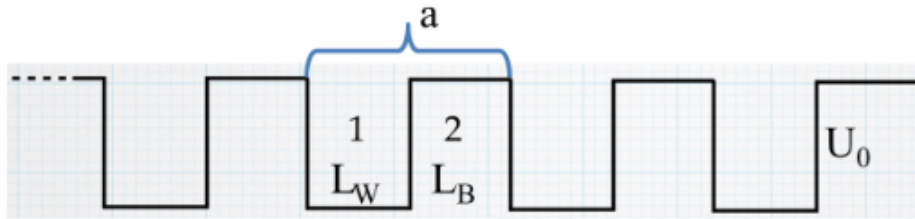# Homework6

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1 Problem1: 1D Kronig-Penney model

1.1 problem description

One-dimensional Kronig-Penney problem:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x), \qquad V(x) = V(x+a) \tag{1}$$

$U_0 = 2\text{ eV}, L_W = 0.9\text{ nm}, L_B = 0.1\text{ nm}, a = 1\text{ nm}$

Figure 1: Kronig-Penney potential

Using FFT, find the lowest three eigenvalues of the electric eigenstates that satisfy

$$\hat{H}\psi_k(x) = E_k\psi_k(x), \qquad \psi_k(x+a) = \psi_k(x) \tag{2}$$

1.2 algorithm description

Since here we request that $\psi_k(x+a) = \psi_k(x)$ and from Bloch theorem, we have

$$\psi_k(x+a) = e^{ika}\psi_k(x) \tag{3}$$

which means that $k = 0$, so the eigenvalues we need to compute here are actually from the 3 lowest bands at Γ point.

To solve this problem with FFT, we first discretize fourier transform the periodical potential operator $V(x)$ and $\psi(x)$ in the real space with N grid points in one period $[0, a]$.

$$\psi(x) = \sum_{n=0}^{N-1} c_n e^{i\frac{2\pi n}{a}x}, \qquad V(x) = \sum_{m=0}^{N-1} V_m e^{i\frac{2\pi m}{a}x}, \qquad x = \frac{ja}{N}, \quad (j = 0, 1..N-1) \quad (4)$$

c_n are N unknown coefficients to be determined, while V_m can be calculated with FFT from $V(x)$. Then we can rewrite equation(1):

$$-\frac{\hbar^2}{2m} \sum_{n=0}^{N-1} c_n \left(i\frac{2\pi n}{a}\right)^2 e^{i\frac{2\pi n}{a}x} + \left(\sum_{m=0}^{N-1} V_m e^{i\frac{2\pi m}{a}x}\right) \left(\sum_{n=0}^{N-1} c_n e^{i\frac{2\pi n}{a}x}\right) = E \sum_{n=0}^{N-1} c_n e^{i\frac{2\pi n}{a}x} \quad (5)$$

multiply $e^{-i\frac{2\pi k}{a}x}$, $k = 0, 1..N-1$ on left and sum over x from 0 to a (the N grid-points),

$$\frac{1}{N} \sum_x e^{-i\frac{2\pi k}{a}x} e^{i\frac{2\pi n}{a}x} = \delta_{k,n}, \qquad x = \frac{ja}{N}, \quad (j = 0, 1..N-1) \quad (6)$$

we have N equations:

$$-\frac{\hbar^2}{2m} c_k \left(i\frac{2\pi k}{a}\right)^2 + \sum_{m+n=k} V_m c_n = E c_k \quad (7)$$

To solve out non-trivial solution of c_n, the determinant of the coefficient matrix should be zero(which can be viewed as a N-order function $f(E)$), thus we can get N eigenvalues of E by solving the equation $f(E) = 0$.

Here in my code I use $\psi_k(x)$ instead because I want to see the band structure at different k points. I use truncated plane wave basis set to represent the Hamiltonian operator $\hat{H}$ in matrix form, then directly diagonalize the Hamiltonian matrix to get the eigenvalues.

$$\psi_k(x) = \sum_{m=-M}^{M} c_m \phi_m, \qquad N = 2M+1, \quad \phi_m = \frac{1}{\sqrt{a}} e^{i(\frac{2\pi m}{a}+k)x} \quad (8)$$

$$HC = ESC \qquad H_{ij} = \langle\phi_i|\hat{H}|\phi_j\rangle, \quad S_{ij} = \langle\phi_i|\phi_j\rangle, \quad C = [c_1, c_2, .., c_N]^T \quad (9)$$

It's actually the same as equation(7)

1.3 output

run `problem1.py`


```
Requested: first 3 eigenvalues at k=0:
   E_1 = 0.144170 eV
   E_2 = 1.516338 eV
   E_3 = 1.881417 eV
```
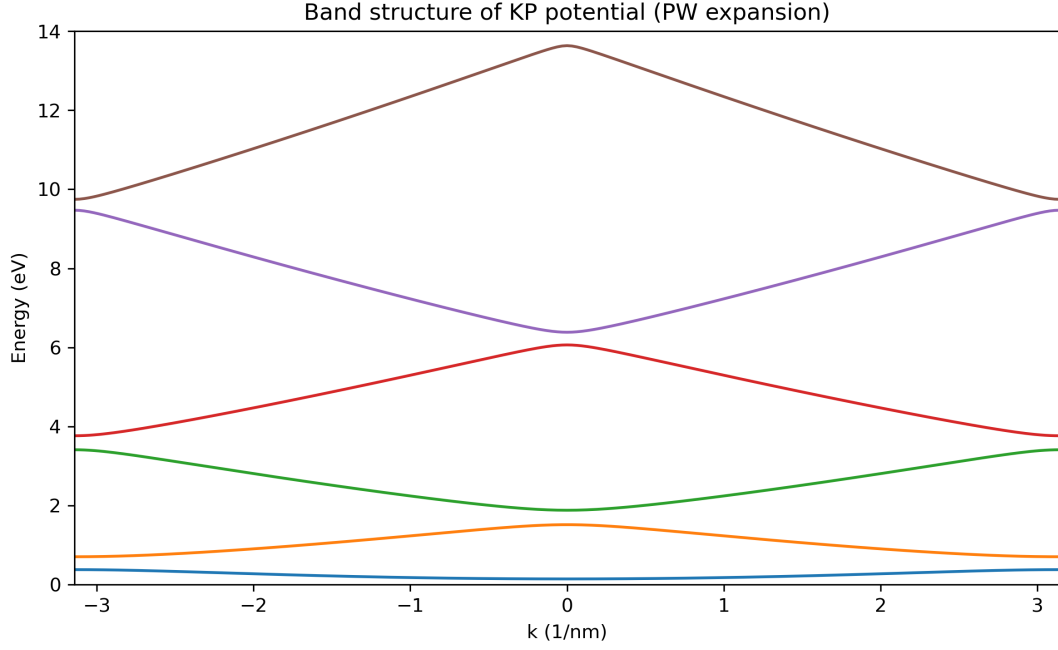
Figure 2: output

Figure 3: Band Structure of Kronig-Penney Model

2 Problem2: Detecting periodicity

2.1 problem description

Download the file called sunspots.txt , which contains the observed number of sunspots on the Sun for each month since January 1749.

Write a program to calculate the Fourier transform of the sunspot data and then make a graph of the magnitude squared $|c_k|^2$ of the Fourier coefficients as a function of k ,also called the power spectrum of the sunspot signal. You should see that there is a noticeable peak in the power spectrum at a nonzero value of k . Find the approximate value of k to which the peak corresponds. What is the period of the sine wave with this value of k?
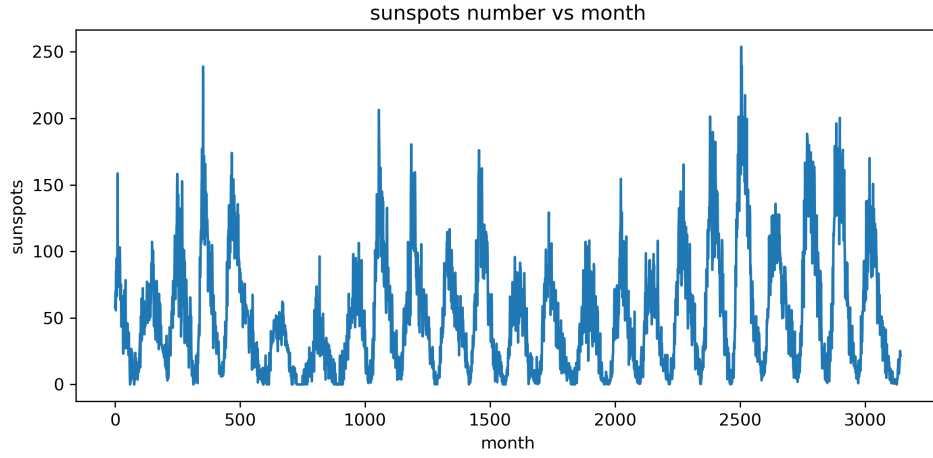
2.2 algorithm description

Figure 4: Sunspot Data

First, we need to cut off the mean value of the sunspot data to eliminate the DC component in the Fourier transform, otherwise the DC component ($k = 0$ contribution) will be too large and cover other frequency components.

$$x'_n = x_n - \frac{1}{N} \sum_{n=0}^{N-1} x_n, \quad n = 0, 1, .., N-1 \tag{10}$$

Then we can fill the data with zero to increase to 2^k sample points for FFT convenience, this procedure has no effect on the frequency result.

$$x' : [0, 1, .., N] \to [0, 1, .., N, 0, 0, .., 0] \quad (total\ length = 2^k) \tag{11}$$

Finally, directly use FFT to calculate the Fourier coefficients c_k of the sunspot data.

$$c_k = \frac{1}{L} \sum_{n=0}^{L-1} x'_n e^{-i\frac{2\pi}{L}kn}, \quad k = 0, 1, .., L-1, \quad L = 2^k \tag{12}$$

2.3 output

run `problem2.py`


```
N=3143,  FFT length L=4096,  mean value≈51.9245
Peak k=31, T≈132.13 months ≈11.01 years
```
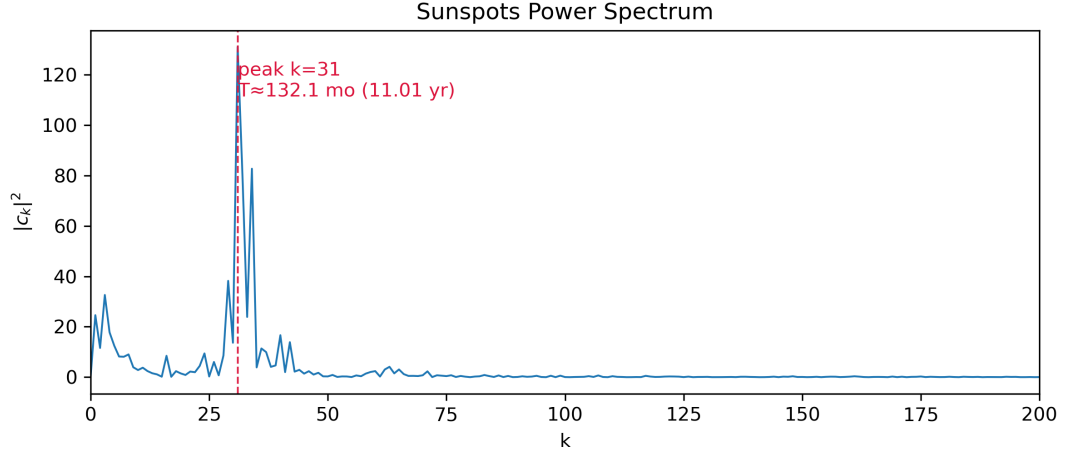
Figure 5: output

Figure 6: Power Spectrum of Sunspot Data

Here $L = 4096, k_{peak} = 31, T = L/k_{peak} \approx 132.13$ months ≈ 11.01 years. Referring to historical data, the solar cycle is about 11 years, which is consistent with our calculation.