PH4101 Assignment — 3
22MS037

Problem 1 — Kronig Penny Model

a)

Problem 2 — Two dimensional tight binding

Problem 3 — Tight Binding with Staggered Potential

The Hamiltonian for a one dimensional chain with staggered potential is given by

$$H = -t \sum_n [|n\rangle\langle n+1| + h.c.] + U \sum_n |n\rangle\langle n| + V \sum_n (-1)^n |n\rangle\langle n| \tag{1}$$

We divide the chain into two sublattices A and B such that even sites belong to A and odd sites belong to B. All "A" sites have on-site potential $U + V$ and all "B" sites have on-site potential $U - V$. One other change takes place, the periodicity of the lattice changes from a to $2a$. This makes the unit cell contain two sites, one from sublattice A and one from sublattice B.

We can now rewrite the Hamiltonian as

$$H = -t \sum_n \left[\underbrace{|n_A\rangle\langle n_B|}_{1} + \underbrace{|n_B\rangle\langle n_A + 1|}_{2} + h.c. \right] + (U+V) \sum_n \underbrace{|n_A\rangle\langle n_A|}_{3} + (U-V) \sum_n \underbrace{|n_B\rangle\langle n_B|}_{4} \tag{2}$$

where n_A and n_B denote the site index for sublattice A and B respectively. The terms (1) and (2) denote hopping between A and B sublattices while terms (3) and (4) denote on-site potentials for A and B sublattices respectively. (1) and (2) are hopping terms where (1) denotes hopping from A to B within the same unit cell while (2) denotes hopping from B to A in the next unit cell.

a) We now need to find the dispersion relation for this system. To do this, we write the Hamiltonian in the k-space basis $|k\rangle_A$ and $|k\rangle_B$ where

$$|k\rangle_A = \frac{1}{\sqrt{N/2}} \sum_{n \in A} e^{ikn(2a)} |n\rangle \tag{3}$$

$$|k\rangle_B = \frac{1}{\sqrt{N/2}} \sum_{n \in B} e^{ikn(2a)} |n\rangle \tag{4}$$

Let us note the orthogonality condition

$$\frac{1}{\sqrt{N/2}} \sum_n e^{i(k-k')n(2a)} = \delta(k - k') \tag{5}$$

Plugging in these basis states into the Hamiltonian Equation 2, we get

$$H = \sum_k \Big[(U+V)|k\rangle_A \langle k|_A + (U-V)|k\rangle_B \langle k_B| - t\big(1+e^{-i2ka}\big)|k\rangle_A \langle k|_B \\ -t\big(1+e^{i2ka}\big)|k\rangle_B \langle k|_A\Big] \quad [6]$$

Problem 4 — Parallel Chains

Problem 5 — Bloch Theorem

Problem 6 — Lattice Vectors

Problem 7 — Ultracold atoms