Homework 6

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1 One-dimensional Kronig-Penney problem

1.1 Question

Using the FFT,solving one-dimensional Kronig-Penney problem, finding the lowest eigenvalues of the eigenstates that satisfy periodical condition.$\psi(x) = \psi(x + a)$

1.2 Solution

We take electron as an example.Parameters are as followed.

e/C	$1.602 * 10^{-19}$	$\frac{h}{2\pi}$/Js	$1.054573 * 10^{-34}$
m/kg	$9.109 * 10^{-31}$	$\frac{U_0}{e}$/V	2
L_W/nm	0.9	L_B/nm	0.1
N	2^{11}	fs	$2N + 1$

The eigenstate of Schrödingerequation is:

$$\hat{H}\psi = E\psi \tag{1}$$

where $\hat{H} = \hat{T} + V(x)$,and $V(x) = 0$ when $0 < x < L_W, V(x) = U_0$ when $L_W < x < a = L_W + L_B$.By expanding ψ and$V(x)$ into Fourier series,we can get:

$$\psi = \sum_{q=-N}^{N} C_q e^{iq\frac{2\pi}{a}x} \tag{2}$$

$$V(x) = \sum_{q'=-N}^{N} V_{q'} e^{iq'\frac{2\pi}{a}x} \tag{3}$$

For convenience,we notate $|q\rangle = e^{iq\frac{2\pi}{a}x}$,and we can obtain the Matrix element H_{pq}:

$$H_{pq} = \langle p|\hat{H}|q\rangle = \langle p|\hat{T}|q\rangle + \langle p|V|q\rangle \tag{4}$$

$$\langle p|\hat{T}|q\rangle = \frac{h^2q^2}{2ma^2}\int_{-\infty}^{\infty} e^{i(q-p)\frac{2\pi}{a}x} = \frac{h^2q^2}{4\pi ma}\delta_p^q \tag{5}$$

$$\langle p|\, V \,|q\rangle = \sum_{q'=-N}^{N} V_{q'} \int_{-\infty}^{\infty} e^{i(q'+q-p)\frac{2\pi}{a}x} = \sum_{q'=-N}^{N} \frac{a}{2\pi} V_{q'} \delta_{q'}^{p-q} \tag{6}$$

$$\langle p|\, V \,|q\rangle = \begin{cases} \frac{a}{2\pi} V_{p-q} & -N \leq p-q \leq N \\ 0 & \text{else} \end{cases} \tag{7}$$

We can evaluate $V_{q'}$ by FFT.

1.3 Psudocode

Algorithm 1 One-dimensional Kronig-Penney problem

Input: initial parameters, sample frequecy fs=2N+1

Output: the lowest three energy

$N = 2^{11}$,initial $V(x)$

$V_{q'} = fft(V(x), 0, a, fs)$

$V_{p-q} == \begin{cases} \frac{a}{2\pi} V_{p-q} & -N \leq p-q \leq N \\ 0 & \text{else} \end{cases}$

for i in range(0,len(fs) **do**

  $H[i,i] = factor(i-N)^2$

  for j in range(0,len(fs) **do**

    $H[i,j] += V_{2N+i-j}$

  end for

end for

$E = eigenvalue(H)$

return E

1.4 Results

The lowest three energy(divided by the charge of an electron e) is in Figure 1,and we find that the eigen-energy is linear with n ($n = x^2$,x is the x^{th} lowest energy),see Figure 2.

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[0.14412070818773126, 1.5165542283326152, 1.8814651295689693]
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Figure 1: energy

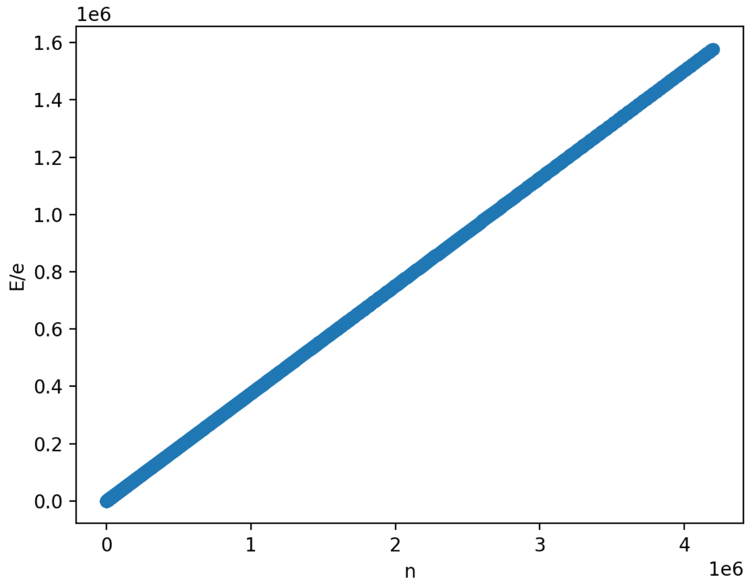

Figure 2: Energy vs. n

2 Detecting periodicity

2.1 Question

Analyze the power spectrum of the sunspot signal.

2.2 Solution

We can use the fft function in Scipy package to process the original data.

2.3 Psudocode

Algorithm 2 FOURIER SERIES

Input: sunspots activity data

Output: its power spectrum

1: $spectrum = abs(fft(sunspots))$

2: **return** spectrum

2.4 Results

In the figure, we can see there is two symmetric peak in the power spectrum. We only focus on the prior one and zoom in to see it. The non-zero peak occurs when k = 24. Since the length of time is 3143, the corresponding period $T = \frac{3143}{2^{24-1}}$. The angular frequency is $\omega = \frac{2^{24}\pi}{3143}$.

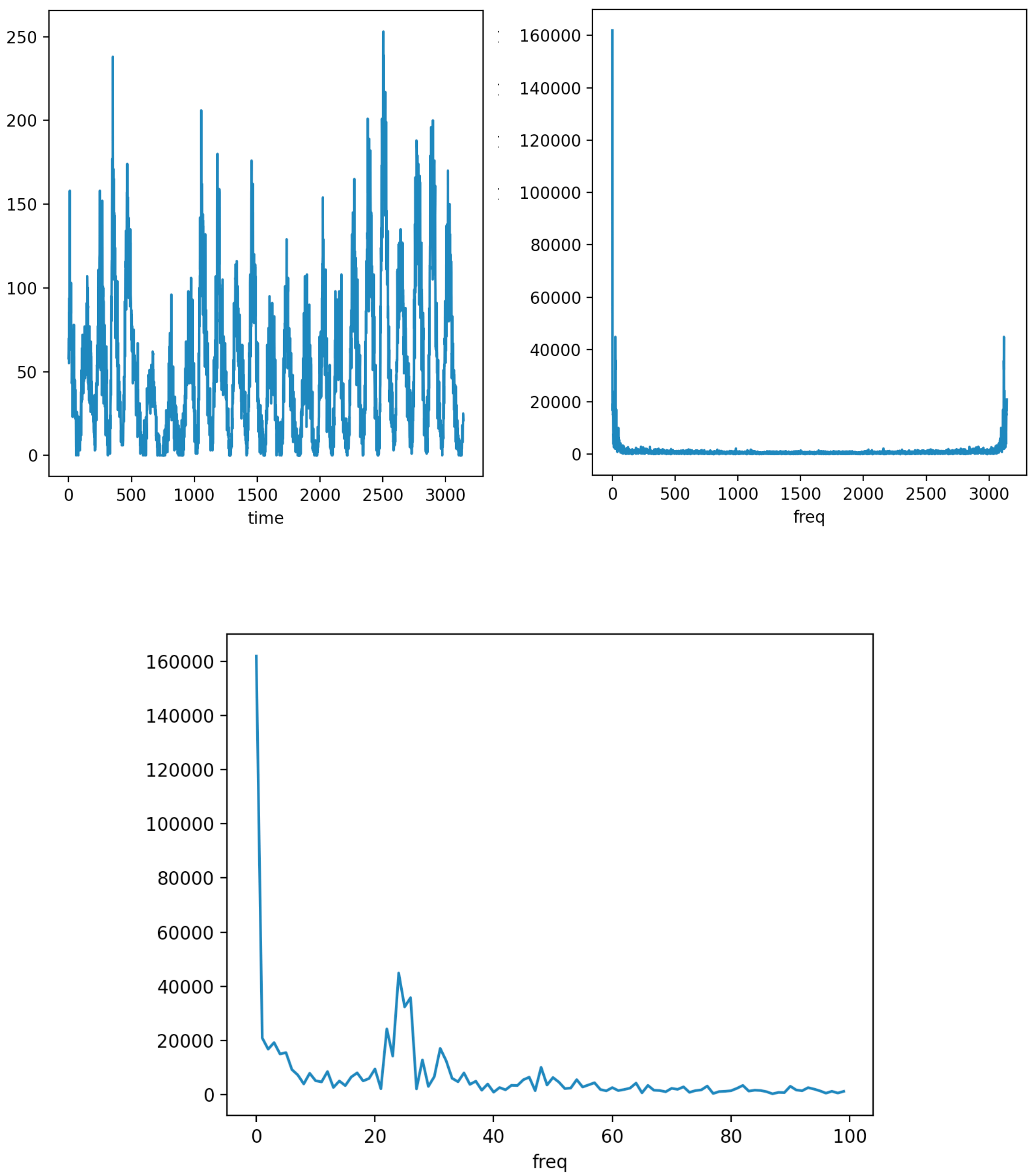

Figure 3: spectrum