计算物理作业 6

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起视四境，而作业又至矣。

1 题目 1：一维 Kronig-Penney 模型的本征值求解。

1.1 题目描述

One-dimensional Kronig-Penney problem. Considering the Hamiltonian of the system as

$$\hat{H} = -\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial x^2} + V(x)$$

with a one-dimensional periodic potential $V(x) = V(x+a)$. The potential can be expressed as

$$V(x) = \begin{cases} 0, & \text{if } 0 \leq x < L_W, \\ U_0, & \text{if } L_W \leq x < a \end{cases}$$

and the period of the potential is $a = L_W + L_B$, which is also shown in the Figure below.

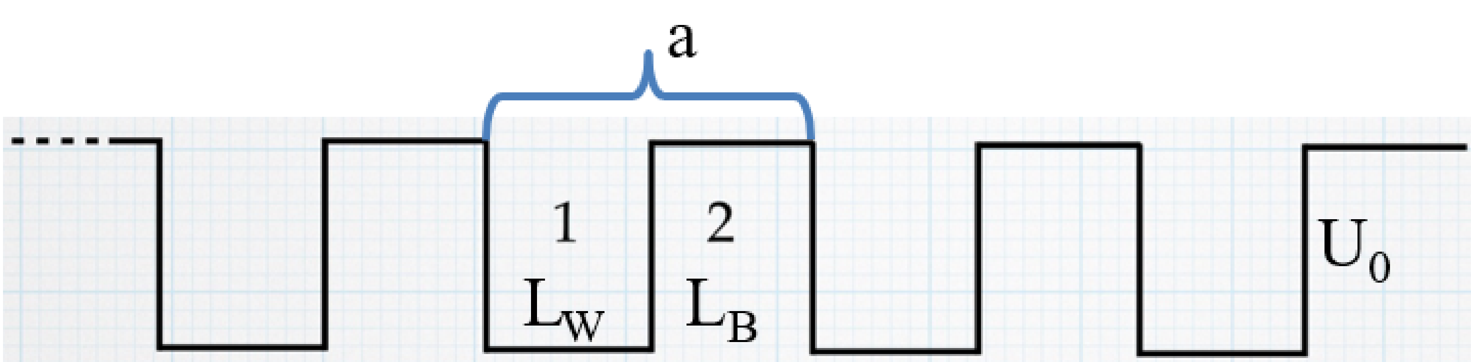

图 1: Kronig-Penney potential well

With parameters:

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

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

$$\hat{H}\psi_i = E\psi_i \quad \text{and} \quad \psi_i(x) = \psi_i(x+a).$$

Explanation: Since the system is translation-invariant, i.e., $\psi_i(x) = \psi_i(x+a)$, we can use the plane wave basis expansion

$$\psi(x) = \frac{1}{\sqrt{a}} \sum_q C_q e^{iq\frac{2\pi}{a}x}, \quad q = -N, -N+1, \ldots, -1, 0, 1, \ldots, N-1, N.$$

In this basis set, the Hamiltonian can be represented in matrix form as

$$H_{pq} = \frac{1}{a} \langle e^{ip\frac{2\pi}{a}x} | \hat{H} | e^{iq\frac{2\pi}{a}x} \rangle_{\text{cell}} = \frac{1}{a} \int_0^a dx e^{-ip\frac{2\pi}{a}x} \hat{H} e^{iq\frac{2\pi}{a}x}.$$

To calculate $\hat{H}e^{iq\frac{2\pi}{a}x}$, the periodic potential $V(x)$ can be expanded in Fourier series as $V(x) \rightarrow V_q$, where

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

The basis wave function can then be written as:

$$\hat{H}e^{iq\frac{2\pi}{a}x} = (\hat{T} + \hat{V}) e^{iq\frac{2\pi}{a}x} = \frac{2\hbar^2 q^2 \pi^2}{ma^2} e^{iq\frac{2\pi}{a}x} + \sum_{q'=-N}^{N} V_{q'} e^{i(q'+q)\frac{2\pi}{a}x}$$

Try constructing the Hamiltonian matrix H_{pq} and solve the eigenvalue equation $\hat{H}\psi_i = E\psi_i$ to obtain the three lowest energy eigenvalues.

Special note: You can use built-in functions to simplify the eigenvalue calculations and FFT transformations.

1.2 程序描述

1.3 伪代码

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1.4 结果示例

2 题目 2：太阳黑子周期性检测

2.1 题目描述

Use 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?

Special note: You may use any built-in functions for the Fourier transform.

2.2 程序描述

2.3 伪代码

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2.4 结果示例