

The matrix equations we are trying to solve can be written explicitly as

$$t\psi_{n-1} + \varepsilon\psi_n + t\psi_{n+1} = E\psi_n \quad \text{for } n = 1, 2, \dots, N$$

These equations are satisfied by $\psi_n = \exp(+ikna)$ and $\psi_n = \exp(-ikna)$

and also by $\psi_n = \cos(kna)$ and $\psi_n = \sin(kna)$

A. Periodic boundary condition: $\psi_0 = \psi_N, \psi_{N+1} = \psi_1$

Use $\psi_n = \exp(+ikna)$ and $\psi_n = \exp(-ikna)$

with $\exp(ikNa) = 1 \rightarrow kNa = \underbrace{\nu}_{\text{integer}} 2\pi$

B. Hardwall boundary conditions: $\psi_0 = 0, \psi_{N+1} = 0$ --- Why ? **

Use $\psi_n = \sin(kna)$

with $k(N+1)a = \underbrace{\nu}_{\text{integer}} \pi$

** Dropping the boundary terms $t\psi_0$ and $t\psi_{N+1}$ amounts to setting the corresponding ψ_0 and $\psi_{N+1} = 0$.