PROPAGATION OF 1D ELECTRON WAVE EQUATIONS IN LATTICE SYSTEM

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Abstract : The propagation of one dimensional electron wave function in periodic potential have been simulated. Gaussian wave function was chose to simulate the wave packet for the electron. The simulation or periodic potential shows that it follows Bloch theorem. Many problems related with the shape of potential are simulated also. Initial energy chose as tested parameter, which correspond to the speed of wave packet and related with the energy of the electron, and its show that for greater energy the spreading of wave packet become slower. The dynamical parameter makes possibilities to evaluate the propagation every time we need.

1. Introduction

The microscopic theory in physics leaded by quantum mechanics had strong relation with solid state physics [1]. Many standard text books of Quantum mechanics serve solutions of many simple systems. For educational aims we build such simulation to make student who take Quantum mechanics classes understand the concept of the top of human being intellectualities, beside the mathematical formalism that can only mastered by practicing and doing.

In the solid state there were many complexities, the idealization was used by physicist by many assumptions which is not change the main poetry of natures. One of the famous approximations which is used in solid state physics is the ion-electron formations. Every single atom in the crystal lattice assumes as Ion and the electron valence correlated with its electron in the Fermi level as the free electron. This electron was moving in the potential which form by interactions of Ion and the neighborhood one. Since Ions in the crystals are periodic, this interaction forming the periodic Coulomb potentials as the interaction is Coulomb interaction.

2. Theory

The Kronig-Penney chosen as it is the simpler form of potential which characterizes physical system. The Purpose of using simpler kind of approximations is to view how the simulations are agree with the concept and the physical meaning of propagation of wave electron in the periodic potential.

Firs we consider one dimensional Schrödinger equation [2,3,4].

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t) \qquad (1)$$

Let V be the periodic potential and follow

$$V(x+a) = V(x). \qquad (2)$$

This potential can be approximate by many kind of functions such as the famous one is the square well periodic potential Kronig-Penney[3]. Ss proved by Bloch that the solutions of the Schrödinger equation for periodic potential must of a special from[5]:

$$\psi_k(x) = u_k(x)\,\mathrm{e}^{(ik.x)}. \qquad (3)$$

Where $u_k(x)$ has the period of the crystal lattice with $u_k(x) = u_k(x+T)$.

The wave equations function was separated in to space term we choose Gaussian wave packet[2,3]:

$$\Psi(x, x_0) = \left[\frac{\Delta k}{\sqrt{\pi}}\right] e^{\left[ik_0(x-x_0) - \frac{1}{2}(x-x_0)^2(\Delta k)^2\right]}$$

and dynamical term, time evolution operator which can be form [1][4]:

$$e^{\left(-i\frac{\Delta t}{\hbar}\hat{M}\right)} = 1 + [\mathrm{e}^{-i\varepsilon}]\frac{ma^2}{\hbar^2}\hat{M} = \frac{1}{2}\left[\frac{1+\mathrm{e}^{-i\varepsilon}}{1-\mathrm{e}^{-i\varepsilon}}\frac{1-\mathrm{e}^{-i\varepsilon}}{1+\mathrm{e}^{-i\varepsilon}}\right] \qquad (4)$$

With

$$\hat{M} = \frac{\hbar^2}{2ma^2}\begin{bmatrix}1 & -1\\ 1 & -1\end{bmatrix} \qquad (5)$$

3. Results and Discussion

The objective of the study is to see how the Bloch theorem was follow by the simulations. Initial energy of wave packet is one of inputs parameter.

After testing the simulations using the establish approximations than the simulations applied to the more complex one, the periodic coulomb potential it is more complex because the shape of the potential functions wasn't discrete.

First consideration of our paper is if the potential Coulomb potential. Our simulations produce the probability density of electron in Coulomb potential as shown in Fig. 1.

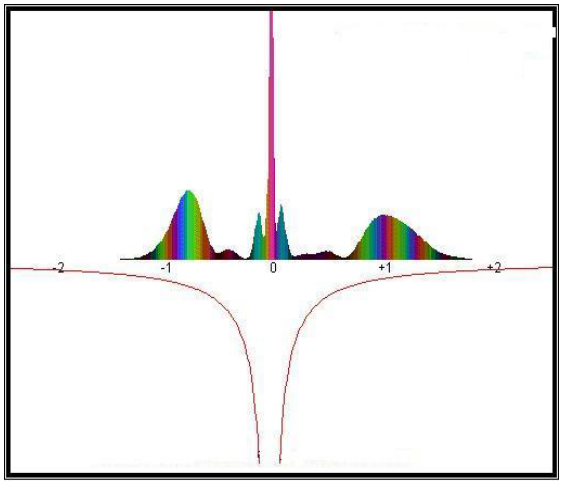
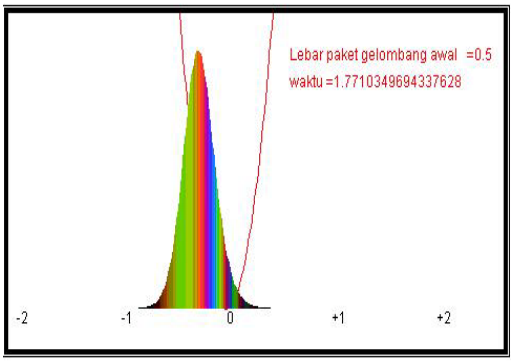


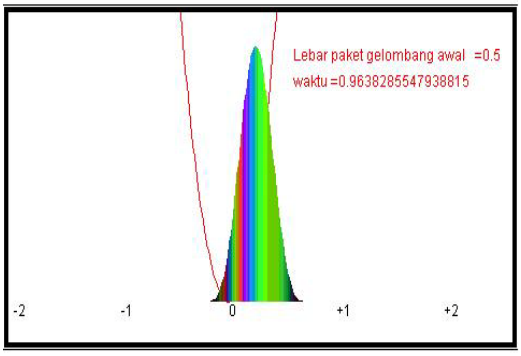
Figure. 1 Probability densities of electron scatter in Coulomb potential.

Further this model could be applied to one electron atom that is Hidrogen atom.

Other potential that can be simulate is electron that is move in harmonic potential. The result of simulation is shown in Fig. 2



(a)



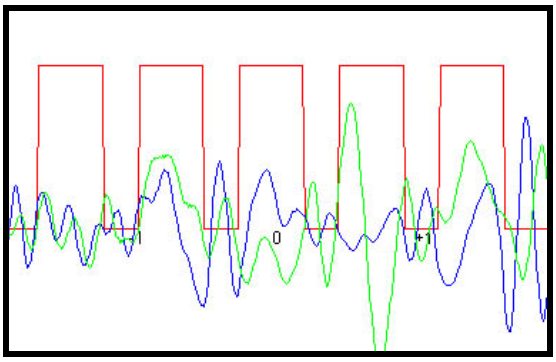
(b)

Figure. 2 Probability densities of electron scatter in Coulomb potential (a) when the probability density function moves to left. (b) the probability density function moves to height.

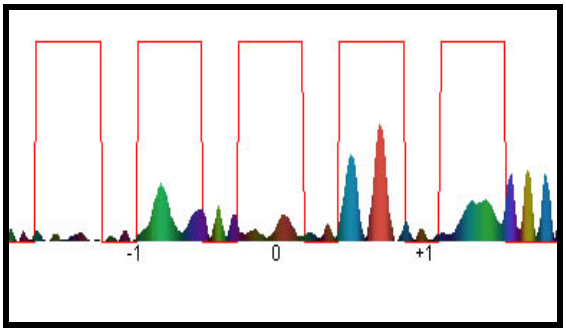
This result is agreed with quantum theory of oscillator harmonic.

The last is our main purpose, that is to simulate the electron wave propagation in lattice modeled by kronig-Penney. Our result is shown in Fig. 3

From Fig. 3 we can see that the wave propagation of electron wave function can be simulated, beside it agreed with Bloch theorems this can be conclude from certain simulation. The longer the simulation time the probability density of the electron has become stationer.



(a)



(b)

Figure 3. Electron wave propagation in Kronig Penney periodic potential (a), probability density correspond to the wave function (b) for initial width of wave packet 0,5.

4. Conclusions

Our main conclusion is that our simulation can be used in many potential that rarely discussed in common quantum mechanics text book. Beside that we prove that Bloch theorem can be simulate by time dependent Schrödinger. We hope our simulation can be used in educational purpose such as for Teaching in quantum Mechanics.

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REFERENCES

[1] Galperin. Y,M., Introduction to Modern Solid State Physics, Blindern, Oslo.

[2] Contantinescue. F, Magyari, E., Problems in Quantum Mechanics, pergamon Press, 1971.

[3] Goswami. A., Quantum Mechanics, WCB Publishers, 1992.

[4] Griffiths. D. J., Introduction to Quantum Mechanics, Prentice Hall Inc, 1995.

[5] Kittel. C, Introduction to Solid State Physics, John Wiley and Sons, Canada, 1986.

[6] Nugroho. F., Nurwantoro, P, Simulasi Hamburan Elektron Pada Potensial Sederhana, Jurnal Fisika Indonesia, Indonesia, 2006.

[7] Muktar. C.J, Visualizing One Dimensional Quantum Scattering for Simple Potential, University of Manchester, Schuster Laboratories, Brunswick Street, M13 9PL, 2004.Introduction