NOTE: Be sure to show your work and explain what you are doing

This homework is about the "tight binding" approximation in a 1D period lattice potential.

1. [20 points] Imagine first a double well (chain with two sites) with one atom. In each site the atom has energy $E_0$ and due to the kinetic energy it can tunnel to the other well with tunneling amplitude $J$. If we think of our basis states as $|R⟩$ and $|L⟩$, representing the states with the atom localized at the right or left site respectively, the Hamiltonian can be written as

$$H = \begin{pmatrix} E_0 & -J \\ -J & E_0 \end{pmatrix}$$

(1)

Calculate the two eigenstates and eigenenergies.

2. Let’s try now to generalize our problem to a chain of $N$ sites. In this case we will assume that an atom on site $|j⟩$ can only tunnel to its nearest neighbor sites. The Schrodinger equation can then be written as

$$E|j⟩ = E_0|j⟩ - J|j+1⟩ - J|j-1⟩$$

with $j = 1, …, N$. Let’s call $a$ the lattice spacing.

(a) [20 points] Show that the eigenstates can be written as $|ψ⟩ = α \sum_j e^{ika} |j⟩$. Use the normalization condition to find $α$ and calculate the eigenenergies.

(b) [20 points] Show that for a periodic chain, where $⟨j=1|ψ⟩ = ⟨j=N+1|ψ⟩$, $k$ can only take the values $ka = 2πn/N$ with $n = 0, 1, …, N-1$ and that for an open chain where $⟨j=0|ψ⟩ = ⟨j=N+1|ψ⟩ = 0$, $k$ can only take values $ka = πn/(N+1)$ with $n = 1, …, N$. For the latter you have to assume $ψ = \sum_j (Ae^{ikja} + Be^{-ikja})|j⟩$ to force the wave function to vanish at sites 0 and $N+1$.

3. [20 points] Imagine that we have $M < N$, $M$ even, noninteracting $S = 1/2$ fermions in the periodic chain. Calculate the Fermi energy and the total energy of the gas. Assume that $N$ is large.