Numerical solution of the Schrödinger equation with periodic Coulomb potential

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Abstract. This paper investigates the energy spectrum of a periodic one-dimensional Coulomb potential. The Schrödinger equation is solved numerically by our newly developed filter method (Phys. Rev E 96(3), 033302 (2017)). We observe that the energy spectrum can be obtained with a limited number of lattice. The results show the presence of an energy band structure as a function of lattice width and edge width. The comparison with the other potential model is also discussed.

1. Introduction
Along with the rapid development of technology, there is an increasing need for the availability of materials with specific mechanical, optical, electrical, and magnetic properties. Because the properties of a material largely depend on its band structure, one of the most important problems in solid-state physics is determining the electronic states in solids [1-2]. This problem is usually solved by assuming a periodic potential for a single electron, which represents a simplified model for a crystal structure [3-4]. More specifically, much theoretical research has focused on the time-independent behavior of the electron in a one-dimensional (1D) periodic potential, which can be obtained by solving the Schrödinger equation for the corresponding case.

Complicated mathematical techniques are often required to find the analytical solutions of the Schrödinger equation for particular potentials. For some cases of potentials, the analytical solutions are even not yet available. Therefore, numerical methods become realistic choices to solve the problem. In this regard, we have developed a numerical method for solving the Schrödinger equation, known as the filter method [5]. The filter method enables us to obtain the eigen-energy and eigen-function of any given potential without the requirement to define any boundary conditions.

The filter method has been applied to solve the Schrödinger equation for a single-particle in single potentials such as an electron in the Coulomb potential and an electron in the harmonic oscillator potential, with great success [5]. Furthermore, this method is also applied to solve multi-particle systems, such as electrons in a helium atom, where acceptable results can be reproduced with precision up to the 9th decimal. Recently, we applied the filter method to solve periodic 1D potential problems, such as a periodic harmonic potential [6] and the Kronig-Penney model [7-8]. In both cases, we observed the energy band structures, as expected from periodic potentials. The numerical results for the Kronig-Penney model well agree with the analytical ones. On the other hand, we have difficulty for checking the results of the periodic harmonic potential due to the absence of the analytical solutions.

Another attractive challenge is the implementation of the filter method for a periodic Coulomb potential. In implementation, the soft-core Coulomb is employed to avoid singularity [9]. The soft-core
Coulomb potential consists of a screening factor, whose value can be determined by optimization \([10-11]\) or variation method \([12]\). However, the Schrödinger equation for the periodic Coulomb potential is often solved in terms of pseudo-Coulomb potential and is rarely solved directly by using the pure Coulomb potential. This article is aimed to implement the filter method to solve the eigen-function and eigen-energy of a single electron in a periodic 1D soft-core Coulomb potential. We analyze the energy spectrum and its dependence on the screening factor, as well as the number and the width of lattice.

2. Methodology

In this study, the Schrödinger equation with the periodic soft-core Coulomb potential is solved by using the filter method. Details of the filter methods are presented in Ref. [5]. Here, we will focus on (i) the main ideas underlying the filter method, (ii) how the filter method generates the solutions of the Schrödinger equation and (iii) how to apply the filter method for a particle in the periodic 1D soft-core Coulomb potential.

The filter method is based on the principle of superposition of waves. Thus, for any given potential, the corresponding wave function must be a superposition of all possible eigen-functions. Each eigen-function can be retrieved using the appropriate operator. Here, we define the filter operator as an inverse of \((H - E_n)\), or

\[
F = \frac{1}{H - E_n}.
\]  

In Equation (1), \(H\) stands for the Hamiltonian operator while \(E_n\) stands for the eigen-energy, whose eigen-function will be retrieved. When the filter operator \(F\) is applied to the wave function, it acts as the Dirac delta function so that only the desired eigen-function with \(E = E_n\) survives, while other eigen-functions whose energies are not matched go to zero. Let us apply the operator \(F\) to the initial guess wave function given by \(\psi(\mathbf{r}) = \sum_n a_n \phi_n(\mathbf{r})\) with a given initial energy \(E_n^0\).

\[
F\psi(\mathbf{r}) = \frac{1}{H - E_n^0} \sum_m a_m \phi_m(\mathbf{r}) = \sum_m a_m \phi_m(\mathbf{r}) \delta(E_m - E_n^0) = \tilde{\phi}_n^1(\mathbf{r})
\]  

The eigen-function \(\tilde{\phi}_n(\mathbf{r})\) obtained from Equation (1) is normalized as follows:

\[
\phi_n^1(\mathbf{r}) = \frac{\tilde{\phi}_n^1(\mathbf{r})}{\sqrt{\int d^3r |\tilde{\phi}_n^1(\mathbf{r})|^2}}
\]  

Having the normalized eigen-function, we can calculate the eigen-energy given by

\[
E_n^1 = \int d^3r \ \phi_n^1(\mathbf{r}) H \ \phi_n^1(\mathbf{r})
\]  

We note here that \(\phi_n^1(\mathbf{r})\) and \(E_n^1\) are the initial guess of the eigen-function and the eigen-energy, respectively. To obtain the eigen-energy that is closer to the correct value, we repeat the same process, with the initial wave function \(\phi_n^1(\mathbf{r})\). Thus, we apply the filter method on \(\phi_n^1(\mathbf{r})\) to obtain the second unnormalized guess eigen-function, \(F\phi_n^1(\mathbf{r}) = \tilde{\phi}_n^2(\mathbf{r})\). We normalize \(\tilde{\phi}_n^2(\mathbf{r})\) using Equation (2) to obtain \(\phi_n^2(\mathbf{r})\), and use \(\phi_n^2(\mathbf{r})\) to calculate the next guess of eigen-energy \(E_n^2\) according to Equation (3). This iterative process is repeated until the eigen-energy converges to a particular value \(E_n\) with the corresponding eigen-function \(\phi_n(\mathbf{r})\). In this study, the filter method can be implemented for two different purposes, i.e. (i) to find a single eigen-energy above a given initial energy, and (ii) to find all possible eigen-energies in a given range of energy.

In this study, we investigate the behaviour of a single electron in the periodic 1D soft-core Coulomb potential. The potential is shown on Figure 1, where \(n\) and \(\alpha\) represent the number and the width of the crystalline lattice, respectively. By defining \(t\) as the edge or surface width, the crystal width is given by
\[ L = na + 2t. \] Here, the soft-core Coulomb potential of a nuclei with atomic number of \( Z \), measured at a distance \( x \) from the nuclei is given by [9]

\[ V(x) = -k \frac{Ze^2}{(|x|^p + \epsilon^p)^{1/p}}. \] (5)

In Equation (5), \( \epsilon \) is the screening constant to avoid singularity, while \( p = 1,2,3 \ldots \) is the optimization number. We begin with the initial wave function \( \psi(x) = \sin(x) + \cos(x) \) to provide both odd and even eigen-functions. Hereafter, we use Hartree atomic units where \( e = m = h = k = 1 \) and \( c = 137 \). We also choose \( Z = 1 \) and \( p = 1 \).

3. Results and Discussion

Before discussing the energy spectrum, let first discuss the shape of the wave function and the eigen-energy in the periodic 1D Coulomb potential, as shown in Figure 2. The results are justified because the wave function is close to zero at the points where the potential is maximum, and vanishes at the edge of the crystal.

![Figure 1](image1.png)

**Figure 1.** The profile of the periodic 1D Coulomb potential, characterized by the lattice width \( a \), the lattice number \( n \), the edge width \( t \), and the screening constant \( \epsilon \). The crystal width is given by \( L = na + 2t \).

![Figure 2](image2.png)

**Figure 2.** Wave function (upper panel, blue color) and its modulus square (lower panel, blue color), from the first energy level. As a comparison, we also plot the potential (red color). In the calculation, we choose \( a = 12 \) a.u., \( n = 20 \), \( t = 60 \) a.u. and \( \epsilon = 10^{-4} \).
Next, we investigate the effect of the screening constant $\varepsilon$ by analyzing the energy spectrum obtained with various $\varepsilon$, as shown in Figure 3. The calculations are performed for $\varepsilon = 10^{-6} - 10^{-1}$. From Fig. 3, we see that there is no significant change in the energy spectrum as long as $\varepsilon \leq 10^{-3}$. These results allow us to use $\varepsilon = 10^{-4}$. The greater screening factor shifts up the eigen-energy, as in the case of a single Coulomb potential [5].

Figure 3. Energy levels for the periodic 1D Coulomb potential with $a = 12$ a.u., $n = 80$, $t = 0$ a.u. with various $\varepsilon$.

Now, we analyze the effect of number of lattice $n$ on the energy spectrum, by varying the calculation with $n = 100, 80, ..., 20$, as shown in Figure 4. It is interesting to note that the energy spectrum does not change when we reduce the number of lattices from 100 to 20. This shows the great efficiency of the filter method as it works well even with a limited number of lattice. Figure 4 also shows that the first eigen-energy is $-0.47$ a.u., that is close to the first eigen-energy for single Coulomb potential, $-0.5$ a.u. [13]. However, the second eigen-energy is $-0.33$ a.u., which is lower than the second eigen-energy for the single Coulomb potential, $-0.125$ a.u. Moreover, the periodic Coulomb potential produces a discrete energy states for $E > 0$, in contrast to the continuum states for the single Coulomb potential. Unfortunately, we do not observe the band pattern for $a = 12$ a.u.

Figure 4. Energy levels for the periodic 1D Coulomb potential with $a = 12$ a.u., $t = 0$ a.u. and $\varepsilon = 10^{-4}$ with various $n$. 
To obtain the energy band structure we vary the lattice width $a$, from 6 a. u. to 30 a. u., as shown in Figure 5. The figure shows that for $a \geq 18$ a. u., most of the energy level are degenerated, creating a dense energy levels in a certain energy range and an energy level vacancies in another range. The dense energy levels can be interpreted as an energy band, while the vacancies energy levels can be interpreted as a band gap. This model confirms the existence of energy bands.

**Figure 5.** Energy levels for the periodic 1D Coulomb potential with $n = 80$, $t = 0$ a. u. and $\varepsilon = 10^{-4}$ with various $a$.

**Figure 6.** Energy levels for the periodic 1D Coulomb potential with $n = 80$, $a = 12$ a. u. and $\varepsilon = 10^{-4}$ with various $t$. 
We also analyze the effect of edge’ width, $t$. To this end we perform the calculation with various values of $t$, from 0 to 120 a.u. The results are shown in Fig. 6. In general, the greater $t$ produces a denser energy levels, so that the energy band structure is easier to observe.

Now, we come to an important question concerning the validity of the results. Unfortunately, we were unable to compare the results due to the absence of the analytical solutions. On the other hand, the filter method succeeded in getting numerical solutions for the Kronig-Penny model which were exactly the same as the analytical results [7]. For this reason, we have compared the energy spectrum of the periodic 1D Coulomb potential with the energy spectrum of the Kronig-Penny model, the sawtooth potential and the periodic 1D harmonic oscillator potential. We observed that the energy spectrum is quite sensitive to the potential shape. This fact inspired the application of the filter method for optimization of potential models in crystals.

4. Conclusion
To conclude, we have demonstrated that the filter method can be used to obtain the energy spectrum of the 1D Schrödinger equation with the periodic Coulomb potential. The results show the existence of energy band structure. We also observe that the energy spectrum depends on the lattice width and the edge width. However, we can not evaluate the results due to the lack of analytical solution of this problem.

Acknowledgement
This work was financially supported by Faculty of Mathematics and Natural Sciences Brawijaya University through “Penelitian DPP/SPP Tahun Akademik 2019-2020” with the contract number: 30/UN10.F09.01/PG/2019

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