Simple quantum mechanical models literature reviews examples

1. 1 Overview

Quantum mechanics is a branch of Physics that deals with the behaviors of energy and matter in the smallest perspective such as the nuclear, atomic, and microscopic levels. Quantum, meaning " how much", refers to the quantifiable units to energy and matter as observed and predicted through physics. This branch of studies stated with mathematical reasoning of certain experiments that are non-explainable through the classical mathematical methods. Physics revolutionized during the early 20th century (Coolman, 2014). Various models has been developed by scientists since them to help them in their experiments in studying particular behaviors of reaction mechanisms and chemical reactions. This paper deals with the simple models for quantum mechanics that includes Kronig and penny model, harmonic oscillator model, and tunneling across modulated single and double barriers.

1. 2Kronig and Penney Model

The Kronig-Penney model offers a simple model for quantum mechanics that provides simple approximations of solids. This model consists of delta functions periodic arrangements and Coulombs well potentials. The realization of the semiconductor super-lattices is done via epitaxial growth techniques with behaviors that are closely similar with the behavioral assumptions shown in the Kronig-Penny mode (Vasileska and Klimeck, 2008). The superlattices are the epitaxial layers that are ultrathin and alternatingly superimposed in a one-dimensional crystal potential (Esaki, 1986). The potential in a one-dimensional background is formed via the heterolayered band offsets in the compositional superlattice. It can also be formed through the periodic rowing of the n and the p-doped layers of the semiconductor

(Yuh and Wang, 1988).

The Kronig-Pennery model is an ideal model that presents that calculation of the crystalline solids energy bands having periodic varying potentials (Cho and Prucnal, 1987). The model can be presented in a one dimensional solid-state periodic potential. Despite the single dimensional state of the model, the crucial property that reveals the structure of electronic band yield is the periodicity of the potentials. This can be presented through the figure (Figure 1) and mathematical form (Equation 1) (McQuarrie, 1996).

Figure 1: The Kronig-Penney Model (McQuarrie, 1996)

Equation 1:

The assumption in the Kronig-Penney model one-electron includes the finite array of quantum wells that are rectangular and separated by barriers as shown in Figure 1. In the band structure engineering, the miniband structures of the super-lattices having various parameters such as space of the quantum well thickness, barrier energy, and the barrier thickness allow various designs for the artificial band structures. These three parameters involved can be defined with the following terms (Goncharuk, 2006).

do = the quantum well width

dw = the barrier thickness

Vo = the barrier height

In a one dimensional crystal, there are only certain resonant transmission or reflectance wavelengths that can pass through creating " standing waves".
In the figure 2, the various certain wavelengths passing through the 1D crystal are presented (Doolittle, nd).

Figure 2: Wavelengths passing through 1D crystal (Doolittle, nd).

Figure 3: Wavelengths characteristics

Most of the applications involving this model is the bulk semi-conductors. It has also been used in the calculation of the quantum energy confined subbands. There is discontinuity of the valence band and conduction in this case where the smaller gap of energy layers stand as the potential wells to those larger layers of energy gaps (Cho and Prucnal, 1987). In the field of bulk semi-conductor, the different crystal potentials will result in different primitive cells or bases resulting to varying energy bands. Likewise, in the superlattices, it is expected that the minibands will change along with the changes of the superlattice basis (Yuh and Wang, 1988).

Kronig and Penny derived their model from the work of Bloch, with higher and advanced understanding of the behaviors of electrons in the crystal lattice. Bloch's theory assumes the interaction of a certain electron to have particles in the lattice that can be replaced even at the first approximation by the periodicity of the potential. Various parameters such as the thermal conductivity, specific heat, electrical conductivity, optical properties, and the Hall effect of the metals are obtained by the model. Kronig and Penny model considers the concept of Bloch, but with higher understanding. In this model, it presents the wave-equation that represents the electron's motion in the periodic field of potential. The equation is integrated into the elementary functions as the potentials forms with the series of the rectangular barriers that are equidistant from each other. As the breadth b is turned smaller and the height Vo turned larger, the results bVo become simple as influenced by the barriers. In the one dimensional cases, the spectrum of values for energy consists of continuous regions that are separated with defined and finite intervals. The variation of the value of bVo from nil to infinity passing from

cases of free to bounded electrons, allows for the study of the various changes of energy and the transitional wave functions. In the linear momentum matrix of elements, the model presents the electron's capacity to pass through the lattice and that the possibility of the transition to other stationary states is existent under the absorption or emission of radiation. Thus, these electrons have the characteristic of both the bound and free electrons at the same time. Lastly, the model provides an investigation of the electron's reflection sown in the field of potential that leads to the results of qualitative agreement with the facts from experimentation. This phenomenon is observed by Rupp and with connection of the measurements of Rudberg (Kronig and Penney, 1931).

1. 3 The Harmonic Oscillation Motion

The harmonic oscillation motion model is one of the models in quantum mechanics. The model is mathematically simple and is very effective in the teaching about instruments. It presents that a harmonic oscillator is a particle that is subjected to a restoring force proportional to its displacement. In the form of equation, this is stated as equation [2]:

The constant k is the force constant. As the force constant increases, the restoring force for any displacement from the state of equilibrium also increases. In the basic mathematical foundational equation for a certain displacement x given by the equation [3]:

The angular frequency considered is given by

In these equations, given with large force constants yield to oscillation frequency that is high. Given with large mass will result to small oscillation frequency (Hill, 2006).

The simple harmonic oscillator equation states that: q̈(t) + ω2 q(t) = 0, with ω = √ k/m, the equation can be written as [4]:

q(t) = A cos(ωt + φ).

This equation is in second order, with constant coefficients, and simple homogenous solutions.

A= amplitude

ω = the natural frequency

φ= phase of the motion

In the field of quantum mechanics, the adaptation for the concept of harmonic oscillation model is higher and more complex. In quantum mechanics, the quantum physical properties occupy discrete values in space and are not really continuous. The atomic bonds considered in the quantum space do not have rigid structures. Rather, they involve mobile electrons nd vibrational motions. The harmonic oscillator is then used for the modeling of these particle's behaviors. Considering if the bonds between molecules to behave in accordance to the classical harmonic oscillators, the electron's energies of the bonds can have any energy, as well as the probability of the density of locating the endpoints of the oscillators would likely be found where there is a slowing down of the electrons and on the areas where the directions are changed. Oscillators in this case get only discrete values where the probability of locating the electron density is found at the center. This reasoning is in congruence with the concept of wavelengths by de Broglie and the wave functions of Schrodinger (Jensen et al, nd).

The concept of the quantum harmonic oscillator has higher implications from that of the diatomic molecules. The model served as foundation to the

understanding of the complex vibration behaviors of the large molecules, the understanding of their lattice surfaces, heat capacity, and other. The main difference with the quantum harmonic oscillation with the classical theory is the concept of " zero-point vibration". With quantum mechanics, there is no such thing as complete rest for molecules even at temperatures at absolute zero (Beiser, 1995).

In quantum mechanics, the simple conservation of energy equations stated in Equation [2] can be transformed into:

The potential and kinetic energies in the quantum mechanics are transformed into Hamiltonian. The wave functions are acted upon for the generation of the wave functions applicable in space and time (Nave, 2000).

1. 4 Tunneling across modulated single and double barriers

In the field of quantum mechanics, the usual mechanical tunneling is with the rectangular barrier found in one-dimension (Beiser, 1984). The tunneling across double barriers is applicable in various areas. One of the areas where it is highly useful is the quantum heterostructures. In this area, the heterostructures of the semiconductors are found with layers, with nano-thin sandwich structures derived from diverse materials for semiconductors. There are junctions of different materials also that allows for the occurrence of wells and barriers sequences. In these structures, the control of the parameters inside the devices and crystals are made possible. For instance, the measurement of the band gaps, charge masses and mobilities, electron energy spectrum, and the refractive indices are made possible. Applications include telecommunications, transistors, satellite television, and others (Mitin et al, 1999; Alferov, 2001).

The concept of double tunneling is also applicable in the high energy physics, where there is a developed barrier penetration model for heavy ion fusion. The Coulombs potential's realistic features are being considered in the nuclei for this concept (Descouvemont et al, 1982). Another field which is the Extra dimensions also applies the double tunneling. Particularly, this concept is applicable in the localization of the fields and particles in the brane, or the four-dimensional hypersurface. The brane models are viewe with quasi-bound or bound states in double barrier effective potentials that are spread across the extra dimensional coordinates (Randall and Sundrum, 1999). The equation for nonlinear schrodinger equation also applies to this concept. The equation is used in the macroscopic quantum tunneling probing as well as in the gravity surfaces (Rapedius and Korsch, 2008, Ishkhanyan et al, 2009).

The Tunelling Across double Barriers can be stated in this simple function equation, equation [5].

V (x) = Vsingle(x, V1, w1) + Vsingle(x − a, V2, w2),

Where V1, 2 = height of the barriers 1 and 2

W1, 2 = width of the two barriers

a = is the separation of the barrier heights

This concept is defined through the Figure 2:

Figure 2: Tunneling across double barriers

In the figure shown, the solid line shows the double rectangular barrier with two widths separated by quantity a (Dutt and Kar, 2010).

The tunneling effect in the quantum mechanics allows for the transport of charges across gaps in nanometric scales between conducting electrodes.

The voltage applications between these electrodes have tunneling currents that are measured and are highly sensitive to the sizes of the gaps, applied voltage, and the gap medium. There is high potentiality of its applicability in the liquid environments (Albrecht, 2012).

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