

SOLVING SCHRÖDINGER EQUATION FOR A PARTICLE IN ONE-DIMENSIONAL LATTICE: AN HOMOTOPY PERTURBATION APPROACH

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In this paper, a novel approach for an approximate solving Schrödinger equation for a particle in the one-dimensional lattice with the periodic potential is described. This approach, based on the homotopy perturbation method (HPM), gives an approximate analytic solution which has a high degree of convergence, and at the same time high degree of accuracy. The convergence of the HPM is examined and formally confirmed. In addition, the efficiency of the HPM method is illustrated in two examples.

Key words: Homotopy perturbations, Schrödinger equation, periodic potential, wave function, periodic boundary conditions, approximation.

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1. INTRODUCTION & DEFINITION OF THE PROBLEM

A nontrivial problem of the computation of electronic states in a solid can be greatly simplified in the case of a crystal, i.e. in the case of a regular, periodic and infinite arrangement of atoms. In this case, under the suitable assumptions, the many-electron problem turns into much simpler problem of an electron under a periodic potential. Periodicity can be mathematically formalized in a simple and general way in any number of dimensions. In the following we will assume a one-dimensional array of atoms of the same kind, regularly spaced by a distance a . Let us emphasize that a is the lattice parameter, while $a_n = na$, where n is an integer, are the vectors of the crystal lattice. We suppose that system has a discrete translational invariance, that is: it is equal to itself if translated by a or multiples of a . Furthermore, crystal potential will be labeled as $V(x)$, where x is the position of the particle in the lattice. For this potential which is formed by the superposition of atomic-like potentials $V(x) = \sum_n V_n(x - a_n)$, the following symmetry holds: $V(x + a) = V(x)$. Thanks to such symmetry the infinite line which represents considered one-dimensional space can be decomposed into finite space regions of length a , periodically repeated. That finite region $[-a/2, a/2]$ defines the so-called *unit cell*.

For an electron moving in the potential $V(x)$, the one-dimensional, time independent Schrödinger equation is given by:

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} (E - V(x))\psi(x) = 0. \quad (1)$$

Here, $\psi(x)$ is *the wave function*, in general complex, m is mass of electron, E is its total energy, and \hbar is reduced Planck's constant. In the following, the aforementioned idealized modeling will be applied to a crystal of finite length L , i.e. it will be assumed that $x \in [-L/2, L/2]$. It can be achieved by introducing *the periodic boundary conditions (PBC)* $\psi(-L/2) = \psi(L/2) = 0$. Further, also, will be assumed that wave function satisfies the probability density normalized condition:

$$\int_{-L/2}^{L/2} \psi(x)\psi^*(x)dx = \int_{-L/2}^{L/2} |\psi(x)|^2 dx = 1.$$

In spite of the PBC which enable that the system can be treated as a one-dimensional segment of finite length L , still retaining the discrete translational invariance, the solution of Eq.(1) for a periodic potential is not a simple problem. There is still a need for finding a number of single-particle states equal to at least half the number of electrons in the system. Due to the translational symmetry of the problem, solution of Eq.(1) satisfies the Bloch's condition $\psi(x+a) = \psi(x)e^{ika}$, with $\psi(x) = U(x)e^{ikx}$, where k is the wave vector and $U(x)$ is a periodic function of lattice period a . Also, it can be easily verified that wave function obeys the condition of translational symmetry $\psi(x) = \psi(x+L)$. Thus, the Bloch's condition and last equality imply that only values of k such that $\exp(ikL) = 1$ are compatible with PBC, that is, k must be an integer multiple of $2\pi/L$.

However, the time-independent Schrödinger Eq.(1) for periodic potential has not been solved exactly even for infinitely large periodic systems despite the simplification that Bloch's theorem provides. On the other hand, its solutions for one dimensional finite systems are obtained by using various numerical techniques in some special cases [1,2]. In this paper, we used the homotopy perturbations method (HPM) as a novel approach to find approximate analytical solutions of the Schrödinger equation for arbitrary one-dimensional periodic potentials. The HPM, firstly introduced by He [3–6], is an approximate-analytical method, different from other similar ones, because it provides a simple way to adjust and control the convergence region of the solution series by choosing the proper values for auxiliary parameters. In recent years, the HPM has been intensive developed and it was the subject of extensive studies [7–10]. This method is also found a very useful application in (approximate) solving the various kind of nonlinear equations, mostly in the physical sciences [11–15]. Especially, the HPM has been used in solving the different forms of the non-linear Schrödinger equation [16, 17].

2. HPM SOLUTION OF THE SCHRÖDINGER EQUATION

In order to solve the Eq.(1) using HPM, let us consider the following *homotopy equation*:

$$(1-p) \left[\frac{\partial^2 \Psi(x;p)}{\partial x^2} - \frac{d^2 \psi_0(x)}{dx^2} \right] + p \xi \left[\frac{\partial^2 \Psi(x;p)}{\partial x^2} + \frac{2m}{\hbar^2} (E - V(x)) \Psi(x;p) \right] = 0, \quad (2)$$

where $p \in [0, 1]$ is the *embedding (homotopy) parameter*, and $\xi \neq 0$ is the *auxiliary parameter*. When $p = 0$, the homotopy Eq.(2) has the so-called *initial solution* $\Psi(x; 0) = \psi_0(x)$, which can be chosen arbitrarily, but such that satisfies the PBC $\psi_0(\pm L/2) = 0$. On the other hand, when $p = 1$, Eq.(2) becomes equivalent to the Schrödinger Eq.(1), whereby we assume that the same PBC are valid.

The basic assumption of the HPM is that solution of homotopy Eq.(2) can be expressed as the power series in p :

$$\Psi(x;p) = \sum_{j=0}^{\infty} p^j \psi_j(x). \quad (3)$$

According to this, the solution of the Schrödinger Eq.(1) can be obtain as:

$$\psi(x) = \lim_{p \rightarrow 1^-} \Psi(x;p) = \sum_{j=0}^{\infty} \psi_j(x), \quad (4)$$

provided that the series in Eq.(4) converges. Substituting Eq.(3) in the homotopy Eq.(2), it follows:

$$\begin{aligned} \sum_{j=1}^{\infty} p^j \frac{d^2 \psi_j(x)}{dx^2} + (\xi - 1) \sum_{j=1}^{\infty} p^j \frac{d^2 \psi_{j-1}(x)}{dx^2} + p \frac{d^2 \psi_0(x)}{dx^2} \\ + \frac{2m\xi}{\hbar^2} (E - V(x)) \sum_{j=1}^{\infty} p^j \psi_{j-1}(x) = 0. \end{aligned} \quad (5)$$

Now, by equating in Eq.(5) the expressions with identical powers p^j , $j = 1, 2, \dots$, the following differential equations get ones:

$$\frac{d^2 \psi_1(x)}{dx^2} + \xi \left[\frac{d^2 \psi_0(x)}{dx^2} + \frac{2m}{\hbar^2} (E - V(x)) \psi_0(x) \right] = 0, \quad (6a)$$

$$\frac{d^2 \psi_j(x)}{dx^2} + (\xi - 1) \frac{d^2 \psi_{j-1}(x)}{dx^2} + \frac{2m\xi}{\hbar^2} (E - V(x)) \psi_{j-1}(x) = 0, \quad (6b)$$

where $j = 2, 3, \dots$. Also, we assume that the PBCs $\psi_j(\pm L/2) = 0$ hold for each $j = 1, 2, \dots$. In that way, the Eqs.(6a)-(6b) can be solved recursively on $\psi_j(x)$ using

the double integration:

$$\begin{cases} \psi_1(x) = \frac{2m\xi}{\hbar^2} \int dx \int (V(x) - E) \psi_0(x) dx - \xi \psi_0(x), \\ \psi_j(x) = \frac{2m\xi}{\hbar^2} \int dx \int (V(x) - E) \psi_{j-1}(x) dx + (1 - \xi) \psi_{j-1}(x), \end{cases} \quad (7)$$

where $j = 2, 3, \dots$. Finally, according to Eq.(4), the HPM approximations of the unknown wave function $\psi(x)$ will be:

$$\widehat{\psi}_n(x) := \sum_{j=0}^n \psi_j(x), \quad n = 0, 1, 2, \dots \quad (8)$$

where the normalized condition $\int_{-L/2}^{L/2} |\widehat{\psi}_n(x)|^2 dx = 1$ holds. In the following, some sufficient conditions for the existence and convergence of HPM approximations has been given.

Theorem 1 Let $\{\psi_j(x)\}_{j=0}^{\infty}$ be the sequence of functions defined, for an arbitrary $L > 0$, on the interval $[-L/2, L/2]$ by the recurrence relations in Eqs.(7). In addition, assume that the following conditions are satisfied:

(i) The function $\psi_0(x)$ is an uniformly bounded on $[-L/2, L/2]$, i.e. there exists constant $M > 0$ such that the inequality

$$\|\psi_0(x)\| := \max_{|x| \leq L/2} |\psi_0(x)| \leq M$$

holds.

(ii) Potential $V(x)$ is a periodic, integrable function on $[-L/2, L/2]$, with period $a \in (0, L)$ and Fourier expansion:

$$V(x) = \sum_{\ell \in G} v_\ell e^{i\ell x}, \quad (9)$$

where $G = \{\frac{2\pi n}{a} \mid n = 0, \pm 1, \pm 2, \dots\}$ and $v_\ell = \frac{1}{a} \int_{-a/2}^{a/2} V(x) e^{-i\ell x} dx$ are the Fourier coefficients of the function $V(x)$.

(iii) For some value of $\xi \neq 0$, series $C := \frac{2m}{\hbar^2} \sum_{\ell \in G} \frac{|v_\ell|}{\ell^2}$ satisfies the condition $0 < \xi(1 - C) < 1$.

Then, for an arbitrary $L > 0$, the sequence $\{\widehat{\psi}_n(x)\}_{n=0}^{\infty}$, defined by Eq.(8), uniformly converges on $[-L/2, L/2]$ to the solution of the Schrödinger Eq.(1).

Proof. According to assumptions (i)–(ii) of the theorem, as well as Eqs.(7), it follows:

$$|\psi_1(x)| \leq M\xi \left(1 + \frac{2m}{\hbar^2} \left| \sum_{\ell \in L} v_\ell \int dx \int e^{i\ell x} dx \right| \right) \leq M\xi(C+1),$$

$$|\psi_2(x)| \leq M\xi(C+1) \left(1 - \xi + \frac{2m\xi}{\hbar^2} \left| \sum_{\ell \in L} v_\ell \int dx \int e^{i\ell x} dx \right| \right)$$

$$\leq M\xi(C+1) [1 + \xi(C-1)], \quad \text{etc.}$$

In general, using the induction method, it can be easily proved that inequalities:

$$|\psi_j(x)| \leq M\xi(C+1) [1 + \xi(C-1)]^{j-1} \tag{10}$$

hold for each $j = 1, 2, \dots$. Now, for an arbitrary but fixed $x \in [-L/2, L/2]$, let $r(x)$ be the radius of convergence of the power series in Eq.(3). Applying the Cauchy-Hadamard theorem, as well as Eqs.(10) and the assumption (iii), we find that:

$$r(x) = \left[\limsup_{j \rightarrow \infty} |\psi_j(x)|^{1/j} \right]^{-1} \geq \lim_{j \rightarrow \infty} [M\xi(C+1)]^{-1/j} [1 + \xi(C-1)]^{-1+1/j}$$

$$\geq [1 + \xi(C-1)]^{-1} > 1.$$

for some $\xi \neq 0$. Thus, this power series converges at $p = 1$.

On the other hand, according to Eqs.(7)-(10), for the HPM approximations $\{\widehat{\psi}_n(x)\}_{n=0}^\infty$ we obtain:

$$\begin{aligned} |\widehat{\psi}_0(x)| &= |\psi_0(x)| \leq M, \\ |\widehat{\psi}_1(x)| &\leq |\widehat{\psi}_0(x)| + |\psi_1(x)| = M [1 + \xi(C+1)], \\ |\widehat{\psi}_2(x)| &\leq |\widehat{\psi}_1(x)| + |\psi_2(x)| = M [1 + \xi(C+1)(1 + (1 + \xi(C-1)))], \end{aligned}$$

and, in general,

$$|\widehat{\psi}_n(x)| \leq M \left[1 + \xi(C+1) \frac{1 - (1 + \xi(C-1))^n}{\xi(1-C)} \right], \quad n = 1, 2, \dots \tag{11}$$

In the limit case, when $n \rightarrow \infty$, inequalities (11) imply:

$$\begin{aligned} \left| \sum_{j=0}^\infty \psi_j(x) \right| &= \lim_{n \rightarrow \infty} |\widehat{\psi}_n(x)| \leq M \lim_{n \rightarrow \infty} \left[1 + \xi(C+1) \frac{1 - (1 + \xi(C-1))^n}{\xi(1-C)} \right] \\ &= \frac{2M}{1-C} < +\infty. \end{aligned}$$

Thus, the power series in Eq.(3) is absolutely convergent at $p = 1$, and uniformly converges on $[-L/2, L/2]$, for an arbitrary $L > 0$. According to Abel's theorem, it follows that homotopy function $\Psi(x, p)$, defined by Eq.(3), is continuous from the left at $p = 1$. Therefore, the Eq.(4) holds, i.e. the series $\sum_{j=0}^{\infty} \psi_j(x)$ is a solution of Eq.(1). \square

Remark 1 Thanks to the appropriate choices of the initial wave function $\psi_0(x)$, the condition (i) of the previous theorem can be easily fulfilled. Moreover, the condition (ii) is provided for an arbitrary periodic and integrable function $V(x)$. Finally, according the well-known results of the Fourier theory (see, for instance [18]), for the Fourier coefficients v_ℓ of the function $V(x)$ is valid $v_\ell/\ell^2 = w_\ell$, where w_ℓ are the Fourier coefficients of the function $W(x) := \int dx \int V(x) dx$. Obviously, $W(x)$ is also periodic and continuous on $[-L/2, L/2]$, for an arbitrary $L > 0$, so the series C is (always) convergent. Thus, the condition (iii) can be satisfied for some values of the auxiliary parameter $\xi \neq 0$.

3. VALIDATION OF THE HPM PROCEDURE

To justify application of the aforementioned HPM procedure in solving the Schrödinger equation with periodic potential two important cases will be considered:

A.) *Kronig-Penney model* representing a periodic arrangement of rectangular potential wells and potential barriers [20]. Assuming that potential barrier width is $a - b$ and the width of potential well is b , the potential can be described as:

$$V(x) := V_0 \left(1 - \sum_{n=-\infty}^{+\infty} \Pi \left(\frac{x - na}{b} \right) \right),$$

where a is the period, V_0 is the amplitude of potential (i.e. the depth of well or the height of the barrier), and

$$\Pi(x) := \begin{cases} 1, & |x| \leq 1/2, \\ 0, & |x| > 0, \end{cases}$$

is the so-called *rectangle function*. To obtaining HPM approximations of the wave function $\psi(x)$ on $[-L/2, L/2]$, we have taken the auxiliary parameter $\xi = 1$, and the initial approximation $\psi_0(x) = U_0(x) \exp(ikx)$. Here, $U_0(x) = \sqrt{2/L} \sin(N\pi x/L)$ with $N = 1, 2, \dots$, is the periodic wave function corresponding also to the solution of the Schrödinger Eq.(1) with the so-called *empty potential* $V(x) \equiv 0$ (see, for instance [21]).

To demonstrate the implementation of the HPM procedure in the considered case of rectangular wells and barriers we have chosen next values: the period $a = 2$, the width of barriers and wells $a - b = b = 1$, as $L = 12$ for the length of crystal (all

of these values are referred to E-10m), as it is shown in Fig. 1. (above left plot). From $L = Na$ follows that the number of unit cells is $N = 6$, while the wave number is $k = 2\pi/L = \pi/6$. Taking these values as well as $V_0 = \pi/a = \pi/2$ for amplitude of potential, numerical computation gives the corresponding value of electron energy $E = 2.621\text{eV}$. The convergence of thus obtained the HPM approximations $\hat{\psi}_n(x)$, of the order $n = 0, 1, 2, \dots, 6$, is shown in Fig. 1, where their density functions $|\hat{\psi}_n(x)|^2$, as well as the real and imaginary parts are plotted. As it can be easily seen, for $n \geq 1$, the HPM approximations $\{\hat{\psi}_n(x)\}$ show a high degree of convergence, which is also formally confirmed (see Table 1, below).

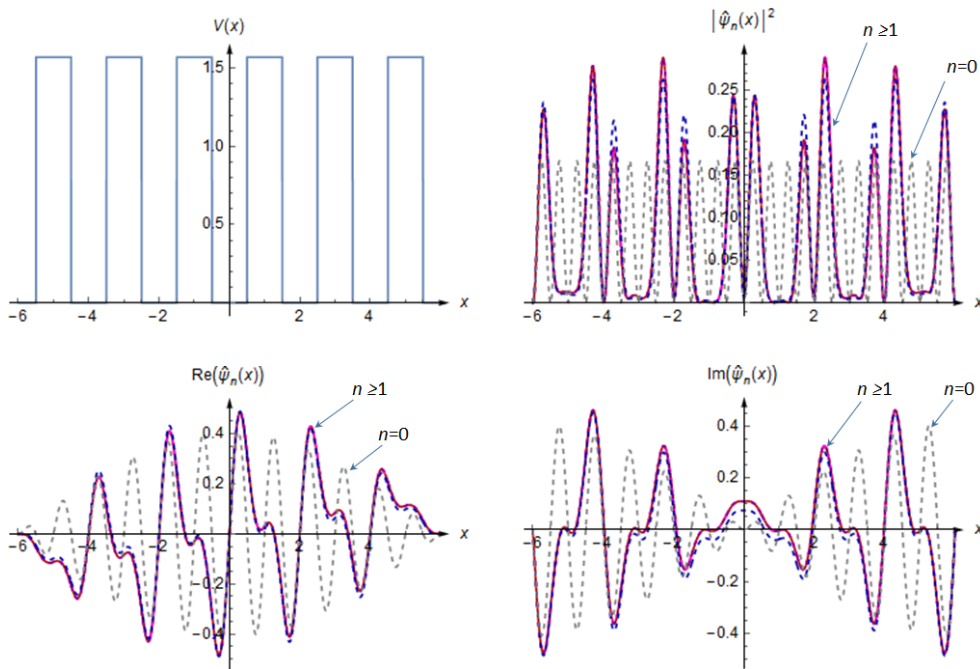


Fig. 1 – Graphs of the Kronig-Penney potential (above left), as well as the HPM-approximations $\hat{\psi}_n(x)$ of the wave function $\psi(x)$: density functions (above right), real parts (bellow left) and imaginary parts (bellow right).

Notice that in original Kronig-Penney model there are two wave functions calculated by solving Schrödinger equation separately for the regions of barrier and well. Using HPM procedure does not require the separate solving of Schrödinger equation in mentioned regions, but along the whole length of observed interval. We can conclude that HPM approximations obtained here are appropriate for the both of potential regions: they take the form of wave function for empty potential in the well, while ones represent the transmitted particles through barrier region.

B.) Considered, as the second case, the periodic potential given by following function $V(x) := V_0 \cos(\omega x)$. This function, in general, corresponds to the well-known *Mathieu equation*, which has found important applications in describing, for instance, the flux lattice in superconductors, the wave motion in optical lattice, or in some other periodic media [22]. With the aim to illustrate the application of the HPM procedure to the case of a particle in considered periodic potential, we have chosen that value of the amplitude of the potential be $V_0 = 1$, as well as $\omega = 2$ which implies the period $a = \pi$ (Fig. 2, above left plot). For comparison with the previously considered Kronig-Penney model, also is assumed that $N = 6$, i.e. the length of the observed interval is $L = 6\pi$, and value of the wave vector is $k = 2\pi/L = 1/3$, which implies the appropriate energy $E(k) = 2.209\text{eV}$. Further on, the HPM approximations were computed with the same auxiliary parameter $\xi = 1$ and the initial approximation $\psi_0(x)$. The HPM approximations $\{\hat{\psi}_n(x)\}$, when $n \geq 1$, obtained in the case of this periodic potential also fast converge to the exact solution of the Eq.(1), as it can be easily seen in Fig. 2.

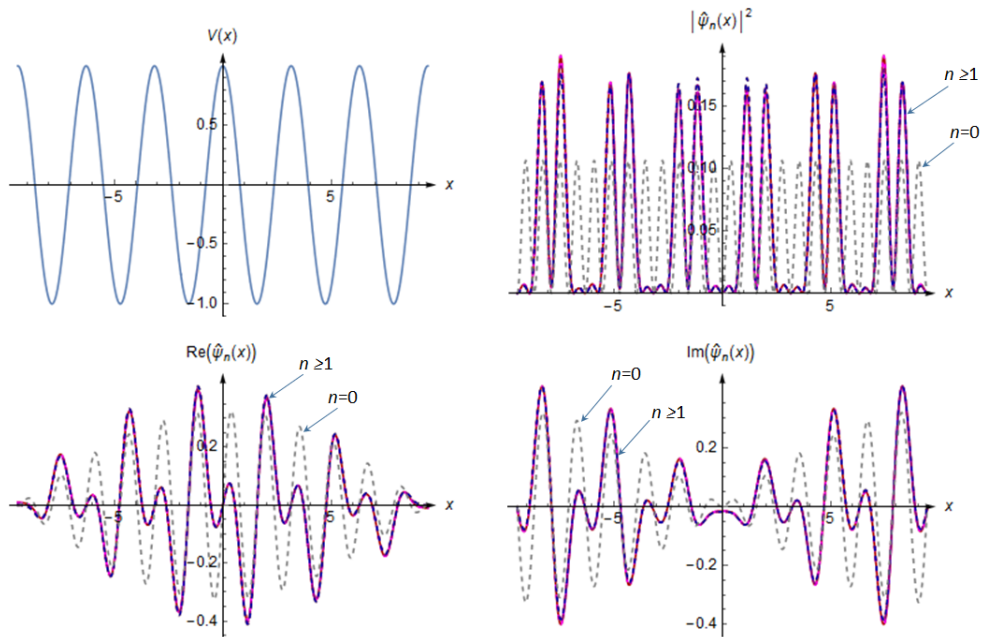


Fig. 2 – Graphs of the Mathieu's periodic function (above left), as well as the HPM-approximations: density functions (above right), real parts (bellow left) and imaginary parts (bellow right).

In addition, for each of the HPM approximation $\hat{\psi}_n(x)$, $n = 1, 2, \dots, 6$, it was computed *the maximum approximation errors*:

$$Err(\widehat{\psi}_n) := \max_{|x| \leq L/2} \left| \frac{d^2 \widehat{\psi}_n(x)}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)] \widehat{\psi}_n(x) \right|,$$

as well as *the maximum iteration differences*:

$$\left\| \widehat{\psi}_n - \widehat{\psi}_{n-1} \right\| := \max_{|x| \leq L/2} \left| \widehat{\psi}_n(x) - \widehat{\psi}_{n-1}(x) \right|.$$

Let us emphasize that both of these values represent the measures of convergence of the HPM approximations $\{\widehat{\psi}_n(x)\}$, in comparison to their approximations order $n \geq 1$. These measures obtained for both of the aforementioned series of the HPM approximations, labeled as *A* and *B*, respectively, are given in Table 1. The whole computation procedure has been realized and implemented in the software package MATHEMATICA 11.0. As it can be easily seen, the HPM approximations converge somewhat faster in the case of *B*-series. However, it should be pointed out that the both series of the HPM approximations have approximately the same level of accuracy, of the order 10^{-5} , which they achieve already for $n \geq 5$.

Table 1.

Maximum approximation errors and iteration differences of the HPM approximations $\{\widehat{\psi}_n(x)\}$.

Approximation order (n)	$Err(\widehat{\psi}_n)$		$\left\ \widehat{\psi}_n - \widehat{\psi}_{n-1} \right\ $	
	A-series	B-series	A-series	B-series
1	1.82E-02	1.72E-02	7.44E-01	3.53E-01
2	2.26E-03	1.65E-03	3.92E-02	5.79E-03
3	7.92E-04	2.30E-04	1.05E-03	4.88E-04
4	1.64E-04	9.77E-05	2.76E-04	8.76E-05
5	9.02E-05	2.50E-05	8.31E-05	5.14E-05
6	8.48E-05	2.13E-05	8.27E-06	6.07E-06

4. CONCLUSION

In this work, the electron moving in one dimensional lattice with an arbitrary periodic potential is considered. By using periodic boundary conditions (PBC) and Bloch's theorem the system has been treated as the one-dimensional one of finite length which shows the discrete translational invariance. For approximate analytical solving the appropriate Schrödinger equation, the Homotopy Perturbation Method (HPM) has been proposed. The existence and convergence of the so-called HPM approximations was discussed and shown in general case. Also, two illustrative examples were given to confirm the suitability and the applicability of the HPM in solving this kind of problem.

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