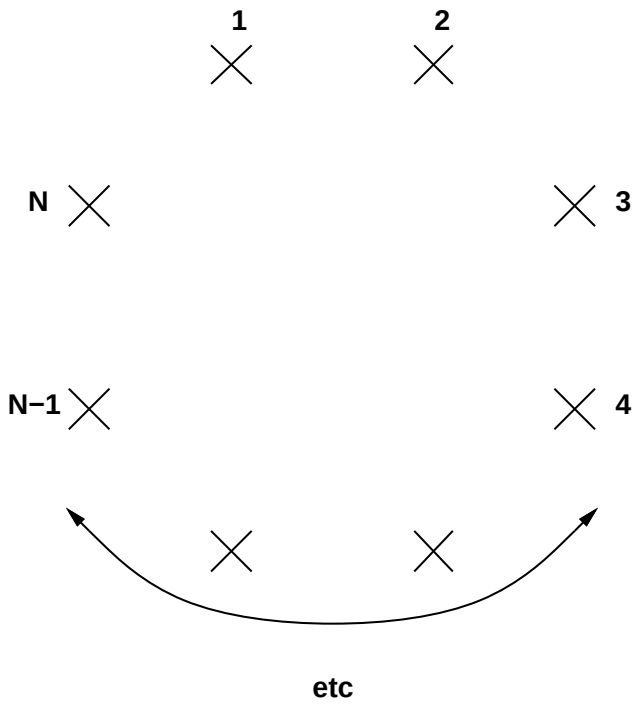
Physics 3: Bloch's Theorem and 'Tight Binding'

Many problems in physical systems involve *periodicity*: A symmetry of the system where a particular translation maps the 'problem' onto itself. The simplest example involves a 'ring':



with a single number associated with each site. For a tight-binding model, this number denotes the *wavefunction*, the modulus square of which is the probability of the electron residing on the site.

To describe the problem we need a basis of states and we elect to use the basis where an electron is isolated on a particular atom, $\mid i >$, for the i'th atom. A general state of the system is then:

$$\mid \psi >= \sum_{i=1}^{N} \psi_i \mid i >$$

What is required here is to provide a new basis in terms of which the translation operator, $\hat{T}$ say, is diagonal. Acting on the vectors, the translation operator yields:

$$\hat{T} \mid i >= \mid i+1 >$$

where $\mid N+1 >\equiv \mid 1 >$, and so acting on an arbitrary state:

$$\hat{T} \mid \psi >= \sum_{i=1}^{N} \psi_i \hat{T} \mid i >= \sum_{i=1}^{N} \psi_i \mid i+1 >= \sum_{i=2}^{N+1} \psi_{i-1} \mid i >$$

where we have relabeled the summation in the final step. It is now clear that the *components* transform as:

$$\psi_i \mapsto \psi_{i-1}$$

under the action of $\hat{T}$, which can be accomplished by the matrix:

$$\hat{T} = \begin{bmatrix} 0 & 1 & 0 & 0 & ... & 0 & 0 \\ 0 & 0 & 1 & 0 & ... & 0 & 0 \\ 0 & 0 & 0 & 1 & ... & 0 & 0 \\ 0 & 0 & 0 & 0 & ... & 0 & 0 \\ . & . & . & . & ... & . & . \\ . & . & . & . & ... & . & . \\ 0 & 0 & 0 & 0 & ... & 0 & 1 \\ 1 & 0 & 0 & 0 & ... & 0 & 0 \end{bmatrix}$$

which moves each component to its anti-clockwise neighbour. This matrix is diagonalised by vectors:

$$\mid x >= \begin{bmatrix} 1 \\ x \\ x^2 \\ x^3 \\ . \\ . \\ . \\ x^{N-2} \\ x^{N-1} \end{bmatrix}$$

with eigenvalue x, *provided* that $x^N = 1$, ie that x is an n'th root of unity.

The N'th roots of unity, ie the solutions of $x^N = 1$, are best annotated by:

$$x = e^{ik}$$

with $k = 2\pi n/N$ and $n \in \{0, 1, 2, ..., N-2, N-1\}$ and in the continuum limit (viz $N \mapsto \infty$), $k \in (-\pi, \pi]$ is required. With this choice:

$$\hat{T} \mid k >= e^{ik} \mid k >$$

and a translation picks up a phase, the so-called Bloch phase. The corresponding wavefunctions are just:

$$\psi_j = \frac{1}{\sqrt{N}} e^{ikj}$$

which all have equal modulus but have a uniformly spiraling phase.

The tight-binding problem in one-dimension, restricted to nearest-neighbour bonding, is simply:

$$\hat{H} = -t \left[\hat{T} + \hat{T}^{-1} \right]$$

which is diagonalised by $\mid k >$:

$$\hat{H} \mid k >= -t \left[e^{ik} + e^{-ik} \right] \mid k >= -2t \cos k \mid k >$$

leading to a dispersion of:

$$\epsilon(k) = -2t \cos k$$

The tight-binding problem on a two-dimensional square-lattice, restricted to nearest-neighbour bonding is just:

$$\hat{H} = -t\left[\hat{T}_1 + \hat{T}_1^{-1} + \hat{T}_2 + \hat{T}_2^{-1}\right]$$

combined with:

$$\hat{T}_1 \mid i,j> = \mid i+1,j> \qquad \hat{T}_2 \mid i,j> = \mid i,j+1>$$

which is diagonalised by:

$$\mid k_1,k_2> = \frac{1}{N}\sum_{j_1,j_2} e^{ik_1j_1+ik_2j_2} \mid j_1,j_2>$$

with eigenvalues, e^{ik_1} for $\hat{T}_1$, and e^{ik_2} for $\hat{T}_2$. The nearest-neighbour problem yields:

$$\hat{H} \mid k_1,k_2> = -t\left[e^{ik_1} + e^{-ik_1} + e^{ik_2} + e^{-ik_2}\right] \mid k_1,k_2> = -2t\left[\cos k_1 + \cos k_2\right] \mid k_1,k_2>$$

leading to a dispersion of:

$$\epsilon(k_1,k_2) = -4t\frac{1}{2}\left[\cos k_1 + \cos k_2\right]$$

When there are 'internal' degrees of freedom, such as spin or many atoms per unit cell as in Project 0.V, then the analysis still applies, but for each internal degree of freedom independently. The internal degrees of freedom must then be diagonalised for each Bloch phase.