A Hyper-Block Self-Consistent Approach to Nonlinear Schrodinger Equations: Breeding, Metamorphosis and Killing of Hofstadter Butterflies

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Abstract

Nonlinear Schrödinger equations play essential roles in different physics and engineering fields. In this paper, a hyper-block finite-difference self-consistent method (HFDSCF) is employed to solve this stationary nonlinear eigenvalue equation and demonstrated its accuracy. By comparing the results with the Sinc self-consistent (SSCF) method and exact available results, we show that the HFDSCF method gives quantum states with high accuracy and can even solve the strongly nonlinear Schrodinger equations. Then, by applying our method to Hofstadter butterfly problem, we describe the breeding, metamorphosis and killing of these butterflies by using nonlinear interactions as well as two constant length multi-well and sinusoidal potentials.

Keywords: Nonlinear Schrodinger equation, Hyper-block finite difference self-consistent method, Stationary states, Constant length multi-well potentials, Hofstadter butterflies.

1. Introduction

Hofstadter butterfly was first reported by Douglas Hofstadter in 1976 [1]. The Hofstadter butterfly can be obtained as the fractal energy spectrum if we solve the Schrodinger equation for an electron under a uniform magnetic field in a two dimensional quantum system [2]. The self-similarity takes place with the frustrated competition between the lattice constant and the magnetic length scale. In order to experimentally

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realize the Hofstadter butterflies, many attempts have been done. The first investigation of the Hofstadter spectrum in semiconductor superlattice was reported by Schlosser et al. [3]. Then it realized in graphene moiré superlattices [4], and one-dimensional optical superlattices [5-6]. Hofstadter butterfly also realized in ultracold atoms [7-8], Grapheme [9], and superconducting qubits [10]. Effects of interactions on the Hofstadter butterfly have also been discussed previously [11-12].

The numerical solution of nonlinear Schrödinger equations usually needs complicated numerical programming [13]. In recent research by Tsoy et al [14], it is explicitly specified that "*direct numerical solution of such a problem is a difficult task*". Some of the existing methods to solve this problem are: transfer matrix [15], time-splitting schema [16], inverse scattering approach [17], compact finite difference method [18], neural network [19] and relaxation procedure [20], etc.

Among different numerical approach to study the physical differential equations, the finite difference methods have been among the most appealing ones. These methods have been applied to Schrodinger equations from long time ago [21-27]. However, the nonlinear Schrodinger equation appears by adding a nonlinear term to the Schrodinger equation. This nonlinear term can have different interesting sources due to the many-body interactions or the coupling with the environment. For instance the nonlinearity can be seen in the system including of electron-electron interactions [28], electron-phonon interactions or polaronic problems [29], spin domains of spinor Bose-Einstein condensates in an optical lattice [30], nonlinear theory of elementary particles [31], plasma physics [32], biomolecular dynamics [33], solitons properties [34], nonlinear excitations in magnets [35], nonlinear crystals [36], etc.

In the current study, we present a direct, simple and efficient hyper-block finite difference self-consistent method to solve the nonlinear Schrödinger equation which has two important characteristics: A) in addition to the ground state eigenvalue, it can evaluate the excited states in a more accurate manner than the conventional finite difference self-consistent methods can do. B) It can provide us the correct energy spectrum of a more strongly nonlinear systems than that of the finite difference self-consistent methods can do.

2. Formalism

We start with the following nonlinear Schrodinger equation [37-38],

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)+V(x)\psi(x)+G\left|\psi(x)\right|^2\psi(x)=E\psi(x), \qquad (1)$$

Where $\hbar$ and m are the Planck constant and effective mass of electron in each mono-layer, respectively. The parameter Q is a nonlinear parameter which in a semiconducting system it can determine the strength of the electron-electron interaction. The potential function can also be defined as,

$$V_1(x)=2\ \mathrm{Cos}\ (2\pi\alpha x+\theta) \qquad (2\text{-}1)$$

$$V_2(x)=\begin{cases}V_{conf} & i=1,3,\ldots\\ 0 & i=2,4,\ldots\end{cases};\quad \frac{i-1}{2NOW+1}L<x<\frac{i}{2NOW+1}L \qquad (2\text{-}2)$$

$$V_3(x)=\mathrm{A\ Sin}\ (\omega x) \qquad (3\text{-}1)$$

Where *NOW* is the number of wells, V_{conf} is a piecewise potential function, 2L in the system length. 'i' shows the i'th well or barrier in the system. The parameter θ is the phase. 'A' and ω are also two parameters that we try to find this effects on the Hofstadter Butterflies. Here, we use the potential $V_1(x)$ to plot the Hofstadter Butterflies and by adding the $V_2(x)$ or $V_2(x)$ (separately) we try to handle it.

In the procedure of plotting the Hofstadter Butterflies, we choose a rational $\alpha = p/q$ with p and q coprime. Therefore, Equation (1) is periodic under x $\rightarrow$ x + q. Now, the wave-functions are Bloch functions ($\psi_k(x)=e^{ikx}u_k(x)$), where produce q bands in the k-space. For a specified $\alpha = p/q$, q bands can exist in the butterfly spectrum. In order to solve the equation (1), we have used a finite difference method. However, since there is a nonlinear term in this equation, we uses a self-consistent iteration to find its energy eigenvalues and eigenfunctions.

3. Hyper-block finite difference self-consistent method

We solve the equation (1) by means of a finite difference self-consistent method (FDSCF). For this purpose, first we assume $\mu=-\hbar^2/m(\Delta x)^2$ and discretize the x-domain with step size Δx. Therefore, equation (1) can be written as,

$$\mu(\psi_{i-1}-2\psi_i+\psi_{i+1})+V_i\psi_i+G\left|\psi_i\right|^2\psi_i=E\psi_i, \qquad (3)$$

This equation is a tri-diagonal nonlinear matrix eigenvalue problem. The diagonal Hamiltonian matrix elements are $-\mu+V_i+G\left|\psi_i\right|^2$ and the off-diagonal Hamiltonian

matrix elements are $-\mu/2$. We show the j[th] eigen-value and j[th] eigen-function at k[th] iteration with $E^{(j,k)}$ and $\psi^{(j,k)}$, respectively. In a nutshell, equation (2) could be written as,

$$-\mu\left(\psi_{i-1}^{(j,k)}-2\psi_i^{(j,k)}+\psi_{i+1}^{(j,k)}\right)+V_i\psi_i^{(j,k)}+G\left|\psi_i^{(j,k-1)}\right|^2\psi_i^{(j,k)}=E\,\psi_i^{(j,k)}, \qquad (4)$$

We can use a self-consistent iteration scheme to solve this nonlinear equation whose steps are presented in the following:

1- Set G= 0 and solve equation (3) and ontain $E^{(0,0)}$ and $\psi^{(0,0)}$.

2- Put $\psi^{(0,0)}$ in equation (3) as a coefficient of G and solved this equation again.

3- Repeate the above steps to achieve the desired accuracy in energy eigen-values and eigen-functions. Moreover, wrote the convergence criterion as $\left|E^{(j,k)}-E^{(j,k-1)}\right|<\varepsilon$, where ε was the desired accuracy. In this study, we set $\varepsilon=0.0001$.

Here, just a state contributes in the SCF procedure (i.e. the ground state). This SCF method gave us the ground state with maximum accuracy and the excited sates had ascending errors with respect to the excited state index. Now, we present a novel hyper-block approach to remove this deficiency. For this purpose, we use the following approach. At first, by assuming N number of discretization points we rewrite the equation (3) as,

$$\left[H_0\right]_{N\times N}\left[\psi^{(j,k)}\right]_{N\times 1}+G\left[\left|\psi^{(j,k-1)}\right|^2\right]_{N\times N}\left[\psi^{(j,k)}\right]_{N\times 1}=E\left[\psi^{(j,k)}\right]_{N\times 1}, \qquad (5)$$

By assuming M participating states in the SCF procedure, we can build the following $(NM)\times(NM)$ hyper-block,

$$\begin{bmatrix} H_0 & 0 & 0 & \cdots \\ 0 & H_0 & & \\ 0 & & H_0 & \\ \vdots & & & \ddots \end{bmatrix}_{NM\times NM}\left[\psi^{(k)}\right]_{NM\times 1}+$$

$$G\begin{bmatrix} \left|\psi^{(0,k-1)}\right|^2 & 0 & 0 & \cdots \\ 0 & \left|\psi^{(1,k-1)}\right|^2 & & \\ 0 & & \left|\psi^{(2,k-1)}\right|^2 & \\ \vdots & & & \ddots \end{bmatrix}_{NM\times NM}\left[\psi^{(k)}\right]_{NM\times 1}=E\left[\psi^{(k)}\right]_{NM\times 1}, \qquad (6)$$

Again, we use the above-mentioned iteration schema and convergence criterion $\left|E^{(j,k)} - E^{(j,k-1)}\right| < \varepsilon$, where ε was the desired accuracy. However, this method produces some fake eigenstates that can simply be identified. If we use the M number of states participating in the SCF procedure, each eigenstate will has (M-1) fake eigenstates that place exactly after the corresponding true eigenstate and can easily be removed. Another numerical concern can be the size of the hyper-block which grows rapidly by increasing the number of states participate in the SCF procedure. Fortunately, since the Hamiltonian matrix H_0 is a tridiagonal which is very sparse, therefore the resulting hyper-block matrix is also a sparse tri-diagonal matrix which its diagonalization is very simpler than diagonalization of dense matrices.

In the tables (1) and (2), we have presented four smallest energy levels of a one dimensional Schrodinger equation with G=1 and G=5, respectively. There, we have compared the results obtained by HFDSCF, FDSCF, SSCF and exact results of the Ref. [39]. As these tables show, our new algorithm HFDSCF has maximum accuracy among the implemented methods.

Table 1: Four smallest energy levels of a one dimensional Schrodinger equation with G=1 obtained by HFDSCF and FDSCF approaches and compared with SSCF and exact results of the Ref. [39]. In the parenthesis, we have given the number of nodes (in the SCF) and discretization points (in the HFDSCF and FDSCF) methods.

Energy levels	SSCF (61)	Ref.[39]	FDSCF(3000)	HFDSCF (3000)
E_0	0.462733782	0.462579418	0.461433722	0.461433722
E_1	4.445020299	4.179929550	4.437927578	4.177151742
E_2	10.60881429	10.35117007	10.59235808	10.33829948
E_3	19.24464308	18.98801387	19.21509222	18.96298325

Also, table (2) shows that our new method HFDSCF has very higher accuracy than other studied methods when the Schrodinger equation is more nonlinear. This fact is more visible when we compare these methods at higher excited states of the table (2).

Table 2: Four smallest energy levels of a one dimensional Schrodinger equation with G=5 obtained by HFDSCF and FDSCF approaches and compared with SSCF and exact results of the Ref. [39]. In the parenthesis, we have given the number of nodes (in the SSCF) and discretization points (in the HFDSCF and FDSCF) methods.

Energy levels	SSCF (61)	Ref. [39]	FDSCF(3000)	HFDSCF(3000)
E0	-3.399698328	-3.400181294	-3.399742399	-3.399742399

E1	2.799662851	1.049048570	2.794608728	1.1423848234
E2	8.756412749	7.297398975	8.741640092	7.3236563228
E3	17.32571098	15.95895638	17.29740312	15.955561130

3. Results and Discussions

In the previous section, we have solved the nonlinear Schrödinger equation (1) by using the described hyper-block finite-difference self-consistent method and compared the results with the conventional finite difference self-consistent method, Sink method and exact results. Thus, we have verified the accuracy of our method.

In the present section, we have applied the HFDSCF to the equation (4) and studied the Hofstadter butterflies. In the figure (1), we have depicted the Hofstadter butterfly for a linear system with G=0. This figure can help us to compare the effect of different parameters on it. In this figure, we observe a butterfly that has two major minigaps in each wing as well as few minor minigaps. Here, each Bloch band divides into q bands. The gaps between these bands lead to a butterfly-like pattern and therefore known as Hofstadter butterfly.

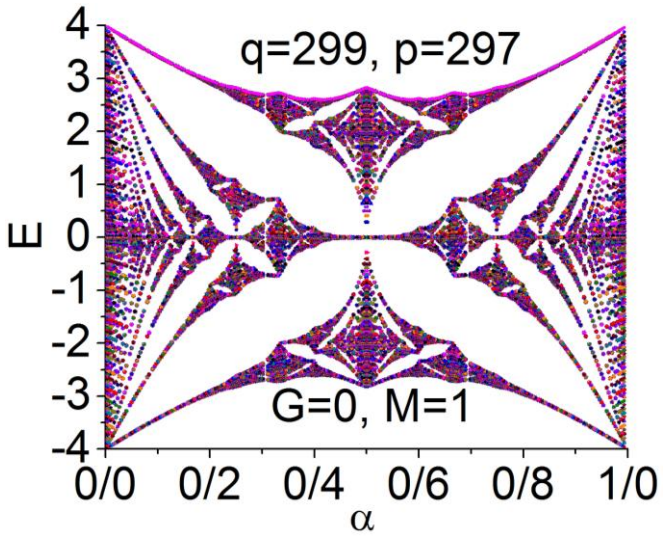

Figure 1: Variation of the energy eigenvalues of the equation (4) as a function of the parameter α. Here, a linear system with G=0 is assumed.

In the figure (2), we have presented the variation of the energy eigenvalues of the equation (4) as a function of the parameter α for two nonlinear systems with nonlinearity strengths G=1 and G=5. The assumed integer numbers p and q, the number of participating states in the SCF procedure M and nonlinearity parameter G are specified on the corresponding panel. Comparing the panel (A) of the figure (2) with the figure (1)

reveals that by adding a small nonlinearity to the system of the figure (1), few allowed states in the energy gaps of the figure (1) is produced. However, by increasing the nonlinearity strength to 5 (see panel B of figure 2), the number of these allowed state increases their position extend to central parts of the energy gaps. In the interacting systems, the interaction itself can introduce a new length scale in the problem which can affect the Hofstadter butterfly topology.

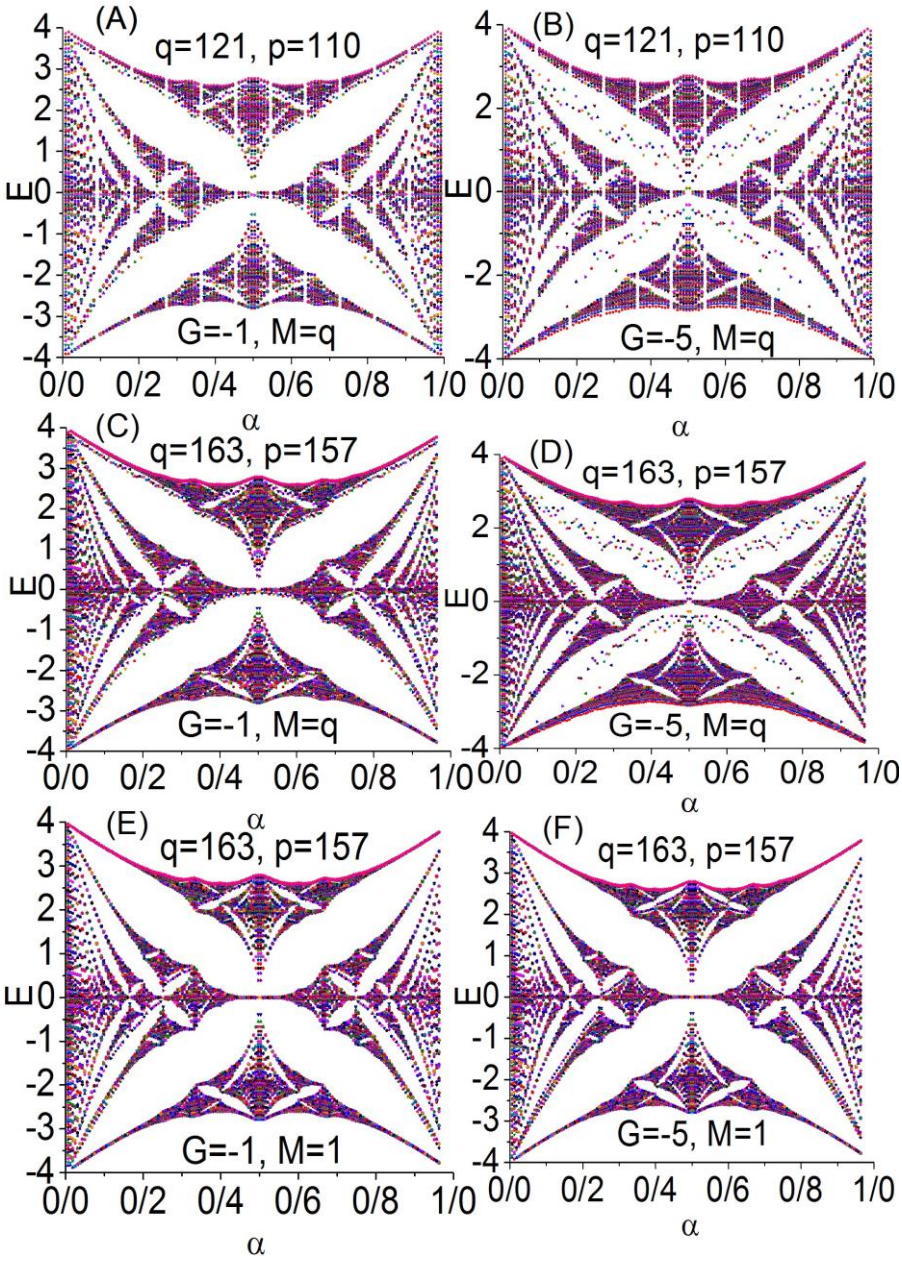

Figure 2: Variation of the energy eigenvalues of the equation (4) as a function of the parameter α. The assumed p, q, M and G are specified on the corresponding panel.

This fact shows that the nonlinearity can play an essential role in the energy band structures and subsequently on the physical properties of the assumed system. Panels (C)

and (D) are the same as the panels (A) and (B), respectively. However, in these new panels we have assumed larger values for the parameters p and q and more clearly show the new allowed stated in the gap regions. Also, panels (E) and (F) are the same as the panels (C) and (D), respectively. However, in these new panels we have sown the effect of the number of participating states in the SCF procedure, i.e. M, on the Hofstadter butterfly. As these panels show, using 'one' state in the procedure of the SCF does not lead to correct energy eigenvalues and therefore the Hofstadter butterfly does not correctly produce (see table 2). This is because the allowed states in the gap regions does not appear in the panels (E) and (F).

In the figure (3), we have shown the effect of the number of wells NOW (in Eq. 2-2) on the variation of the energy eigenvalues of the equation (4) as a function of the parameter α. Here, we assumed p=157, q=163, M=1 and G=0. The number of wells NOW is specified on the corresponding panel. To plot this figure, we have used the potential $V_1(x)+V_2(x)$ in the Schrodinger equation (4). As these panels show, we can tune the number of gaps, their widths, and their positions by changing the number of wells NOW.

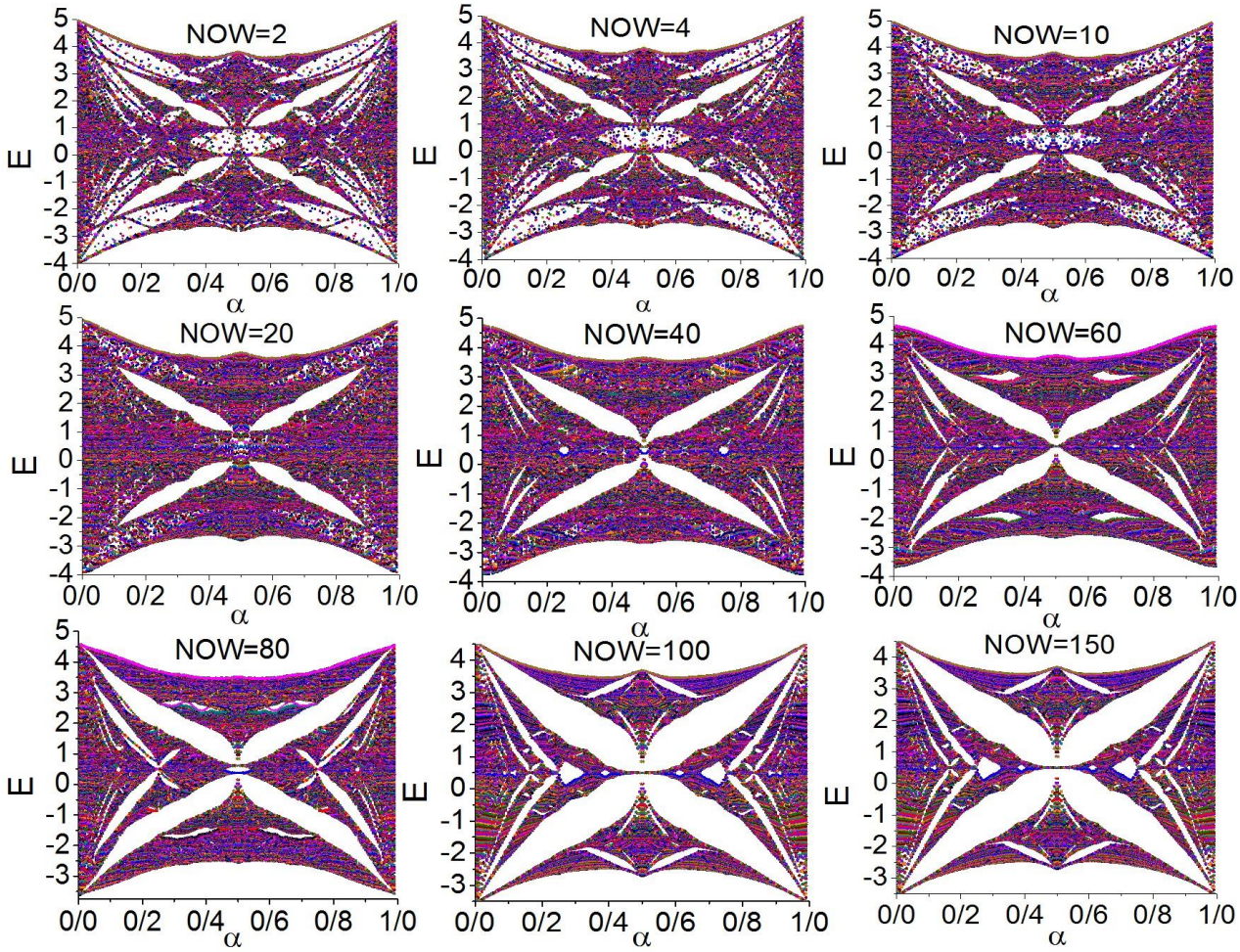

Figure 3: Variation of the energy eigenvalues of the equation (4) as a function of the parameter α. We assumed p=157, q=163, M=1 and G=0. The number of wells NOW in Eq. 2-2 is specified on the corresponding panel.

Therefore, of the increasing the NOW leads to evolution Hofstadter butterflies to new shapes of them. The behavior of the Hofstadter butterflies can be described by merging and splitting of the energy bands which are among the signatures of the change in the symmetry properties of the assumed system.

Now, we study the effect of the potential depth V_{conf} in the equation (2-2) on the variation of the energy eigenvalues of the equation (4) as a function of the parameter α. The results have been shown in figure (4). Here, we have assumed p=157, q=163, M=1, and G=0. The corresponding V_{conf} in Eq. 2-2 is specified on the corresponding panel. As these panels show, by increasing the parameter V_{conf}, two distinct Hofstadter butterflies appear (i.e. breeding). Another fact is that in all of the studied panels the symmetry of the butterflies with respect to axes α=0.5 and E=0 is still preserved.

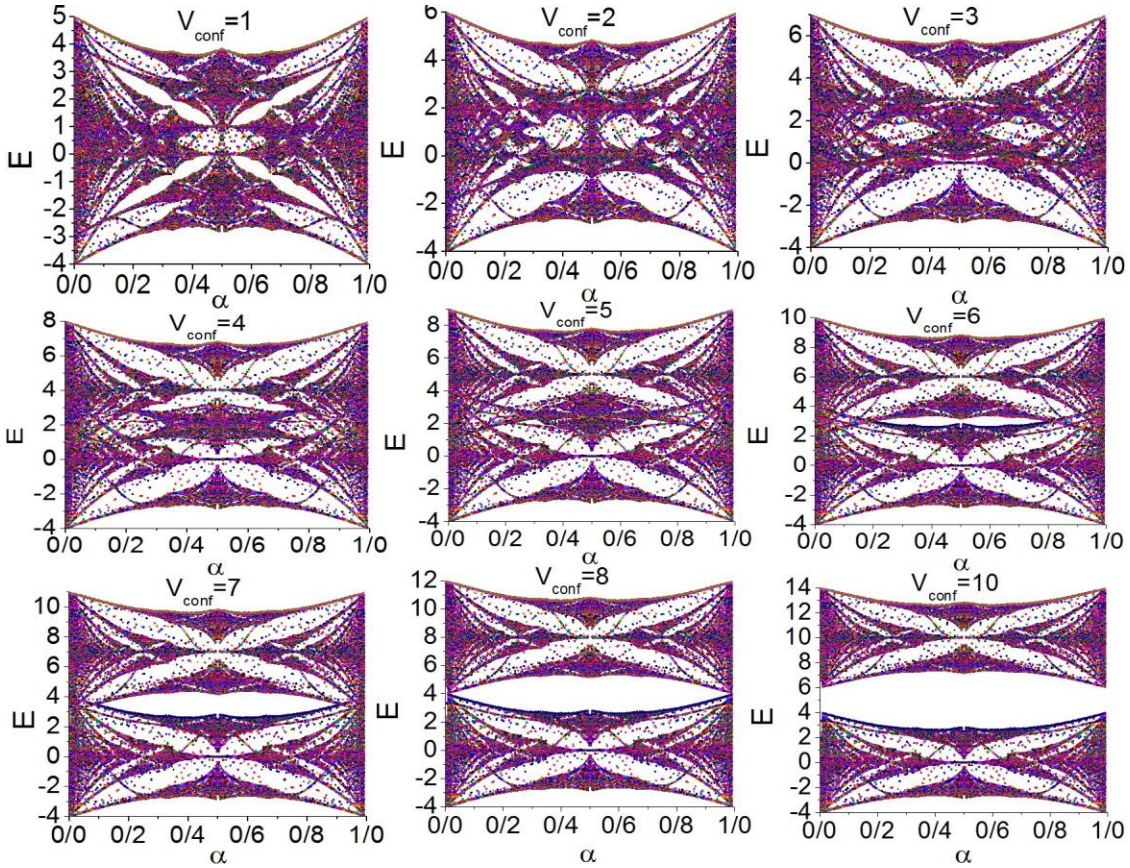

Figure 4: Variation of the energy eigenvalues of the equation (4) as a function of the parameter α. We assumed p=157, q=163, M=1 and G=0. The number of wells NOW in Eq. 2-2 is specified on the corresponding panel.

At this point, we use the potential $V_1(x)+V_3(x)$ in the Schrodinger equation (4) to explore the effect of sinusoidal external potential on the Hofstadter butterflies. As these panels show, by increasing the coefficient 'A' in the equation 2-3, the number of gaps decreases and consequently the butterfly will be killed. However, this additional potential cannot break the symmetries of the Hofstadter butterfly. Also, if we decrease the parameter 'A', the metamorphosis of the Hofstadter butterfly from a Gaussian gap to a perfect butterfly is visible.

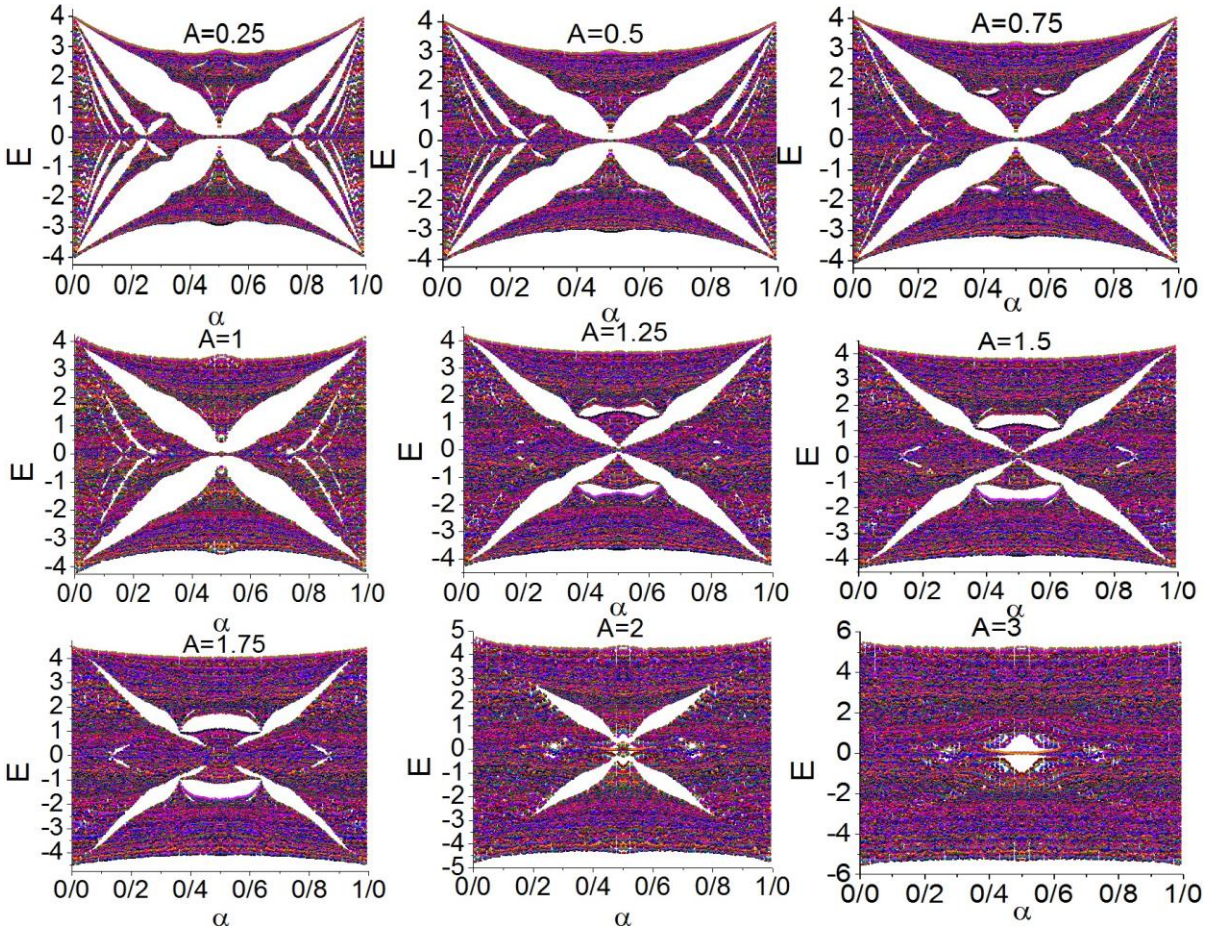

Figure 5: Variation of the energy eigenvalues of the equation (4) as a function of the parameter α. We assumed p=157, q=163, M=1 and G=0. The coefficient 'A' in Eq. 2-3 is specified on the corresponding panel.

Finally, in figure (6) we have plotted the variation of the energy eigenvalues of the equation (4) as a function of the parameter α. Again, we assumed p=157, q=163, M=1 and G=0. The argument 'ω' in Eq. 2-3 is specified on the corresponding panel. As these panels show, the effect of this parameter on the Energy spectrum evolution (i.e. Hofstadter butterfly) is very complicated. The major energy gaps of the butterfly disappears by changing the argument 'ω'. Thus, by using the argument 'ω', we can kill the

Hofstadter butterfly or change its shape and its number of wings. However, the symmetries of the Hofstadter butterfly do not break by changing the arguments 'ω'. The evolution of the Hofstadter butterfly occurs by using the closing procedure which is achieved by infinitely many closures and re-openings of the new gaps.

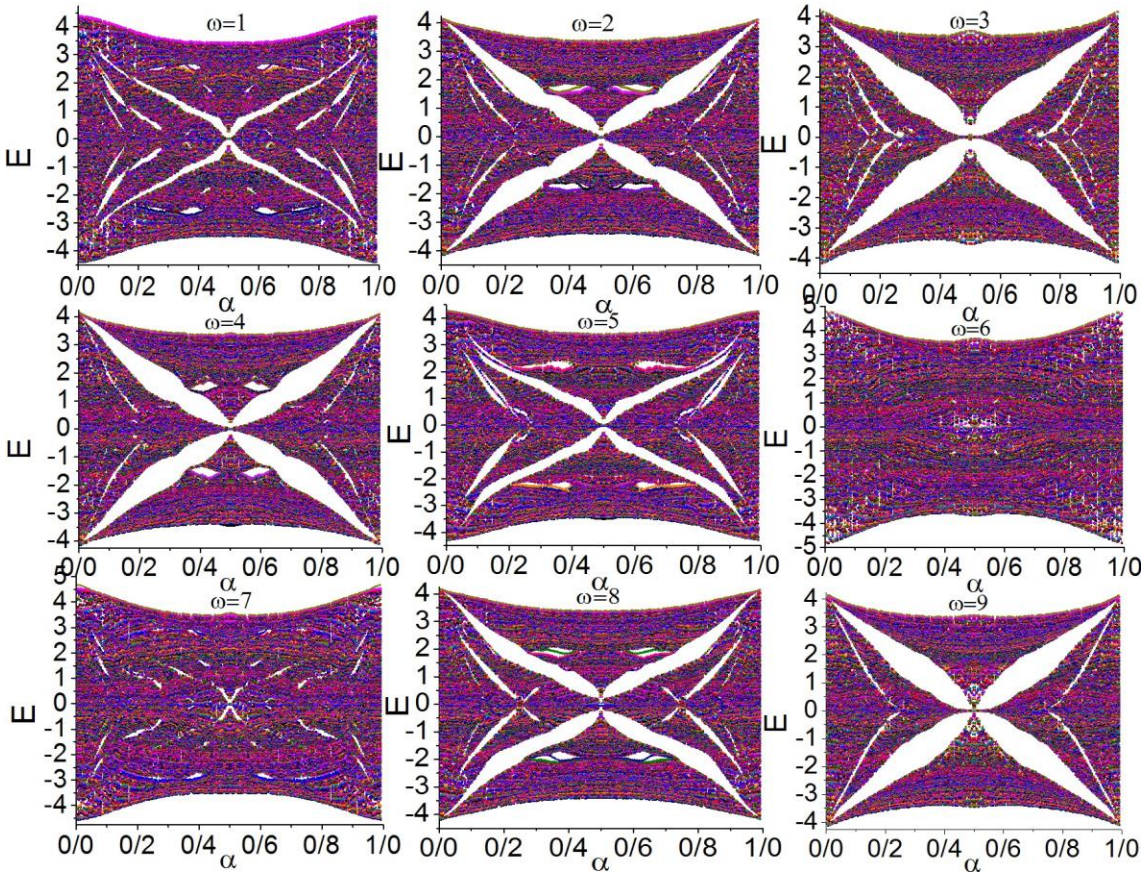

Figure 6: Variation of the energy eigenvalues of the equation (4) as a function of the parameter α. We assumed p=157, q=163, M=1 and G=0. The parameter 'ω' in Eq. 2-3 is specified on the corresponding panel.

Conclusion

In the current study, we used a hyper-block finite-difference self-consistent approach to solving a nonlinear Schrödinger equation. We showed that the hyper-block finite-difference self-consistent method was convergent, accurate, simple and efficient to obtain the energy spectrum of the nonlinear Schrodinger equations. Our new approach gave us the ground and excited states with good accuracies. It also could provide us the energy spectrum of strongly nonlinear Schrodinger equations. By using our new method in the Hofstadter butterfly problem, we showed that the nonlinearity can produce some new allowed state which their position can extend to central parts of the energy gaps. The

number of gaps and their positions could be tuned by adjusting the number of wells NOW. By using an additional sinusoidal potential we described the breeding, metamorphosis and killing of the Hofstadter butterflies.

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