

# PH4505/PAP723 Homework 3

AY17/18 Semester 2

**Instructions for PH4505 students:** You are to choose 2 of the 3 questions to submit as your graded assignment. Every plot produced by your programs should have clear x and y axis labels. If more than one curve is shown on a single plot, the two curves should be labeled clearly. For full marks, code must follow good programming style. Your code should be commented; there should be no cryptic variable and function names (like abc); and the program structure should be modular (e.g. numerical constants should be defined in one place instead of being scattered throughout the code).

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## 1. The Harper Model

The Harper model is a theoretical quantum system consisting of a particle existing along a discrete one-dimensional “chain”. The chain consists of a set of discrete points labeled by  $n = 0, 1, \dots, N - 1$ . A quantum state is described by a complex vector,

$$\psi = \begin{bmatrix} \psi_0 \\ \vdots \\ \psi_{N-1} \end{bmatrix}, \text{ where } \sum_{n=0}^{N-1} |\psi_n|^2 = 1. \quad (1)$$

For each  $n$ , the complex number  $\psi_n$  gives the “quantum wavefunction” at position  $n$ ; the probability to observe the particle at that position  $|\psi_n|^2$ .

An “energy state” is a quantum state that satisfies the eigenvalue problem

$$H\psi = E\psi, \quad (2)$$

where  $E \in \mathbb{R}$  is the energy and  $H$  is an  $N \times N$  matrix called the “Hamiltonian”. The Hamiltonian has the form

$$H = \begin{bmatrix} V_0 & 1 & & \\ 1 & V_1 & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & V_{N-1} \end{bmatrix}, \text{ where } V_n = W \cos(2\pi\alpha n + \phi). \quad (3)$$

The diagonal entries  $V_n$  represent the potential along the 1D chain. This potential varies sinusoidally, with amplitude  $W$  and phase parameters  $\alpha$  and  $\phi$ . If  $\alpha$  is irrational, the potential function is “aperiodic” (i.e. it does not repeat with  $n$ ).

- (a) Write a function that takes in 4 arguments: **N**, the Hamiltonian size, **W**, the amplitude of the potential function, **phi** the parameter  $\phi$  in the potential function and **alpha**, the parameter  $\alpha$  in the potential function. The function should return the Harper model’s Hamiltonian matrix in sparse matrix form.
- (b) Write a function that plots the “energy-level diagram” of  $E$  versus  $\alpha$ : i.e., for each value of  $\alpha$  on the horizontal axis, plot the discrete energies  $E$  (the eigenvalues of  $H$ ) on the vertical. Set  $N = 199$ ,  $W = 2.0$  and  $\phi = 0.0$ .
- (c) Write a function which plots the probability density  $|\psi_n|^2$  for the ground state

versus position  $n$ . Do this for several choices of  $W$ , in the range  $1.2 \leq W \leq 2.5$ . Label all plots clearly; you may use subplots for clarity. Set  $N = 199$ ,  $\alpha = 1.618034$  and  $\phi = 0.0$ .

*Discuss in code comments:* How does the behavior of  $|\psi_n|^2$  change with  $W$ ?

- (d) The “inverse participation ratio” (IPR) of a wavefunction is the quantity

$$IPR[\psi] = \sum_n |\psi_n|^4 . \quad (4)$$

It is a crude measure of whether a wavefunction is “localized” (i.e., concentrated near a few points) or “extended” (i.e. spread out over the whole chain). Write a function which plots the mean IPR of the Harper model’s energy states, versus  $W$ . Use the same arguments as 1c.

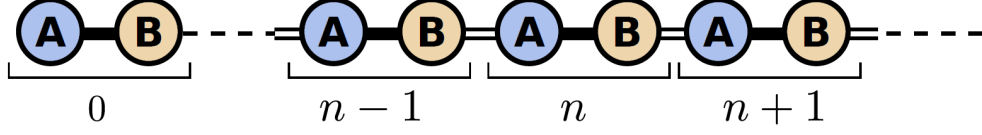
*Discuss in code comments:* Is the IPR large or small for localized states? Estimate the critical  $W$  where localization begins to occur.

- (e) We now consider the  $\phi$  parameter. Write a function which plots the energy levels versus  $\phi \in [-\pi, \pi]$ . Choose appropriate values for the other parameters, but let  $\alpha$  be irrational. You should find that most of the energies cluster into “bands”. However, there exist some states lying outside the bands. In a separate subplot or figure, plot the probability density for one or more of these “out-of-band” states. In the energy level plot, use markers to indicate the states you are plotting.

*Discuss in code comments:* How do the in-band and out-of-band states differ? How does this phenomenon vary with  $\alpha$ ?

## 2. The Su-Schrieffer-Heeger Model

The Su-Schrieffer-Heeger (SSH) model describes a theoretical quantum particle that occupies discrete sites along a one-dimensional “chain”. The chain alternates periodically between “A sites” and “B sites”, as shown below:



We enumerate pairs of sites with a “cell index”  $n \in \mathbb{N}$ , as shown. Cell 0, at the chain’s left edge, is assumed to start with an  $A$  site. (We will discuss the right edge later.)

The “wavefunction” of the particle on this chain consists of a set of complex numbers  $\{\psi_{\mu,n}\}$ , where  $\mu \in \{A, B\}$  and  $n \in \mathbb{N}$  is the aforementioned cell index. The probability of observing the particle at a given point is  $|\psi_{\mu,n}|^2$ , and these probabilities sum to unity:

$$\sum_{\mu=A,B} \sum_{n=0,\dots} |\psi_{\mu,n}|^2 = 1. \quad (5)$$

We can group  $\{\psi_{\mu,n}\}$  into a complex vector, called the “quantum state vector”:

$$\vec{\psi} = \begin{bmatrix} \psi_{A,0} \\ \psi_{B,0} \\ \vdots \\ \psi_{A,n} \\ \psi_{B,n} \\ \vdots \end{bmatrix} \quad (6)$$

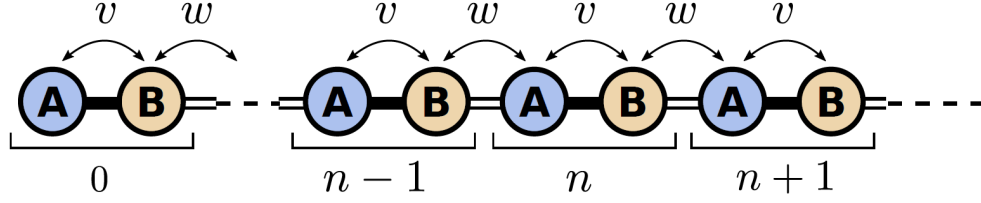
An “energy state” of energy  $E$  is a quantum state that satisfies the Schrödinger equation

$$H\vec{\psi} = E\vec{\psi} \quad (7)$$

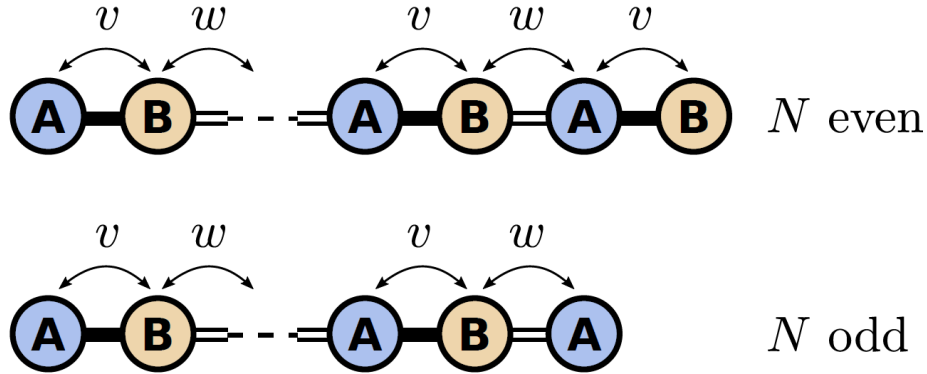
where  $H$  is the Hamiltonian, a Hermitian matrix. The non-zero elements of  $H$  are

$$H_{A,n;B,n} = H_{B,n;A,n} = \nu, \quad H_{A,n+1;B,n} = H_{B,n;A,n+1} = w, \quad (8)$$

for some  $\nu, w \in \mathbb{R}$ . All other elements are zero. This can be thought of  $A - B$  links having “hopping amplitude”  $\nu$ , and  $B - A$  links having hopping amplitude  $w$ :



As mentioned, the chain's left edge always start with an  $A$  site. As for the right edge, it ends on a  $B$  site if the total number of sites,  $N$ , is even; and on an  $A$  site if  $N$  is odd:



- (a) Write a function that takes 3 arguments  $N$ , the total number of sites and  $v$  and  $w$ , the hopping amplitudes defined in Eq. (8). The function should return the SSH model's Hamiltonian in sparse matrix format.
- (b) For an  $N$ -site chain, the Schrödinger equation in Eq. (7) defines  $N$  energy levels  $\{E_0, \dots, E_{N-1}\}$ . To study how these vary with the models parameters, write a function that plots the energy levels with  $N = 50$ ,  $vspan = (-2, 2, 100)$  and  $w = 1.0$ . The function should generate an “energy-level plot” of  $E_n$  (vertical axis) versus  $v$  (horizontal axis), with  $w$  fixed. All energy levels should be shown in the same plot.

*Discuss in code comments:* Describe the differences between the even  $N$  and odd  $N$  cases.

- (c) Write a function to study the spatial characteristics of the energy states. The function should have an additional argument  $E_0$  which is a target energy for which the energy closest to this value will be plotted. The function should plot

the probability density  $|\psi_{\mu n}|^2$  versus position, for the energy state with  $E$  closest to the specified value  $E_0$ . If two energy states have the same  $E \approx E_0$  (up to some reasonable numerical precision), show *both* in the same plot.

Next, use this function to study the probability densities of the energy states for chains with even and odd  $N$ . Write a function which calls the function that plots the probability density versus position for a few parameter choices, showing the results in different subplots.

*Discuss in code comments:* How do the probability densities of  $E = 0$  states behave for different values of  $N$ ,  $v$  and  $w$ ? How do the zero-energy states differ from those with  $E \neq 0$ ?

- (d) Now let us characterize the performance of the sparse matrices against the standard numpy array. Write a function that does the same thing as 2a but instead of returning the Hamiltonian in a sparse matrix format, the full Hamiltonian is returned.
- (e) Write a function to call the two functions which you have written that returns the Hamiltonian of the SSH model for varying system sizes. The function should record the time taken to perform the calculations for  $N = 100, 1000, 10000$  sites. You may use the `timeit` library to obtain the time taken to perform the calculations. The results should be plotted in a graph with the y-axis being the time taken and x-axis being the system size. You should decide if a linear or logarithmic scale is better to represent the results.

*Discuss in code comments:* What do you notice in the results?

### 3. The Quantum Harmonic Oscillator Revisited

Let us revisit the quantum harmonic oscillator (QHO) that we have seen in Homework

2. The equation for the quantum harmonic oscillator can be written as:

$$-\frac{\hbar}{2m} \frac{d^2\psi(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi(x) = E\psi(x) . \quad (9)$$

The energy of level  $n$  for the quantum harmonic oscillator can be analytically solved to give

$$E = (n + \frac{1}{2})\hbar\omega \quad (10)$$

Taking  $m$ ,  $\hbar$  and  $\omega$  to be equal to 1,

- (a) Write a function that is able to return the Hamiltonian of the QHO in the form of a sparse matrix.
- (b) Write a function which calls the Hamiltonian of the QHO and solves for the eigenvalues and eigenvectors for the lowest 3 eigenvalues and eigenvectors. You are to plot the wavefunctions in subplots.
- (c) Write another function that solves Eq. (9) using the Scipy's inbuilt ODE solvers. You may also use your own ODE solving algorithms if you feel more comfortable.
- (d) Modify your functions in 3b and 3c to include the `timeit` libraries. Perform the calculation for the QHO using both methods such that the energies are of the same degree of accuracy. You have to decide the condition required for the energy values returned to be considered equal. Repeat the calculations for varying accuracies and compare the time taken by the different methods.

*Discuss in code comments:* What do you think about the complexity/difficulty in implementing the different methods? Which is more straightforward? Which method would be better for achieving a higher degree of accuracy?