



Research article

Application of Schrödinger equation in quantum well of $\text{Cu}_2\text{ZnSnS}_4$ quaternary semiconductor alloyC.A. Onate^{a,*}, O. Ebomwonyi^b, D.B. Olanrewaju^a^a Department of Physical Sciences, Landmark University, Omu-Aran, Nigeria^b Department of Physics, University of Benin, Benin City, Nigeria

ARTICLE INFO

Keywords:

Quantum mechanics
Quantum well
Energy band gap
Supersymmetry
Schrödinger equation
Potential models

ABSTRACT

An approximate solution of the radial Schrödinger equation is obtained with a generalized group of potentials in the presence of both magnetic field and potential effect using supersymmetric quantum mechanics and shape invariance methodology. The energy bandgap of the generalized group of potentials was calculated for s – wave cases at the ground state. By varying the numerical values of the potential strengths, the energy band gap of Hellmann's potential and Coulomb-Hulthén potential respectively were obtained. It is noted that the inclusion of the potential effect greatly affects the accuracy of the results. Our calculated results are in agreement and better than the existing calculated results. The present results approximately coincide with the standard bandgap of $\text{Cu}_2\text{ZnSnS}_4$ (CZTS).

1. Introduction

Over the years, petroleum has been the wide source of energy generation in almost all the countries of the world. The use of petroleum products however has been reported to be harmful to human health due to hazardous by-products. Thus, the need for affordable and environmentally friendly sources of energy has greatly increased the interest in the study of renewable sources of energy. The most available and abundant source of renewable energy that is less harmful to human health is solar energy. Solar energy as a source of energy generation is known to have been using semiconductor materials. The semiconductor materials suitable for the effective conversion of solar energy have a minimum band gap of 1.3eV [1, 2, 3]. It has been observed that the effectiveness of the semiconductor materials can be improved by the combination of the materials. On this basis, Cadmium telluride (CdTe) and Copper indium gallium selenide (CIGS) was used as a buffer in thin-film solar cells with power conversion efficiencies of about 20% [4]. However, these compounds (CdTe and CIGS) are faced with high cost and unavailability for popular use. Thus, a recent study focuses on the use of $\text{Cu}_2\text{ZnSnS}_4$ (CZTS) as the thin-film solar cell material. This compound is known to have direct band gap energy between 1.4eV to 1.6eV [5, 6, 7] with an optical absorption coefficient of 10^{-4} cm^{-1} , which suggests a high use of the material for suitable photovoltaic. The use of this

compound was studied experimentally by Guo et al. [8] and Steinhagen et al. [9] with a result of 1.5eV and 1.3eV respectively. In Ref. [10, 11, 12], it was calculated using the first principle method. These authors have result of 0.86eV, 1.06eV and 1.48eV respectively. However, the experimental results though in fair agreement with the calculated results, are better than the calculated results so far. Recently, Ejere and Ebomwonyi [13], calculated the energy band gap of $\text{Cu}_2\text{ZnSnS}_4$, using parametric Nikiforov-Uvarov method in the presence of a magnetic field with a Hylleraas type of potential. Though their result agreed with the existing result, their calculations were faulty. In all the studies, no result is approximately equal to the maximum band gap of $\text{Cu}_2\text{ZnSnS}_4$.

Thus, further study on the energy band gap for this compound is required to obtain a result that is approximately equal to the maximum band gap of 1.6eV. In this study, we intend to calculate the energy band gap of the same compound under a group of physical potential functions by solving the radial Schrödinger equation for any ℓ – state using the elegant methodology of supersymmetric quantum mechanics. To have a better result in this study, we intend to include a potential effect in addition to the magnetic field which no author has studied yet. Our choice of potential is the interaction of different types of potential models known as a generalized group of potentials. The generalized group of potentials is of the form:

* Corresponding author.

E-mail addresses: oaclms14@physicist.net, onate.clement@lmu.edu.ng (C.A. Onate).

$$V(r) = -\frac{H_1}{r} - \frac{H_2 e^{-\delta r}}{r} - \frac{H_3 e^{-\delta r}}{1 - e^{-\delta r}} + \frac{H_4}{(1 - e^{-\delta r})^2} \tag{1}$$

where $H_1 = \lambda_1 (2\delta)^{-1} e^{\delta r}$, $H_2 = \lambda_2 (2\delta)^{-1} e^{\delta r}$ and H_i ($i = 1, 2, 3, 4$) characterised the strength of the potential, r is the internuclear distance and δ is the screening parameter. The screening parameter can easily change the form of the potential as it tends to zero. The generalized group of potentials has a different subset. For instance, when $\delta \rightarrow 0$, potential (1) turns to multiple constant and Coulomb potential of the form:

$$V(r) = H_4 - H_3 + \frac{H_1 - H_2}{r} \tag{2}$$

By varying the numerical values of the potential strengths, the following potentials, Coulomb, Yukawa, Hulthén, and Hellmann potentials can be obtained. These potentials however have wide applications in different areas of physics. The main reason for choosing this potential is that the energy band gap of other potentials can easily be obtained by changing the numerical values of the potential strength without undergoing the tedious calculation any more as will be seen in the discussion section. It also gives wider applications different potentials are its subset. For instance, Yukawa potential has been used to describe the nuclear interaction between protons and neutrons due to pion exchange [14, 15, 16, 17, 18, 19]. It was also used to stabilize the local fluid structure that provides a good expression for the free energy and the pair correlation function for a system [14]. Similarly, Hulthén potential is an important molecular potential that has been used extensively to describe the molecular structure of an atom and nuclear interaction [20, 21]. These potentials are widely used in nuclear and particle physics, atomic physics, condensed matter physics, chemical, and solid-state physics.

2. Schrödinger equation and the generalized group of potential models

The Schrödinger equation with spherically symmetric potential and non-relativistic energy $E_{n\ell}$ for $\ell \neq 0$ takes the form [22, 23].

$$\left[-\frac{\hbar^2}{2m} \nabla_D^2 + V(r) - E_{n\ell} \right] \psi_{D\ell m}(r, \theta, \varphi) = 0, \tag{3}$$

where the representation of the Laplacian operator ∇_D^2 in spherical coordinates is

$$\nabla_D^2 = \frac{\partial^2}{\partial r^2} + \frac{(D-1)}{r} \frac{\partial}{\partial r} - \frac{\ell(\ell+D-2)}{r^2} \tag{4}$$

Setting the wave function $\psi_{D,\ell,m}(r, \theta, \varphi) = r^{-(D-1)/2} R(r) Y_\ell^m(\theta, \varphi)$, Eq. (3) becomes

$$\frac{d^2 R_{n\ell}(r)}{dr^2} + \frac{2m}{\hbar^2} \left[E_{n\ell} - V(r) - \frac{l(l+1)\hbar^2}{2mr^2} \right] R_{n\ell}(r) = 0 \tag{5}$$

Eq. (5) and Eq. (1) contained a term of centrifugal barrier in each case which does not admit the solution of $\ell = 0$, though, the computation must be done at the ground state for $\ell = 0$. To address this issue, the equation is solved for any n and ℓ by considering the potential effect. The values of n and ℓ respectively are put to zero during numerical computation. Thus, the presence of the centrifugal term resorts to the use of a suitable approximation scheme to deal with the centrifugal term. For a short-range potential, Dong et al. [24, 25, 26], suggested the following as the suitable approximation scheme to the centrifugal term $\frac{1}{r^2}$ for potential (1)

$$\frac{1}{r^2} \approx \frac{4\delta^2 e^{-2\delta r}}{(1 - e^{-\delta r})^2} \tag{6}$$

The main aim of this work is to calculate the energy band gap of CZTS using the parameters of the semiconductor materials such as the

cyclotron frequency ω_c and the potential effect μ_{pe} on the system. Substituting Eqs. (1) and (6) together with the cyclotron frequency and the potential effect into Eq. (5), we have

$$\frac{d^2 R_{n\ell}(r)}{dr^2} = \left[\frac{V_T e^{-\delta r} - \frac{2m\lambda_1}{\hbar^2}}{1 - e^{-\delta r}} + \frac{4\ell(\ell+1)\delta^2 e^{-2\delta r} + \frac{2mH_4}{\hbar^2}}{(1 - e^{-\delta r})^2} + E_{eff} \right] R_{n\ell}(r), \tag{7}$$

where

$$E_{eff} = -\frac{2mE_{n\ell}}{\hbar^2} + \frac{2m\lambda_1}{\hbar^2} + \frac{m\omega_c}{2} \left(\frac{\omega_c}{4} - \frac{4\mu_{pe}}{\omega_c \hbar^2} \right), \tag{8}$$

$$V_T = m\omega_c \delta \hbar - \frac{2m(\lambda_2 + H_3)}{\hbar^2} \tag{9}$$

$$\omega_c = qBm^{-1} \tag{10}$$

for mathematical simplicity with B as magnetic field and q as particle charge and μ_{pe} is the mean of the potential strengths. In this work, we are going to solve Eq. (7) using the methodology of supersymmetry quantum mechanics. Supersymmetric quantum mechanics (SUSY QM) is a powerful tool for generating new potentials with known spectra departing from an initial solvable one. In 1983, shape invariant potential (SIP) was introduced in SUSY QM by Gendenshten [27]. For any shape invariant potential, the energy bound state spectra could be obtained algebraically. The formalism of SUSY QM plus shape invariance was intimately connected to the factorization method [28]. The bound state solutions, the energy eigenfunctions, and the scattering matrix can easily be obtained for the generalized operator method for such potentials. This approach is equivalent to Schrödinger's method of factorization [28, 29]. If the partner potential $V_{\alpha,\beta}(x, a_1)$ satisfies the condition.

$V_\alpha(x, a_0) = V_\beta(x, a_1) + R(a_1)$, where a_0 is a set of old parameters, a_1 is a function of a_0 (i.e $a_1 = f(a_0)$) and $R(a_1)$, is the remainder which does not depend on x , the partner potentials $V_\alpha(x, a_0)$ and $V_\beta(x, a_1)$ are invariant. From the condition of the shape invariance, and the hierarchy of the Hamiltonians, it is easy to obtain the energy eigenvalues and the eigenfunctions of any shape invariant potential. In other to proceed with this method, we first propose a superpotential function which is the solution of the differential equation of Eq. (7). However, the proposition of the superpotential function is based on the potential function under consideration [30]. Considering our generalized group of potential models in Eq. (1), we propose a superpotential function of the form:

$$W(r) = \lambda_A + \frac{\lambda_B e^{-\delta r}}{1 - e^{-\delta r}}, \tag{11}$$

where λ_A and λ_B are superpotential constants that will soon be determined. To fully apply the basic concepts of supersymmetry quantum mechanics formalism and shape invariance approach [31, 32, 33, 34, 35] to solve Eq. (7), the ground state function is related to the superpotential function as

$$R_{0,\ell}(r) = e^{-\int W(r) dr} \tag{12}$$

The $W(r)$ has been given in Eq. (11) above. The superpotential function of Eq. (11) relates to a non-linear Riccati equation as

$$W^2(r) - \frac{dW(r)}{dr} = \frac{V_T e^{-\delta r} - \frac{2m\lambda_1}{\hbar^2} e^{-2\delta r} - \frac{2m\lambda_1}{\hbar^2}}{1 - e^{-\delta r}} + \frac{4\ell(\ell+1)\delta^2 e^{-2\delta r} + \frac{2mH_4}{\hbar^2}}{(1 - e^{-\delta r})^2} + E_{eff} \tag{13}$$

Substituting Eq. (11) into Eq. (13) and by comparison, the superpotential parameters of Eq. (11) can be deduced in the following form:

$$\lambda_A^2 = E_{ff} \tag{14}$$

$$\lambda_B = \frac{\delta \left(1 \pm \sqrt{1 + 16\ell(\ell + 1) + \frac{8mH_4}{\delta^2 \hbar^2}} \right)}{2} \tag{15}$$

$$\lambda_A = \frac{\frac{2m(H_4 + \lambda_1 - H_3 - \lambda_2)}{\hbar^2} + m\omega_c \delta \hbar + \lambda_B^2}{2\lambda_B} \tag{16}$$

In terms of the superpotential function $W(r)$, we can construct the supersymmetric partner potentials $V_{\pm}(r) = W^2(r) \pm \frac{dW(r)}{dr}$ as follows:

$$V_+(r) = W^2(r) + \frac{dW(r)}{dr} = \lambda_A^2 + \frac{\lambda_B(2\lambda_A - \lambda_B)e^{-\delta r}}{1 - e^{-\delta r}} + \frac{\lambda_A(\lambda_A - \delta)e^{-\delta r}}{(1 - e^{-\delta r})^2} \tag{17}$$

$$V_-(r) = W^2(r) - \frac{dW(r)}{dr} = \lambda_A^2 + \frac{\lambda_B(2\lambda_A - \lambda_B)e^{-\delta r}}{1 - e^{-\delta r}} + \frac{\lambda_A(\lambda_A + \delta)e^{-\delta r}}{(1 - e^{-\delta r})^2} \tag{18}$$

Putting $\lambda_B = a_0$, we can easily show that Eqs. (17) and (18) satisfied the shape invariance condition and formalism, thus, the following relationship can be established

$$V_+(r, a_0) = V_-(r, a_1) + R(a_1) \tag{19}$$

where a_1 is a new set of parameter uniquely determine from an old set of parameter a_0 i.e. $a_1 = f(a_0) = \lambda_B - \delta$. The residual term $R(a_1)$ also known as the remainder, is independent of the variable r . The remainder term also satisfies the relation

$$R(a_1) = \left(\frac{-V_T - a_0^2 - \frac{2m\lambda_1}{\hbar^2}}{2a_0} \right) - \left(\frac{-V_T - a_1^2 - \frac{2m\lambda_1}{\hbar^2}}{2a_1} \right) \tag{20}$$

$$R(a_2) = \left(\frac{-V_T - a_1^2 - \frac{2m\lambda_1}{\hbar^2}}{2a_1} \right) - \left(\frac{-V_T - a_2^2 - \frac{2m\lambda_1}{\hbar^2}}{2a_2} \right) \tag{21}$$

$$R(a_3) = \left(\frac{-V_T - a_2^2 - \frac{2m\lambda_1}{\hbar^2}}{2a_2} \right) - \left(\frac{-V_T - a_3^2 - \frac{2m\lambda_1}{\hbar^2}}{2a_3} \right) \tag{22}$$

$$R(a_{n-1}) = \left(\frac{-V_T - a_{n-2}^2 - \frac{2m\lambda_1}{\hbar^2}}{2a_{n-2}} \right) - \left(\frac{-V_T - a_{n-1}^2 - \frac{2m\lambda_1}{\hbar^2}}{2a_{n-1}} \right) \tag{23}$$

$$R(a_n) = \left(\frac{-V_T - a_{n-1}^2 - \frac{2m\lambda_1}{\hbar^2}}{2a_{n-1}} \right) - \left(\frac{-V_T - a_n^2 - \frac{2m\lambda_1}{\hbar^2}}{a_n} \right) \tag{24}$$

Thus, the energy spectra of the negative partner potential $V_-(r)$ can be determined by using the shape invariance approach [36, 37].

$$E_{n\ell}^- = \sum_k^n R(a_k) = \left(\frac{-V_T - a_0^2 - \frac{2m\lambda_1}{\hbar^2}}{a_0} \right) - \left(\frac{-V_T - a_n^2 - \frac{2m\lambda_1}{\hbar^2}}{2a_n} \right) \tag{25}$$

$$E_{n\ell} = E_{n\ell}^- + E_{0\ell} = - \left(\frac{-V_T - a_n^2 - \frac{2m\lambda_1}{\hbar^2}}{2a_n} \right) \tag{26}$$

For the consideration of the negative partner potential, $E_{0\ell} = 0$, and thus, the total energy spectra of the system becomes

$$E_{n\ell} = \lambda_1 + \frac{\omega_c^2 \hbar^2}{16} - \mu_{pe}$$

$$\left[\frac{\delta^2 \hbar^2}{2m} \frac{\frac{2m}{\delta^2 \hbar^2} (H_4 + \lambda_1 - H_3 - \lambda_2) + \frac{m\omega_c}{\delta}}{1 + 2n + \sqrt{1 + 16\ell(\ell + 1) + \frac{8mH_4}{\delta^2 \hbar^2}}} \right]^2 \frac{1 + 2n + \sqrt{1 + 16\ell(\ell + 1) + \frac{8mH_4}{\delta^2 \hbar^2}}}{2} \tag{27}$$

To obtain the wave function, we first define $y = e^{-\delta r}$, and then substitute it into Eq. (7) to have

$$\left[\frac{d^2}{dr^2} + \frac{1}{y} \frac{d}{dr} + \frac{\alpha y^2 + \beta s + \gamma}{y^2(1 - y)^2} \right] R_{n,\ell}(y) = 0, \tag{28}$$

where

$$\alpha = \frac{2m(E_{n,\ell} + \mu_{pe} - \lambda_2 - H_3)}{\delta^2 \hbar^2} - \frac{m\omega_c \hbar}{\delta} + \frac{m\omega_c^2}{8\delta^2} + 4\ell(\ell + 1), \tag{29}$$

$$\beta = \frac{2m(\lambda_2 + H_3 - 2E_{n,\ell} + 2\mu_{pe} - \lambda_1)}{\delta^2 \hbar^2} - \frac{m\omega_c \hbar}{\delta} + \frac{m\omega_c^2}{4\delta^2}, \tag{30}$$

$$\gamma = \frac{2m(E_{n,\ell} + \mu_{pe} + \lambda_1 - H_4)}{\delta^2 \hbar^2} - \frac{m\omega_c^2}{8\delta^2}. \tag{31}$$

Analysing the asymptotic behaviour of Eq. (28) at origin and at infinity, it can be tested that when $r \rightarrow 0$ and $r \rightarrow \infty$, Eq. (28) has the solution of the form $R_{n,\ell}(y) = y^\phi$ and $R_{n,\ell}(y) = (1 - y)^\gamma$. Now, taking a trial wave function of the form

$$R_{n,\ell}(y) = y^\phi (1 - y)^\gamma f(y), \tag{32}$$

and substitute this into Eq. (28), we have

$$f''(y) + \left(\frac{2\Phi + 1 - (2\Phi + 2\Upsilon + 1)y}{y(1 - y)} \right) f'(y) - \left(\frac{(\Phi + \Upsilon)^2 + \alpha}{y(1 - y)} \right) f(y) = 0, \tag{33}$$

where

$$\Phi = \left(\frac{2m(H_4 - E_{n,\ell} - \mu_{pe} - \lambda_1)}{\delta^2 \hbar^2} + \frac{m\omega_c^2}{8\delta^2} \right)^{\frac{1}{2}}, \tag{34}$$

$$\Upsilon = \frac{1}{2} + \left(1 + 16\ell(\ell + 1) + \frac{2mH_4}{\delta^2 \hbar^2} \right)^{\frac{1}{2}}. \tag{35}$$

Further analysis/simplification gives a complete wave function as

$$R_{n,\ell}(y) = N_{n,\ell} y^\phi (1 - y)^\gamma {}_2F_1(-n, n + 2\Phi + 2\Upsilon; 2\Phi + 1, y) \tag{36}$$

3. Numerical computation of results and discussion

In other to obtain the energy band gap, we input the values of the following parameters, $\lambda_1 = \lambda_2 = H_4 = 2.10$, $H_3 = H_4 + 0.96$, $m = m_0^2(m_1 m_2)/(m_1 + m_2)m_0$, $m_1 = 0.185$, $m_2 = 0.26$, $B = 10$, $\varepsilon = 5.06$ and $n = \ell = 0$. These values were inputted into Eq. (27), and run with MATLAB 7.5.0. The m_0 is the free electronic mass and m is the effective mass of the compound. The graph of the energy for the ground state and the first two excited states against the screening parameter is shown in Figure 1.

Special cases of the generalized potential models.

- (i) Hellmann-like potential. This is potential is obtained when we put $H_3 = H_4 = 0$ in Eq. (1).

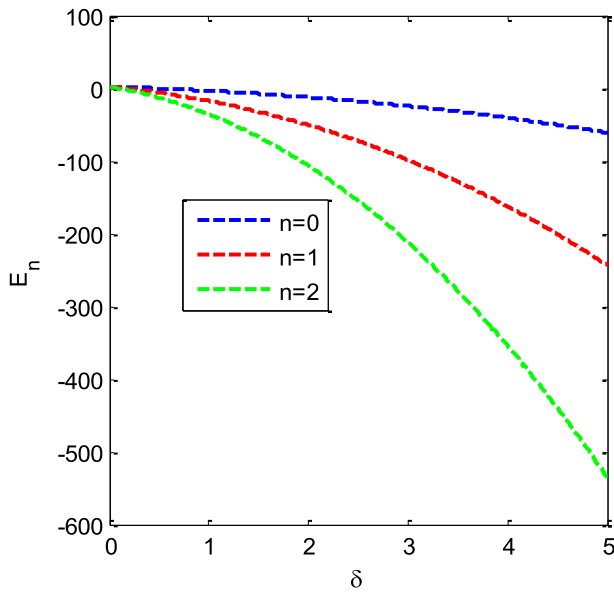


Figure 1. Variation of the energy for the generalized group potential model with the screening parameter in the presence of the cyclotron frequency and potential effect.

$$V(r) = -\frac{\lambda_1 \delta^{-1}}{r} - \frac{\lambda_2 \delta^{-1} e^{-\delta r}}{r} \tag{37}$$

The energy Eq. (27) reduces to

$$E_{n\ell} = \lambda_1 + \frac{\omega_c^2 \hbar^2}{16} - \mu_{pe} - \frac{\delta^2 \hbar^2}{2m} \left[\frac{\frac{2m}{\delta^2 \hbar^2} (\lambda_1 - \lambda_2) + \frac{m\omega_c}{\delta}}{1 + 2n + \sqrt{1 + 16\ell(\ell + 1)}} - \frac{1 + 2n + \sqrt{1 + 16\ell(\ell + 1)}}{2} \right]^2 \tag{38}$$

The graph of energy against the screening parameter is shown in Figure 2.

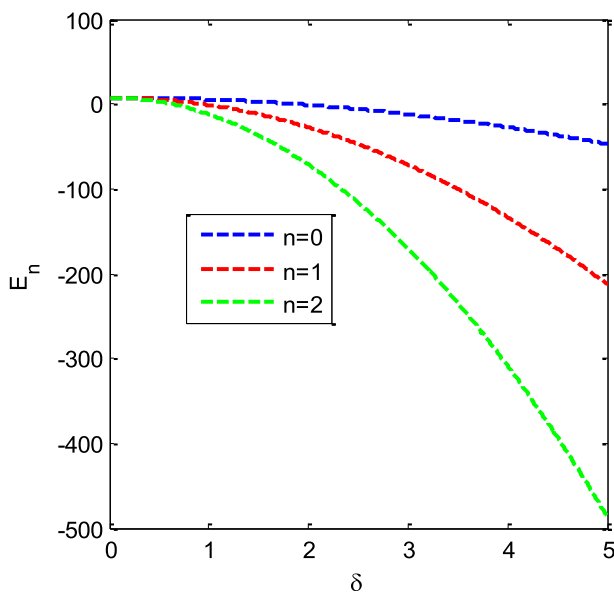


Figure 2. Variation of the energy for Hellmann's potential model with the screening parameter in the presence of the cyclotron frequency and potential effect.

(ii) Coulomb-Hulthén potential. When we put $H_2 = H_3 = 0$, potential (1) reduces to Coulomb-Hulthén potential of the form

$$V(r) = -\frac{\lambda_1 \delta^{-1}}{r} - \frac{H_3 e^{-\delta r}}{1 - e^{-\delta r}} \tag{39}$$

The energy equation then becomes

$$E_{n\ell} = \lambda_1 + \frac{\omega_c^2 \hbar^2}{16} - \mu_{pe} - \frac{\delta^2 \hbar^2}{2m} \left[\frac{\frac{2m}{\delta^2 \hbar^2} (\lambda_1 - H_3) + \frac{m\omega_c}{\delta}}{1 + 2n + \sqrt{1 + 16\ell(\ell + 1)}} - \frac{1 + 2n + \sqrt{1 + 16\ell(\ell + 1)}}{2} \right]^2 \tag{40}$$

(iii) Yukawa-Hulthén Potential. Potential (1) turns to Yukawa-Hulthén potential when $H_1 = H_4 = 0$ which is physically given as

$$V(r) = -\frac{\lambda_2 \delta^{-1} e^{-\delta r}}{r} - \frac{H_3 e^{-\delta r}}{1 - e^{-\delta r}} \tag{41}$$

The energy is given as

$$E_{n\ell} = \frac{\omega_c^2 \hbar^2}{16} - \mu_{pe} - \frac{\delta^2 \hbar^2}{2m} \left[\frac{\frac{2m}{\delta^2 \hbar^2} (-H_3 - \lambda_2) + \frac{m\omega_c}{\delta}}{1 + 2n + \sqrt{1 + 16\ell(\ell + 1)}} - \frac{1 + 2n + \sqrt{1 + 16\ell(\ell + 1)}}{2} \right]^2 \tag{42}$$

(iv) Yukawa potential: Putting $H_1 = H_3 = H_4$ in Eq. (1), we obtain Yukawa potential of the form:

$$V(r) = -\frac{\lambda_2 \delta^{-1} e^{-\delta r}}{r} \tag{43}$$

The energy equation of Eq. (27) turns to be

$$E_{n\ell} = \frac{\omega_c^2 \hbar^2}{16} - \mu_{pe} - \frac{\delta^2 \hbar^2}{2m} \left[\frac{\frac{-2m\lambda_2}{\delta^2 \hbar^2} + \frac{m\omega_c}{\delta}}{1 + 2n + \sqrt{1 + 16\ell(\ell + 1)}} - \frac{1 + 2n + \sqrt{1 + 16\ell(\ell + 1)}}{2} \right]^2 \tag{44}$$

The variation of energy in Eq. (44) against the screening parameter is shown in Figure 3.

(v) Coulomb potential. This potential is obtained from potential (1) when $H_2 = H_3 = H_4 = 0$. The physical form of the Coulomb potential is given below

$$V(r) = -\frac{\lambda_1 \delta^{-1}}{r} \tag{45}$$

Its energy equation obtained from Eq. (27) is

$$E_{n\ell} = \lambda_1 + \frac{\omega_c^2 \hbar^2}{16} - \mu_{pe} - \frac{\delta^2 \hbar^2}{2m} \left[\frac{\frac{2m\lambda_1}{\delta^2 \hbar^2} + \frac{m\omega_c}{\delta}}{1 + 2n + \sqrt{1 + 16\ell(\ell + 1)}} - \frac{1 + 2n + \sqrt{1 + 16\ell(\ell + 1)}}{2} \right]^2 \tag{46}$$

The graph of the energy of Coulomb potential against the screening parameter is shown in Figure 4.

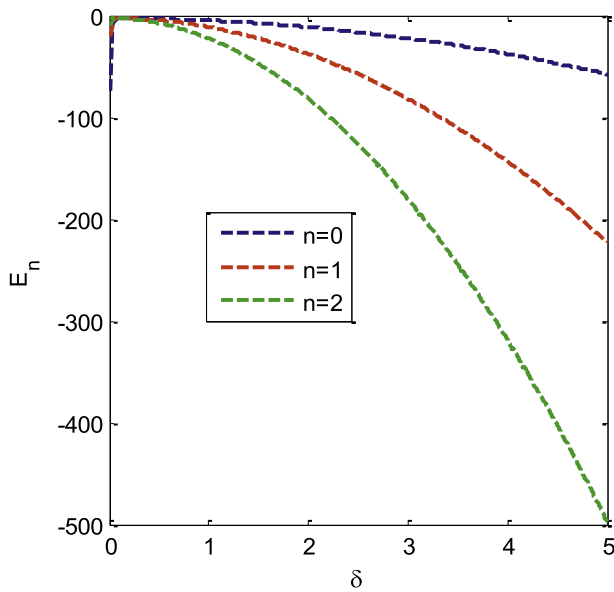


Figure 3. Variation of the energy for Yukawa potential model with the screening parameter in the presence of the cyclotron frequency and potential effect.

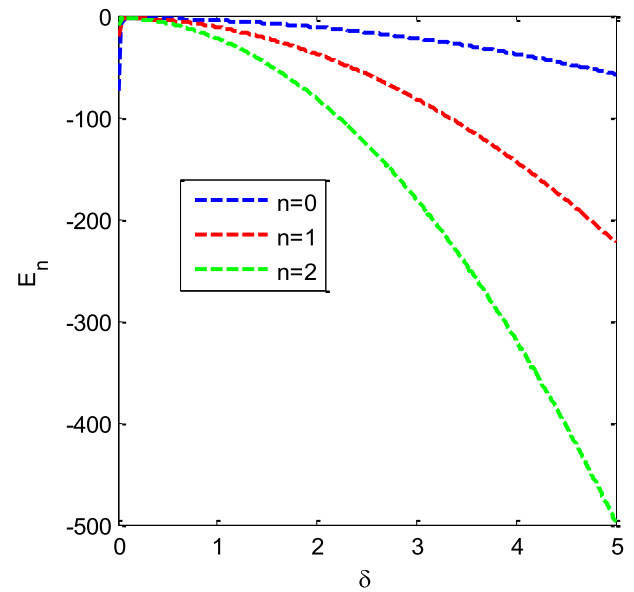


Figure 5. Variation of the energy for Hulthén potential model with the screening parameter in the presence of the cyclotron frequency and potential effect.

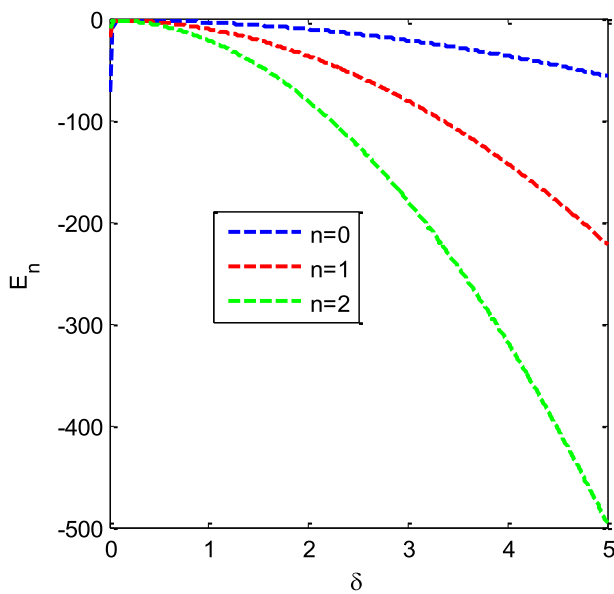


Figure 4. Variation of the energy for the Coulomb potential model with the screening parameter in the presence of the cyclotron frequency and potential effect.

The variation of energy of the Hulthén potential against the screening parameter is shown in Figure 5. In the Figures, an increase in the screening parameter decreases the energy. The decrease is more pronounced as the quantum number increases.

In Table 1, we presented a comparison of the present results and the existing results. It can be seen that the present results for each of the three potentials are in excellent agreement with the existing results. However, the present results seem better than the existing results as it is closer to the maximum band gap of the compound. This is because the potential effect has been considered in the present study. In Table 2, we presented the energy band gap of Cu₂ZnSnS₄ with the presence and absence of a potential effect. As it can be seen from the Table, the presence of potential effect decreases the energy band gap. Similarly, an increase in the potential effect results to decrease in the band gap. Table 3 presents the energy band gap of three different potentials with various quantum and angular momentum quantum number *n* and *ℓ* for four values of the potential effect. It is seen that the energy band gaps for generalized group potential are different from that of the Hellmann and Coulomb-Hulthén potentials. This is because the potential has been reduced and as such the potential effect has also been reduced. In Figures 1, 2, 3, 4, and 5, we examined the variation of the energy band gap with the screening parameter for a generalized group of potential, Hellmann-like potential, Yukawa-like potential, Coulomb-like potential, and Hulthén-like potential respectively. In each case, the energy band gap decreases as the screening parameter increases. This indicates that as the screening parameter increases, the energy band gap becomes narrower. Thus, at a very large value of the screening parameter, the energy band gap becomes too narrow and hence, reduces its efficiency and its effectiveness.

(vi) Hulthén potential. Hulthén potential is obtained when $H_1 = H_2 = H_4 = 0$ in Eq. (1)

$$V(r) = -\frac{H_3 e^{-\delta r}}{1 - e^{-\delta r}} \tag{47}$$

Its energy equation obtained from Eq. (27) is

$$E_{n\ell} = \frac{\omega_c^2 \hbar^2}{16} - \mu_{pe} - \frac{\delta^2 \hbar^2}{2m} \left[\frac{-\frac{2mH_3}{\delta^2 \hbar^2} + \frac{m\omega_c}{\delta}}{1 + 2n + \sqrt{1 + 16\ell(\ell + 1)}} - \frac{1 + 2n + \sqrt{1 + 16\ell(\ell + 1)}}{2} \right]^2 \tag{48}$$

4. Conclusion

The energy band gap of Cu₂ZnSnS₄ calculated from the solution of the *s* – wave Schrödinger equation at the ground state for three different potentials are in excellent agreement with existing results. The present results are better to compare to the already existing results since the present results are closer to the maximum band gap of Cu₂ZnSnS₄. It is noted that the potential effect greatly affects the accuracy of the energy band gap when combining different potentials. Our results also showed that the more potential combined, the smaller the value of the potential

Table 1. Comparison of present results with the existing results for the energy band gap (ineV) of Cu₂ ZnSnS₄.

Present results for three different potentials			[8]	[9]	[10]	[11]	[12]	[13]
$\mu = 2.34$	Generalized group potentials	1.58	1.5	1.3	1.06	1.48	0.86	1.5
$\mu = 8.22$	Hellmann potential	1.56						
$\mu = 8.22$	Coulomb-Hulthén potential	1.56						

Table 2. Energy band gap (ineV) of Cu₂ ZnSnS₄ in the presence and absence of a potential effect.

μ	n	ℓ	Presence of potential field		Absence of potential field	
			Gen. grp. pt.	Hellmann	Gen. grp. pt.	Hellmann
0.5	0	0	3.423794104	9.478031223	3.923794104	9.978031223
	0	1	3.254006353	9.250164886	3.754006353	9.750164886
	0	2	2.913544902	8.853581280	3.413544902	9.353581280
	1	0	2.493259124	9.412124892	2.993259124	9.912124892
	1	1	2.314012233	9.080026316	2.814012233	9.580026316
	1	2	1.954993406	8.593276364	2.454993406	9.093276364
	2	0	1.512495176	9.302281006	2.012495176	9.802281006
	2	1	1.323990938	8.865950191	1.823990938	9.365950191
	2	2	.9467899471	8.289033894	1.446789947	8.789033894

Table 3. Energy bandgap (ineV) of Cu₂ ZnSnS₄ for three different potentials studied with various n, ℓ for four values of the potential effect.

μ	n	ℓ	Generalized group potential	Hellmann potential	Coulomb-Hulthen Potential
0.5	0	0	3.423794104	9.478031223	9.478031223
1.0			2.923794104	8.978031223	8.978031223
1.5			2.423794104	8.478031223	8.478031223
2.0			1.923794104	7.978031223	7.978031223
0.5	0	1	3.254006353	9.250164886	9.250164886
1.0			2.754006353	8.750164886	8.750164886
1.5			2.254006353	8.250164886	8.250164886
2.0			1.754006353	7.750164886	7.750164886
0.5	1	1	2.314012233	9.080026316	9.080026316
1.0			1.814012233	8.580026316	8.580026316
1.5			1.314012233	8.080026316	8.080026316
2.0			0.814012234	7.580026316	7.580026316
0.5	1	2	1.954993406	8.593276364	8.593276364
1.0			1.454993406	8.093276364	8.093276364
1.5			0.954993406	7.593276364	7.593276364
2.0			0.454993406	7.093276364	7.093276364

effect that leads to accuracy. Thus, for the first time, a potential effect is considered in the calculation, a better result is obtained.

Declarations

Author contribution statement

C.A. Onate: Conceived and designed the analysis; Analyzed and interpreted the data; Contributed analysis tools or data; Wrote the paper.
 O.Ebomwonyi: Analyzed and interpreted the data; Wrote the paper.
 D.B. Olanrewaju: Contributed analysis tools or data; Wrote the paper.

Funding statement

This work was supported by Landmark University, Omu-Aran.

Competing interest statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

References

- [1] N.K. Allouche, T.B. Nasar, N.T. Kamoun, C. Guash, Synthesis and properties of chemical bath deposited ZnS multilayer films, Mater. Chem. Physica 624 (2010) 620–624.
- [2] H. Panahi, S. Golshahi, M. Doostdar, Influence of position dependent effective mass on donor binding energy in square and V-shape quantum wells in the presence of a magnetic field, Physics B 418 (2013) 47–51.
- [3] Z. Zongyan, Z. Xiang, Electronic, optical and mechanical properties of Cu₂ZnSnS₄ with four crystal structures, J. Semiconduct. 36 (2015) 45–49.
- [4] I. Repins, M.A. Contreras, B. Egaas, C. Dehart, J. Scharf, C.L. Pikeris, B. To, R. Noufi, 19.9%-efficient ZnO/CdS/CuInGaSe₂ solar cell with 81.2% fill factor, Prog. Photovoltaics Res. Appl. 16 (2008) 235–239.
- [5] H. Katagiri, K. Saitoh, T. Washio, H. Shinohara, T. Kurumadani, S. Miyajima, Development of thin film solar cell based on Cu₂ZnSnS₄. Thin Films Si, Energy Mater. Sol. Cells 65 (2001) 141.
- [6] T. Tanaka, T. Nagatomo, D. Kawasaki, M. Nishio, Q. Guo, A. Wakahala, A. Yoshida, H. Ogawa, Preparation of Cu₂ZnSnS₄ thin films by hybrid sputtering, J. Phys. Chem. Solid. 66 (2005) 1978.

- [7] J.S. Soel, S.Y. Lee, J.C. Lee, H.D. Nam, K.H. Kim, Electrical and optical properties of $\text{Cu}_2\text{ZnSnS}_4$ thin films prepared by rf magnetron sputtering process, *Sol. Energy Mater. Sol. Cells* 65 (2003) 155–162.
- [8] Q. Guo, H.W. Hillhouse, R. Agrawal, Synthesis of $\text{Cu}_2\text{ZnSnS}_4$ nanocrystal ink and its use for solar cells, *J. American Chem. Soc.* 131 (2009) 11672.
- [9] C. Steinhagan, M.G. Panthani, V. Akhavan, Synthesis of $\text{Cu}_2\text{ZnSnS}_4$ nanocrystals for use in low-cost photovoltaics, *J. American Chem. Soc.* 131 (2009) 12554.
- [10] H. Katagiri, N. Sasagushi, S. Hando, Preparation and evaluation of $\text{Cu}_2\text{ZnSnS}_4$ thin films by sulfurization of E-B evaporated precursors, *Sol. Energy Mater. Sol. Cell.* 49 (1997) 407.
- [11] J. Paier, R. Asahi, A. Nagoya, $\text{Cu}_2\text{ZnSnS}_4$ as a potential photovoltaic material: a hybrid Hartree-Fock density functional theory study, *Phys. Rev. B* 79 (2009) 115126.
- [12] S. Batti, D. Kammerlander, M.A.L. Marques, Band structures $\text{Cu}_2\text{ZnSnS}_4$ and $\text{Cu}_2\text{ZnSnS}_4$ from many-body methods, *Appl. Phys. Lett.* 98 (2011) 241915.
- [13] A.L.I. Ejere, O. Ebomwonyi, Hylleraas potential quantum well in $\text{Cu}_2\text{ZnSnS}_4$ quaternary semiconductor alloy in the presence of magnetic field, *Mater. Res. Express* 6 (2019).
- [14] Y. Kadiri, R. Albaki, J.L. Bretonnet, Thermodynamic equivalence between the Lennard-Jones and hard-core attractive Yukawa systems, *Chem. Phys.* 352 (2008) 135–141.
- [15] N. Farzi, S. Hoseini, Study some known regularities for hard core one Yukawa and hard core double Yukawa fluids, *Chem. Phys.* 384 (2011) 9–18.
- [16] H. Farrokhpour, E. Mojtabaic, Fluid containing hard-chain molecules with attractive potential of variable range: extension of mixtures and heteronuclear chain fluids, *Chem. Phys.* 352 (2008) 157–166.
- [17] T. Chakraborti, J. Adhikari, Prediction of fluid-phase behaviour of symmetrical binary Yukawa fluids using transition matrix Monte Carlo, *Fluid Phase Equil.* 415 (2016) 64–74.
- [18] R.L. Hall, Refining the comparison theorem of quantum mechanics, *J. Phys. Math. Gen.* 25 (1992) 1373.
- [19] Y.P. Varshni, Eigenenergies and oscillator strengths for the Hulthén potential, *Phys. Rev.* 41 (1990) 4682.
- [20] M.-C. Zhang, B. An, Analytical solutions of the Manning-Rosen potential in Tridiagonal program, *Chin. Phys. Lett.* 27 (2010) 110301.
- [21] C.A. Onate, O. Ebomwonyi, K.O. Dopamu, J.O. Okoro, M.O. Oluwayemi, Eigensolution of the D-Dimensional Schrödinger equation with inverse trigonometry scarf potential and Coulomb potential, *Chin. J. Phys.* 56 (2018) 2538–2546.
- [22] S.H. Dong, W.C. Qiang, G.H. Sun, V.R. Bezerra, Analytical approximations to the l-wave solutions of the Schrödinger equation with the Eckart potential, *J. Phys. Math. Theor.* 40 (2007) 10535.
- [23] R.L. Greene, C. Aldrich, Variational wave functions for a screened Coulomb potential, *Phys. Rev. A* 14 (1976) 2362.
- [24] C.A. Onate, M.C. Onyeaju, A.N. Ikot, O. Ebomwonyi, Eigen solutions and entropic system for Hellmann potential in the presence of the Schrödinger equation, *Eur. Phys. J. Plus* 132 (2017) 462.
- [25] C.A. Onate, Bound state solutions of the Schrödinger equation with second Pöschl-Teller like potential model and the vibrational partition function, mean energy and mean free energy, *Chin. J. Phys.* 54 (2016) 165–174.
- [26] H. Hassanabadi, E. Maghsoodi, S. Zarrinkamar, Relativistic symmetries of Dirac equation and the Tietz potential, *Eur. Phys. J. Plus* 127 (2012) 31.
- [27] L. Gendenshtein, Semi-classical behavior of Pöschl-Teller coherent states, *JETP Lett.* 38 (1983) 356 (Engl. Transl.).
- [28] L. Infeld, T.E. Hull, The factorization Method, *Rev. Mod. Phys.* 23 (1951) 21.
- [29] E. Schrödinger, A method of determining quantum mechanical eigenvalues and eigenfunction, *Proe Roy. Irish Acad.* 46 (1928) (1928) 9.
- [30] G.F. Wei, S.H. Dong, A novel algebraic approach to spin symmetry for Dirac equation with scalar and vector second Pöschl-Teller potentials, *Eur. Phys. J. A* 43 (2010) 185–190.
- [31] C.S. Jia, P. Guo, Y.F. Diao, L.Z. Yi, X.J. Xie, Solutions of Dirac equations with the Pöschl-Teller potential, *Eur. Phys. J. A* 34 (2007) 41–48.
- [32] H. Hassanabadi, S. Zarrinkamar, H. Rahimov, Approximate solution of D-Dimensional Klein-Gordon equation with Hulthén-type potential via SUSY QM, *Commun. Theor. Phys.* 56 (2011) 423–428.
- [33] S. Zarrinkamar, H. Hassanabadi, A.A. Rajabi, Dirac equation for a Coulomb scalar, vector and tensor interaction, *Int. J. Mod. Phys. A* 26 (2011) 1011–1018.
- [34] C.S. Jia, T. Chen, S. He, Bound state solutions of the Klein-Gordon equation with the improved expression of the Manning-Rosen potential energy model, *Phys. Lett.* 377 (2013) 682–686.
- [35] S. Zarrinkamar, A.A. Rajabi, H. Hassanabadi, Supersymmetric study of the pseudospin symmetry limit of the Dirac equation for a pseudoharmonic potential, *Phys. Scripta* 83 (2011), 015009.
- [36] C.A. Onate, J.O. Okoro, O. Adebimpe, A.F. Lukman, Eigen solutions of the Schrödinger equation and the thermodynamic stability of the black hole temperature, *Results in Phys* 10 (2018) 406–410.
- [37] A.N. Ikot, H.P. Obong, H. Hassanabadi, Relativistic symmetries of (D+1) dimensional Dirac equation with multiparameter exponential-type potentials using supersymmetric quantum mechanics, *Few Body Syst.* 56 (2015) 185.