$ $\mu = 0.114$, $\delta = 0.2$, $A_0 = 0.6$ $A_1 = 0.4$, $B = 4T$ for $D=2, 3, 4$ and 5

n	l	D=2	D=3	D=4	D=5
0	0	-0.7595725805	-0.7516732870	-0.7284839440	-0.6914504580
1	0	-0.4936387123	-0.4882345491	-0.4723339202	-0.4468275193
2	0	-0.3164571209	-0.3125762542	-0.3011372651	-0.2827236782
	1	-0.3011372651	-0.2827236782	-0.2582238077	-0.2287255221
3	0	-0.1939143751	-0.1910222774	-0.1824854666	-0.1687047844
	1	-0.1824854666	-0.1687047844	-0.1502937744	-0.1280099490
	2	-0.1502937744	-0.1280099490	-0.1026798600	-0.07513052490
4	0	-0.1069768302	-0.1047588428	-0.09820410335	0.05609806230
	1	-0.09820410335	-0.08759838125	-0.07338102395	-0.01474646479
	2	-0.07338102398	-0.05609806230	-0.03635053790	-0.02911833679

Table 3: Energy eigenvalues of PbSe (in units of meV) for various values of n, l with $\hbar = 0.1$ $\mu = 0.114$, $\delta = 0.2$, $A_0 = 0.6$ $A_1 = 0.4$, $B = 8T$ for $D=2, 3, 4$ and 5

n	l	D=2	D=3	D=4	D=5
0	0	-0.4954146856	-0.4875153921	-0.4643260491	-0.4272925632
1	0	-0.2294808177	-0.2240766542	-0.2081760254	-0.1826696244
2	0	-0.05229922615	-0.04841835948	-0.03697937035	-0.01856578351
	1	-0.03697937035	-0.01856578351	0.005934087020	0.03543237263
3	0	-0.07024351965	0.07313561735	0.08167242805	0.09545311035
	1	-0.08167242805	0.09545311035	0.1138641204	0.1361479458
	2	-0.1138641204	0.1361479458	0.1614780348	0.1890273698
4	0	0.1571810646	0.1593990520	0.1659537914	0.1765595135
	1	0.1659537914	0.1765595135	0.1907768709	0.2080598324
	2	0.1907768709	0.2080598324	0.2278073568	0.2494114300

Table 4: Energy eigenvalues of PbSe (in units of meV) for various values of n, l with $\hbar = 0.1$ $\mu = 0.114$, $\delta = 0.4$, $A_0 = 0.6$ $A_1 = 0.4$, $B = 0T$ for $D=2, 3, 4$ and 5

n	l	D=2	D=3	D=4	D=5
0	0	-0.3090981838	-0.2992190888	-0.2708270676	-0.2272850794
1	0	-0.1475786928	-0.1414991752	-0.1239151154	-0.09661562575
2	0	-0.06321676280	-0.0591663365	-0.04739824518	-0.02896482790
	1	-0.04739824518	-0.02896482790	0.005353712575	0.02179962542
3	0	-0.02070079102	-0.01786490176	0.009596200935	0.09545311035
	1	-0.009596200935	0.003442254709	0.02030222496	0.1361479458
	2	0.02030222496	0.0399211774	0.06127202120	0.1890273698
4	0	-0.003600135131	-0.001557186982	0.004415407570	0.013882004444
	1	0.004415407570	0.01388200444	0.02621358433	0.04069508047
	2	0.02621358433	0.04069508047	0.05662202905	0.07336758785
	3	0.05662202905	0.07336758785	0.09041641930	0.1073720068

Here are the graphical plots represented in figure 1, 2 and 3 respectively.

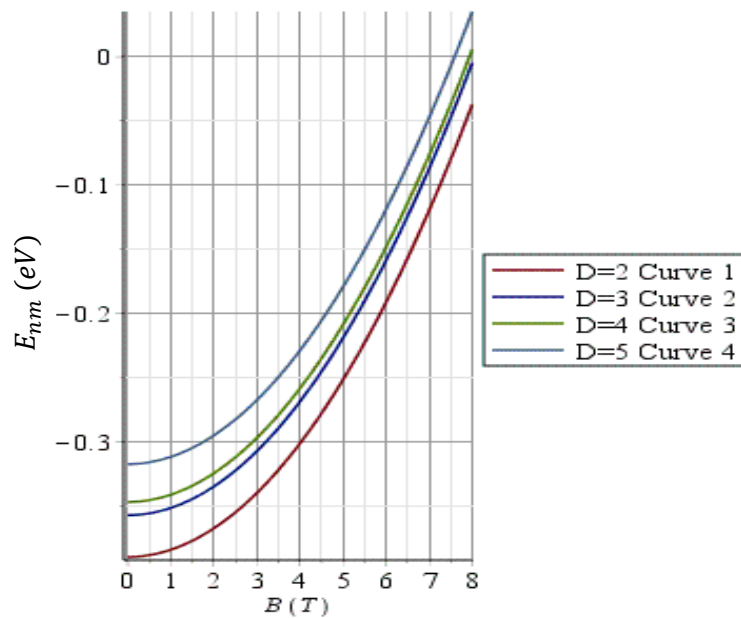


Figure 1: Energy, E versus magnetic field B

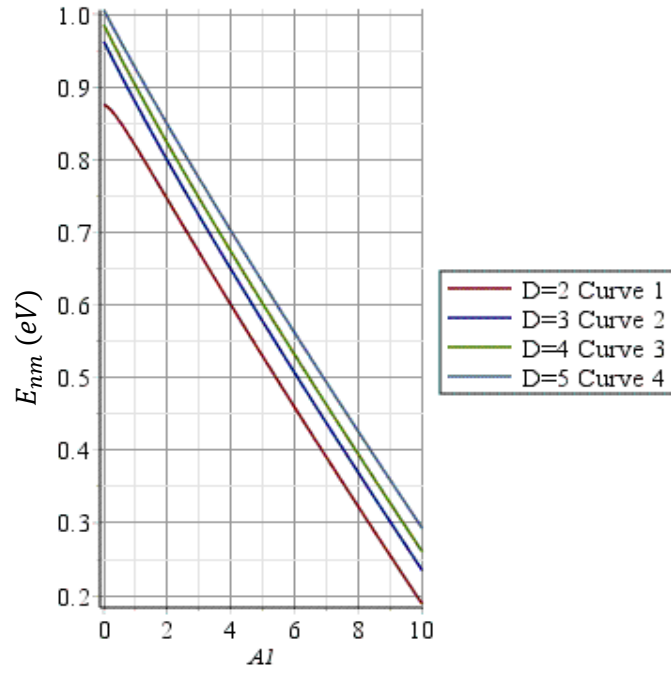


Figure 2: Energy, E versus Potential depth

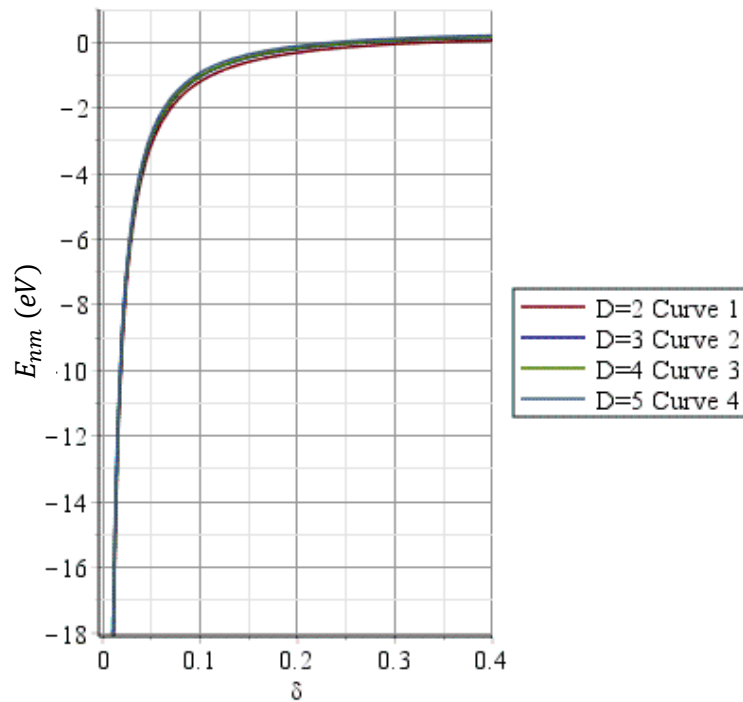


Figure 3: Energy, E against Screening Parameter

3.2 Discussion

For Lead Selenide (PbSe), the effective mass $\mu = 0.114m_o$, m_o is the bare electron mass. The potential depth A_1 is in meV. The magnetic field, B , is e in Tesla (T). From table 1-4, it is observed that as the applied magnetic field values are varied from 0T to 8T, and the screening parameter, δ is varied from 0.2 to 0.4, the energy eigenvalues are seen to increase and tend to be more positive down the table as the orbital quantum numbers are increasing and across the table where the dimensions are also increasing.

Figure 1 depicts the nature of the eigenvalues for various values of the magnetic field ranging from 0-8(T). It is observed that as the values of the magnetic field are increasing, the eigenvalues also rose for the various dimensions. In Figure 2, the energy eigenvalues are observed to decrease proportionally to the potential depth A_1 of the potential well. As the depth of the potential increases, the quantum confinement effect is weakened, thus, the energy eigen values is decreased [Harrison and Kittel (2016, 2005)]. Figure 3 depicts how the screening parameter δ behaves with the eigenvalues. The energy eigen values are seen to increase sharply from negative value towards positive value when the values of the screening parameter δ are between 0.02 to 0.05. It can be deduced that increasing the values of the screening parameter enhance the energy eigen values.

4. CONCLUSION

The energy eigen values have been studied for PbSe in the presence of applied magnetic field with the Hulthen-Yukawa potential in D-dimensions with the NU method. The energy equation and the wave function are gotten by solving the Schrödinger wave equation. The numerical energy eigenvalues are calculated with the help of Maple software and plots for energy eigen values against varying values of magnetic field, potential depth and screening parameter were presented. In the field of electronics and optoelectronics industry, the outcome of our research can be applied.

CONFLICT OF INTEREST

No conflict of interest was declared by the authors.

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