Modelling one-dimensional crystal by using harmonic oscillator potential

IOP Conf. Series: Materials Science and Engineering **546** (2019) 052001 doi:10.1088/1757-899X/546/5/052001

Modelling one-dimensional crystal by using harmonic oscillator potential

Abdurrouf, M. Nurhuda, and Wiyono

Department of Physics, Brawijaya University, Jl. Veteran Malang, Indonesia 65145

*Corresponding author: abdurrouf@ub.ac.id

Abstract. Our recent developed filter method (*Phys. Rev E* **96**(3), 033302, 2017) is applied here to investigate the energy spectrum and their corresponding wave function of one dimensional crystal. The periodic one dimensional potential is modelled by using one dimensional periodic harmonic oscillator, with variation on oscillator potential depth, quasi-potential depth, and crystal width. For energy less than the potential depth of the oscillator, the computational results reveal that the periodic harmonic oscillator produces a discrete spectrum, as the energy spectrum of a single harmonic potential. However, for energy almost equal to or greater than the depth of the potential oscillator, the periodic harmonic oscillator demonstrates the existence of pattern similar to energy band in crystal.

1. Introduction

Current development of technology requires our ability to know and control material properties, including mechanical, electrical, magnetic, and optical properties. In general, the nature of a material is determined by the shape of its energy band, arising from the periodic potential of crystal [1].

To understand the relationship between potential forms in crystals and their energy band patterns, we must know the behavior of electrons. This means we have to solve the Schrödinger equation, with the periodic potential formed by the lattice in the crystal. This process is strongly influenced by its potential form, the dimensions of the problem, and the reliability of the method [2]. For one-dimensional problem, the periodic potential can be modelled as a recurrence of simple harmonic potential, inverted harmonic potential, Kronig-Penney potential, or linear potential [3,4], solved by using matrix method [4,5] wave propagation [6], or variational method [7].

In the previous research, we have successfully developed a computational method for solving Schrödinger equation, called the filter method. The filter method has the advantage of not requiring any boundary conditions. This method gets much success when applied to solve the Schrödinger equation for single potential, such as coulomb and harmonic oscillator potential [8]. Therefore, it is very interesting to apply the filter method for 1-dimensional periodic crystals, formed by a periodic single potential.

This paper is aimed to implement filter method for 1-dimensional crystals, find the energy spectrum, and analyze the results. To this end, the 1-dimensional crystals is modelled by using periodic harmonic oscillator potential, as shown in Fig. 1. The energy spectrum obtained from the model is then compared with an electron energy spectrum from a single harmonic oscillator.

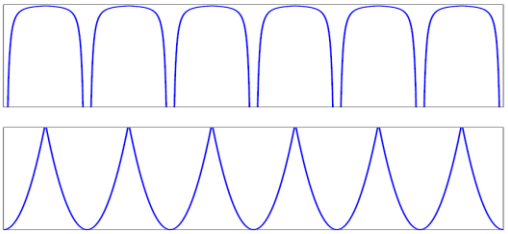

Figure 1. Comparison between periodic Coulomb potential (upper panel) and periodic harmonic oscillator potential (lower panel).

2. Methods

The periodic harmonic oscillator potential used for modelling crystal, is depicted in Fig. 2. The 1-dimensional crystal potential is formed by the arrangement of 1-dimensional harmonic oscillators. In this model, we can control the width of the lattice a, the number of oscillators n, and the width of the edge t. The other variable, such as widh of crystal (L), depth of lattice potensial (V_0), and depth of edge potensial (V_t), are dependent variable could be calculated as follow.

$$L = na + 2t \tag{1}$$

$$V_0 = \frac{1}{2}\left(\frac{a}{2}\right)^2 \tag{2}$$

$$V_t = \frac{1}{2}\left(\frac{a}{2} + t\right)^2. \tag{3}$$

Along the research, the calculation is performed by using atomic units ($\hbar = e = m_e = k = 1$) .

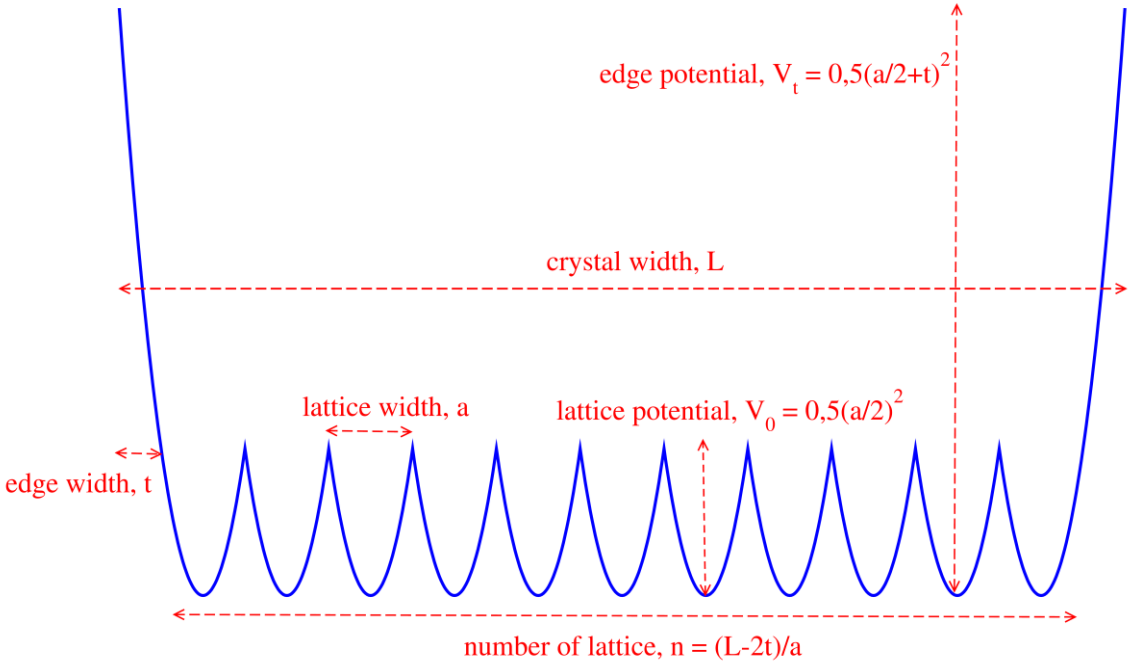

Figure 2. The periodic harmonic oscillator potential

3. Results and discussion

Before discussing the energy spectrum of a periodic harmonic oscillator, let first discuss the shape of wave function and the eigenvalue of energy in one-dimensional periodic harmonic oscillator potential, as shown in Figure 3.

Figure 3 is performed by choosing $\omega = 1$. It can be seen that the energy level $E = 0.5$, $E = 1.5$, and $E = 3.5$ are corresponding to $n = 0$, 1, and 2, respectively. It means that the energy level for periodic harmonic oscillator potential satisfies formula $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$, the same as single harmonic oscillator. However, this formula is no longer holds for higher energy level. Figure 3 also shows that wave function from periodic harmonic oscillator potential differs from wave function of single harmonic oscillator, regarding its shape, period, and parity. For a single harmonic oscillator, the wave function is an odd function for odd n and even functions for even n. This parity does not appear for wave functions from periodic harmonic oscillator potential. In this paper, we will focus on the energy spectrum and neglect to discuss the discrepancies on wave function.

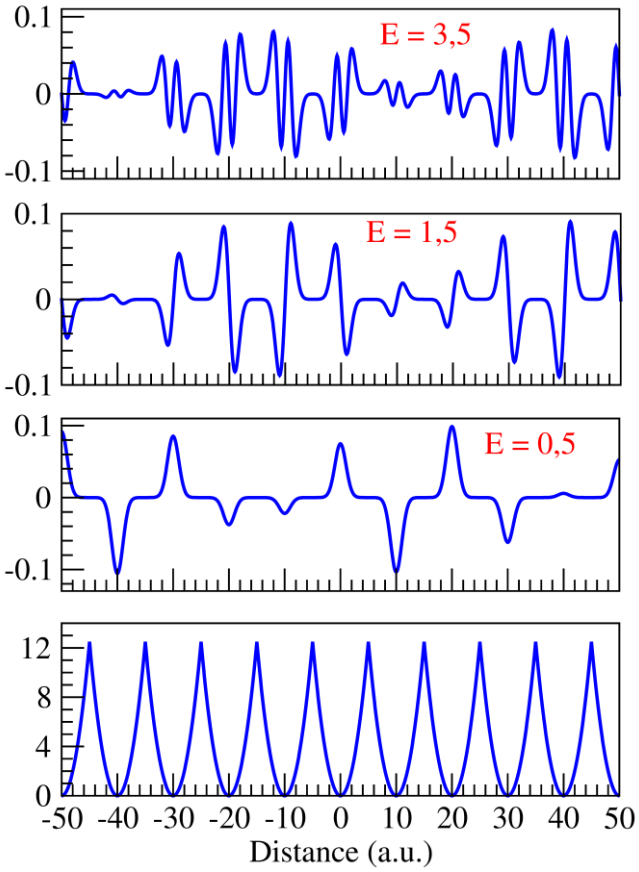

Figure 3. Wave functions and eigenvalues of energy in 1-dimensional periodic harmonic oscillator potential for three lowest energy levels, plotted as a function its position towards the center of the crystal. The bottom panel shows the periodic harmonic oscillator potential in the corresponding position.

Next we discuss the effects of the number of oscillators. The calculation was performed for fixed width of the oscillator (which is also the width of the lattice) $a = 10$ and fixed width of edge $t = 10$, with the number of oscillators $n = 50,100,150$, and 200. The results were depicted in Fig. 4.

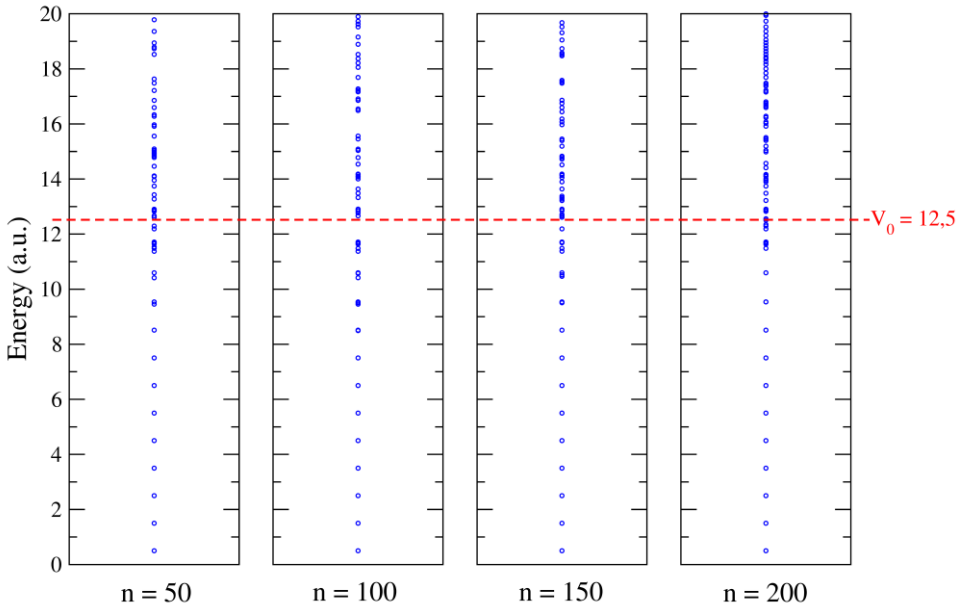

Figure 4. The energy spectrum of one dimensional lattice with a periodic harmonic oscillator potential for lattice widths $a = 10$, and edge widths $t = 10$, at various number of oscillators.

Refer to equations (2-3), it was obtained that the lattice potential depth value is $V_0 = \frac{1}{2}(\frac{10}{2})^2 = 12.5$ and the edge potential depth value is $V_t = \frac{1}{2}(\frac{10}{2} + 5)^2 = 112.5$. This means that electrons experience a periodic potential with a depth of 12.5 and equipotential with a depth of 112.5. Fig. 4. shows that for $E > V_0$, most energy levels are degenerate, creates a dense energy pattern at a certain energy range and emptiness of energy levels in another range. A dense energy pattern can be interpreted as an energy band, while the emptiness of energy levels can be interpreted as band gap. The model confirms the existence of an energy band.

Furthermore, Fig. 4 also demonstrates that the energy band pattern depends on the width of the crystal. According to Eq. (1), our crystal width is $L = 520$ (for $n = 50$), $L = 1020$ (for $n = 100$), $L = 1520$ (for $n = 150$), and $L = 2020$ (for $n = 200$). Comparing those four panels, it is found a tendency for the ribbon structure to tighten when the crystal width increases. It can be interpreted that the electrons almost feel the free potential as the crystal width increase.

Next, we analyze the effects of lattice width a. In this study, we choose number of oscillators $n = 100$ and edge width $t = 10$, with lattice widths $a = 5, 10, 15,$ and 20, corresponds to $V_0 = 3.1, 12.5, 28.125,$ and 50 . The results are shown in Fig. 5. In general, the band structure starts to form at the energy level slightly below V_0. Furthermore, Fig. 5 also shows that the pattern of energy bands depends on the depth of the lattice potential V_0, with the tendency of the structure of the ribbon to be more tight with the addition of V_0.

Lastly we review the effect of the width of the crystal edge t. In this study, we keep the number of oscillators $n = 100$ and lattice widths $a = 10$ with edge effects $t = 10, 20, 30,$ and 40, corresponds to $V_t = 50; 112.5;\ 200,$ and 312.5 . The results are shown in Figure 6.

Referring to the previous discussion, it can be seen that the structure of the energy band starts to form at an energy value less than $V_0 = 12{,}5$, as seen clearly in Figure 6 left panel. In the other panel, the pattern is not clear because the small energy scale. It is worthwhile to note here that there is still an energy band pattern at the energy level above V_t, where electrons feels equipotential only. This problem might be better understood by using Coulomb potential, so we have negative potential energy. As a consequence, the boundary of the bound state and the free state becomes clear. This will be the topic of the next study.

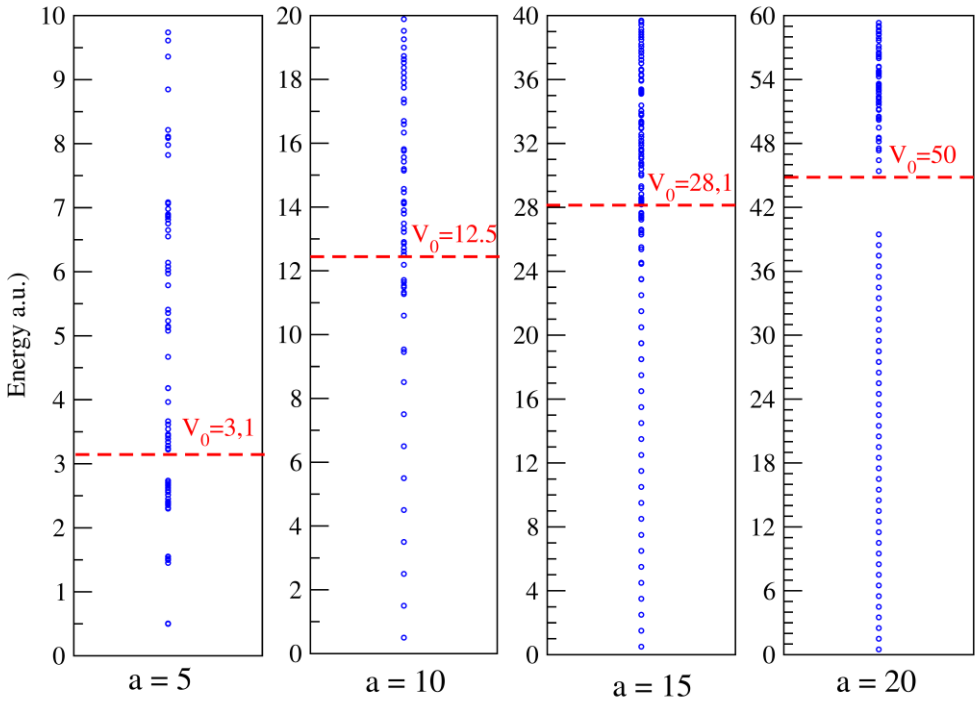

Figure 5. The energy spectrum of one dimensional lattice with a periodic harmonic oscillator potential for lattice number $n = 100$, and edge widths $t = 10$, at various lattice width a..

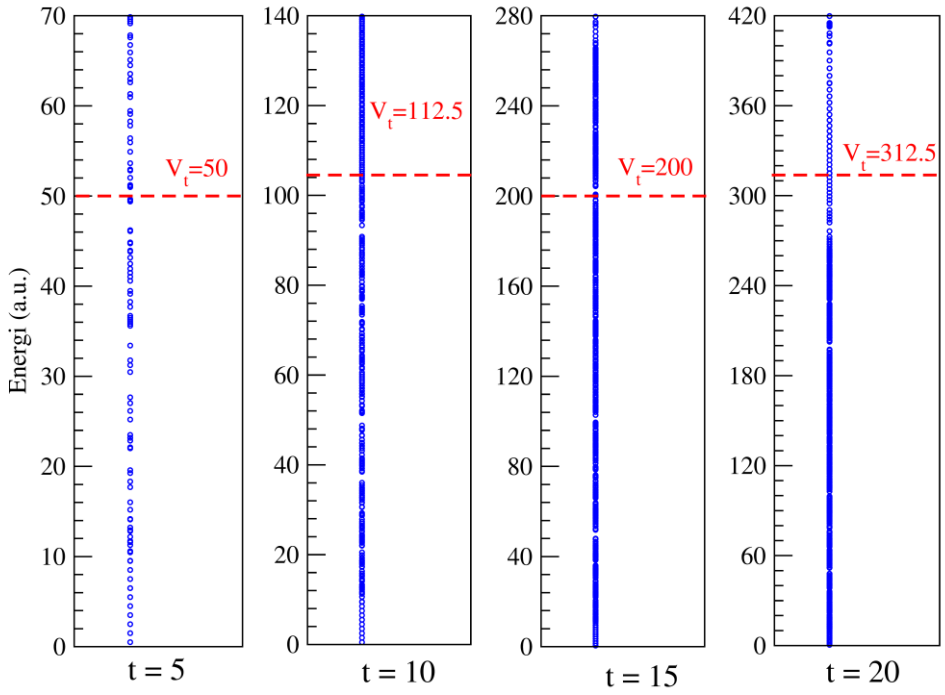

Figure 6. The energy spectrum of one dimensional lattice with a periodic harmonic oscillator potential for lattice number $n = 100$, and lattice width $a = 10$, at various edge widths t.

4. Conclusion

As a conclusion, the implementation of the filter method on a 1-dimensional periodic lattice with a periodic harmonic oscillator potential produces discrete energy patterns, such as a single harmonic oscillator, for the energy level below the lattice potential. For energy level close to or greater than the lattice potential, periodic lattice with a harmonic oscillator potential produce an energy band structure. The structure of the energy band depends on the lattice potential depth, the potential edge depth, and the number of oscillators.

References

[1] M. A. Pamungkas, D. A. Setyowati, and Abdurrouf (2018), Optical properties of Ga-doped silicene and as-doped silicene: First principle calculations, *AIP Conference Proceedings* **2021**, 050014

[2] N. Zettili (2009), *Quantum Mechanics: Concepts and Applications* 2nd Edition, John-Wiley, Chichester, USA

[3] R. L. Pavelich and F. Marsiglio (2015), The Kronig-Penney model extended to arbitrary potentials via numerical matrix mechanics, *Am. J. Phys.* **83**(9), 773-781

[4] P. Markoš and C. M. Soukoulis (Eds) (2008), W*ave Propagation: From Electrons to Photonic Crystals and Left-Handed Materials*, Princeton University Press, Princeton, NJ

[5] F L Vot, J J. Meléndez, and Santos B. Yuste (216), Numerical matrix method for quantum periodic potentials, *Am. J. Phys.* **84**, 426

[6] G. A. Luna-Acosta, F. M. Izrailev, N. M. Makarov, U. Kuhl, and H.-J. Stöckmann (2009), *Phys. Rev. B* **80**, 115112

[7] J.D. A Cardona, O.D. A Echeverri and E. R Parra (2107), *Revista Mexicana de Fısica* E **63,** 12–20

[8] M. Nurhuda dan A. Rouf (2017), Filter method without boundary-value condition for simultaneous calculation of eigenfunction and eigenvalue of a stationary Schrödinger equation on a grid, *Phys. Rev. E* **96**(3), 033302(9).