1. Dispersion and tunneling in a lattice potential
Here we will derive the tunneling energy of particles $t$ in a periodic potential $V(x + d) = V(x)$ with period $d$, and see its connection with the effective mass $m^*$ of the particle. We start with Schrödinger’s equation for a single particle in the potential $V(x)$:

$$i\hbar \partial_t \psi(x, t) = H\psi(x, t) = \left[-\frac{\hbar^2}{2m} \partial_x^2 + V(x)\right] \psi(x, t).$$

Bloch-Floquet theorem states that the eigenstates satisfy $\phi_{nq}(x) = e^{iqx} f_n(x)$, where $f_n(x + d) = f_n(x)$ is a periodic function, and the associated eigenenergies $E_{nq}$ is also called the dispersion. We have $H\phi_{nq}(x) = E_{nq}\phi_{nq}(x)$. The subscripts indicate the quasi-momentum $-\frac{\pi}{d} \leq q \leq \frac{\pi}{d}$ and the band index $n = 0, 1, 2 ...$

To construct a localized wavepacket of particle at the $j$-th site, $j = 1, 2, 3..$, we introduce the Wannier states as the Fourier transform of the eigenstates in the $n$-th band as

$$w_n(x - x_j) \equiv \sqrt{\frac{d}{2\pi}} \int_{-\pi}^{\pi} e^{iqx} \phi_{nq}(x) dq,$$

where $x_j = jd$ and Wannier states form an orthonormal basis $\int w_n^*(x - x_j) w_m(x - x_k) dx = \delta_{nm}\delta_{jk}$.

A. Consider states in the lowest band $n = 0$ and skip the subscript $n$. Show that the Hamiltonian in the Wannier basis can be written in the matrix form as

$$H = \begin{bmatrix}
t_0 & -t_1 & t_2 & \ldots \\
-t_1 & t_0 & -t_1 & t_2 \\
t_2 & -t_1 & t_0 & -t_1 \\
\ldots & t_2 & -t_1 & \ldots \\
\end{bmatrix}

\quad t_m \equiv (-1)^m \int w^*(x - x_j) H w(x - x_{j+m}) dx$$

where $t_0$ is the onsite energy, $t_1$ is the tunneling energy to the nearest neighbors, $t_2$ is the tunneling to the 2nd nearest neighbors and so on.

B. Evaluate the integral and show that the matrix elements $t_m$ are exactly the Fourier coefficients of the dispersion $E_q$

$$E_q = t_0 + 2 \sum_{m=1} (-1)^m t_m \cos qd$$
This is a key and universal result that applies to all periodic lattices. For instance, the width of the band is given by the tunneling as \( \Delta E = 4Dt \), where \( D = 1,2,3 \ldots \) is the dimensionality of the lattice.

C. For low energy particles with small quasi-momenta \(|q| \ll \pi/d\), we may expand the dispersion as \( E_q = \hbar^2 q^2 / 2m^* \), where the effective mass \( m^* \) characterizes the “inertia” of the particle in the lattice. In a deep lattice, a.k.a. tight-binding limit, where we have \( t_1 \gg t_2 \ldots \), show that the effective mass is given by

\[
m^* = \frac{\hbar^2}{2d^2(t_1 - 4t_2 + 9t_3 - \cdots)} \approx \frac{\hbar^2}{2d^2t_1}
\]

Show that in the tight-binding limit, the dispersion is sinusoidal:

\[
E_q \approx -\frac{\hbar^2}{m^*d^2} \cos qd + \text{const.}
\]

2. Quantum phase transition in Bose-Hubbard model

Bose-Hubbard is a simple model that describes the quantum phase transition of bosons in the lattice. It is given by

\[
H = -t \sum_{<i,j>} a_i^+ a_j + a_j^+ a_i + \frac{U}{2} \sum_i n_i(n_i - 1)
\]

Consider \( N \) particles on a 1D ring with \( N \) sites and \( g \equiv U/t \) is the coupling constant. In the limit of large interparticle repulsion \( g \gg 1 \), we expect that each site is occupied by exactly 1 particle. This is the Mott insulator regime and the ground state is expected to be

\[
|MI> = \prod_{i=1} a_i^+ |vac>.
\]

In the opposite limit of \( g \ll 1 \), we expect each atom is in superposition of all \( N \) sites. This is the superfluid regime and the ground state is expected to be

\[
|SF \geq \left[ N^{-\frac{1}{2}} \sum_{i=1} a_i^+ \right]^N |vac>.
\]

A. Evaluate the energy of the two states \( E_{MI} \equiv <MI|H|MI> \) and \( E_{SF} \equiv <SF|H|SF> \).

Show that \( E_{MI} < E_{SF} \) when \( g \gg 1 \) and \( E_{MI} > E_{SF} \) when \( g \ll 1 \). What is the critical value \( g_c \) when the two states have the same energy.

(Hint: You may consider \( N = 2 \) or \( N = 3 \) to gain some intuition.)
B. To determine the critical value more precisely, let’s consider $N = 2$ and the state of the system can be written as $|\psi\rangle = a |2,0 \rangle + b |1,1 \rangle + c |0,2 \rangle$. Determine the ground state as a function of $g$. Does it give a hint where the critical value could be?

C. Attempt the repeat the calculation with $N = 3$ and numerically plot the ground state energy as a function of $g$.

(Hint: For $N = 3$, the Hilbert space is 10 dimensional. In the Fock state basis, we have $|\psi\rangle = a |0,0,3 \rangle + b |0,1,2 \rangle + c |0,2,1 \rangle + d |0,3,0 \rangle + e |1,0,2 \rangle + f |1,1,1 \rangle + g |1,2,0 \rangle + h |2,0,1 \rangle + i |2,1,0 \rangle + j |3,0,0 \rangle$. You may plot all eigenvalues as a function of $g$ and check which state is the ground state.)