PHYS 3142 Spring 2021
Computational Methods in Physics
Assignment 3
Due: 11:59 p.m. 28th Feb 2021

Before you submit your assignment, do remember:

1. the due day
2. submit a report which contains your figures and results along with your code
3. make sure your code can run
4. do not forget to write comments in your codes.
5. label your figures and describle your results

The basic scoring rubric is :

1. **If you submit the assignment after the deadline or do not submit the report, you can only get up to 80% of grade**
2. **If there is any kind of plagiarism, all of the student involving will get zero mark! (except that the one can really prove the code is written by himself or herself and others copied it without telling him or her)**

1. Free energy of two-dimensional electron gas

We consider the electron gas in a two-dimensional square lattice at temperature T. The energy dispersion for the electron is $\epsilon(k_x, k_y) = -2(\cos(k_x) + \cos(k_y)) - \mu$, where k_x, k_y are the two-dimensional momentum wave vector for the electron and μ is the chemical potential.

The free energy $F(T)$ of the electron gas is defined as,

$$F(T) = -k_B T \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \ln\left(1 + e^{\frac{\mu - \epsilon(k_x, k_y)}{k_B T}}\right) dk_x dk_y$$

Using the method of Gaussian quadrature with sample points N = 100 for k_x and k_y respectively and assume the chemical potential $\mu = 0$.

(a)Compute the free energy of the electron gas for $k_B T = 1$ (Answer: ....)

(b)Hence, make a plot of $F(T)$ vs $k_B T$ for $k_B T$ from 0.1 to 10.

2. Two site tight-binding model

For any tight-binding models with two quantum states per unit cell, the Hamiltonian can be written in terms of a two-by-two matrix in the k space:

$$H = \sum_k \left(a_k^\dagger, b_k^\dagger\right) \mathcal{H}(k) \begin{pmatrix} a_k \\ b_k \end{pmatrix}$$

where $\mathcal{H}$ is a 2×2 Hermitian matrix as a function of k. It is called the kernel of the Hamiltonian. Because $\mathcal{H}(k)$ contains all the information of the Hamiltonian H, it is often called the Hamiltonian in literature.

For the model considered in Figure.1, the hamiltonian is as following

$$\mathcal{H}(k) = \begin{pmatrix} V_a & -2t\cos(ka) \\ -2t\cos(ka) & V_b \end{pmatrix}$$

where V_a, V_b is the on-site energy, t is the hopping strength. In this model, the spin of the electron are ignored and the two spin orbitals were degenerated since no spin-dependent potential is present to remove the degeneracy between "up" and "down" spins.

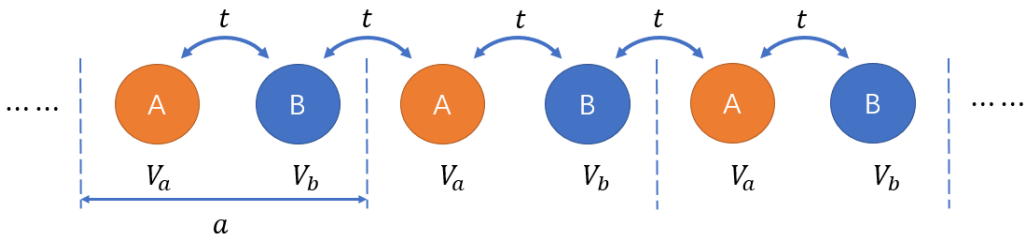

Figure 1: 1D atomic chain with A,B site

The eigenvalues of $\mathcal{H}(k)$ give us the dispersion relations. At each k point, one can define a unitary transformation

$$\begin{pmatrix} c_k \\ d_k \end{pmatrix} = U_k^{-1} \begin{pmatrix} a_k \\ b_k \end{pmatrix}$$
$$\begin{pmatrix} c_k^\dagger & d_k^\dagger \end{pmatrix} = \begin{pmatrix} a_k^\dagger & b_k^\dagger \end{pmatrix} U_k$$

where $U_k^{-1} = U_k^\dagger$

$$H = \sum_k \left(c_k^\dagger, d_k^\dagger\right) U_k^+ \mathcal{H} U_k \begin{pmatrix} c_k \\ d_k \end{pmatrix}$$

If we choose U_k such that $U_k^+ H U_k$ is a diagonal matrix,

$$U_k \mathcal{H} U_k^{-1} = \begin{pmatrix} \epsilon_c & 0 \\ 0 & \epsilon_d \end{pmatrix}$$

Then, the Hamiltonian becomes

$$H = \sum_k \left(c_k^\dagger, d_k^\dagger\right) \begin{pmatrix} \epsilon_c & 0 \\ 0 & \epsilon_d \end{pmatrix} \begin{pmatrix} c_k \\ d_k \end{pmatrix} = \sum_k \epsilon_c(k) c_k^\dagger c_k + \sum_k \epsilon_d(k) d_k^\dagger d_k$$

The group velocity of a wave is the velocity with which the overall envelope shape of the wave's amplitudes. The group velocity v_g is defined by the equation:

$$v_g \equiv \frac{d\omega}{dk}$$

where ω is the wave's angular frequency, and k is the angular wavenumber.

The group velocity of electrons is defined as:

$$\epsilon(k) = \hbar\omega(k), v_g = \frac{1}{\hbar}\frac{d\epsilon(k)}{dk}$$

and has the meaning of the velocity of a wave packet, composed as a superposition of eigenfunctions, having a narrow spread of frequencies about some mean value, ω.

(a) Draw the energy dispersion $\epsilon(k)$ of this two site tight-binding model from $\frac{-\pi}{a}$ to $\frac{\pi}{a}$. Set $V_a = t, V_b = -t$. You can use "numpy.linalg.eigh" to get eigenvalues. (Don't forget there are two bands)

(b) Hence, draw the group velocity $v_g(k)$ of eletron in this two site tight-binding model from $\frac{-\pi}{a}$ to $\frac{\pi}{a}$. (Don't forget there are two bands)

There is analytic result, but please use numerical method to solve both questions. Because for more generic cases, if one have m quantum states per unit cell, $\mathcal{H}(\mathbf{k})$ will be a $m \times m$ Hermitian matrix. There is very little analytic result.