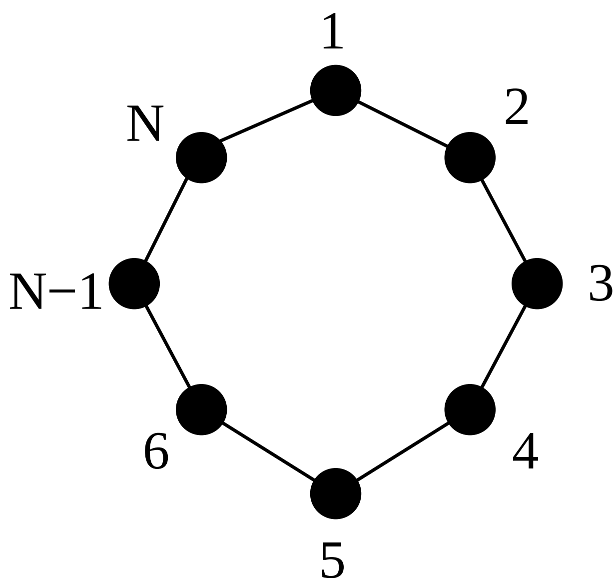
PY4T01 Condensed Matter Theory: Lecture 6

The H$_N$ ring



The Schrödinger equation is identical to that of the chain except for the atoms $|1\rangle$ and $|N\rangle$.

Let's use the trick of adding the *imaginary* atoms $|0\rangle$ and $|N+1\rangle$

The solution is again

$$\psi_j = A\mathrm{e}^{iKj} + B\mathrm{e}^{-iKj}$$

But now the boundary conditions are:

$$\psi_0 = \psi_N \quad \text{and} \quad \psi_{N+1} = \psi_1$$

which give

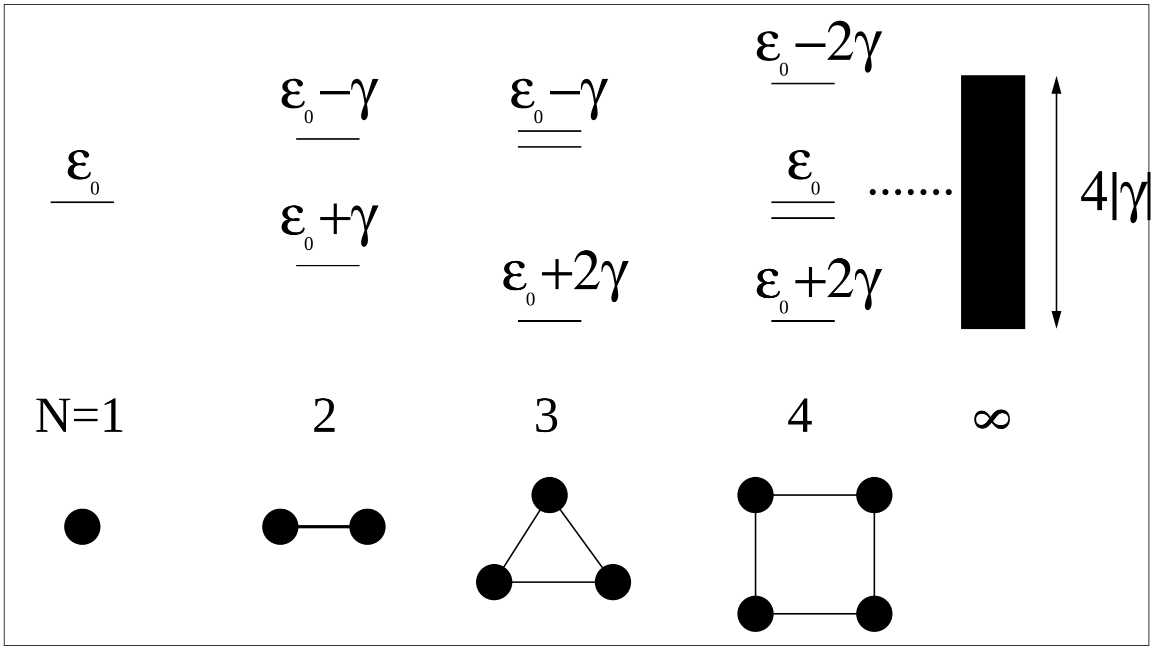
$$\mathrm{e}^{\pm iKN} = 1 \quad \rightarrow \quad K = \frac{2m\pi}{N} \quad \text{with} \quad m = 0, 1, 2, ..., (N-1)$$

The corresponding normalized eigenstates are given by

$$\psi_j^m = \frac{1}{\sqrt{N}}\,\mathrm{e}^{i\frac{2\pi m}{N}j}$$

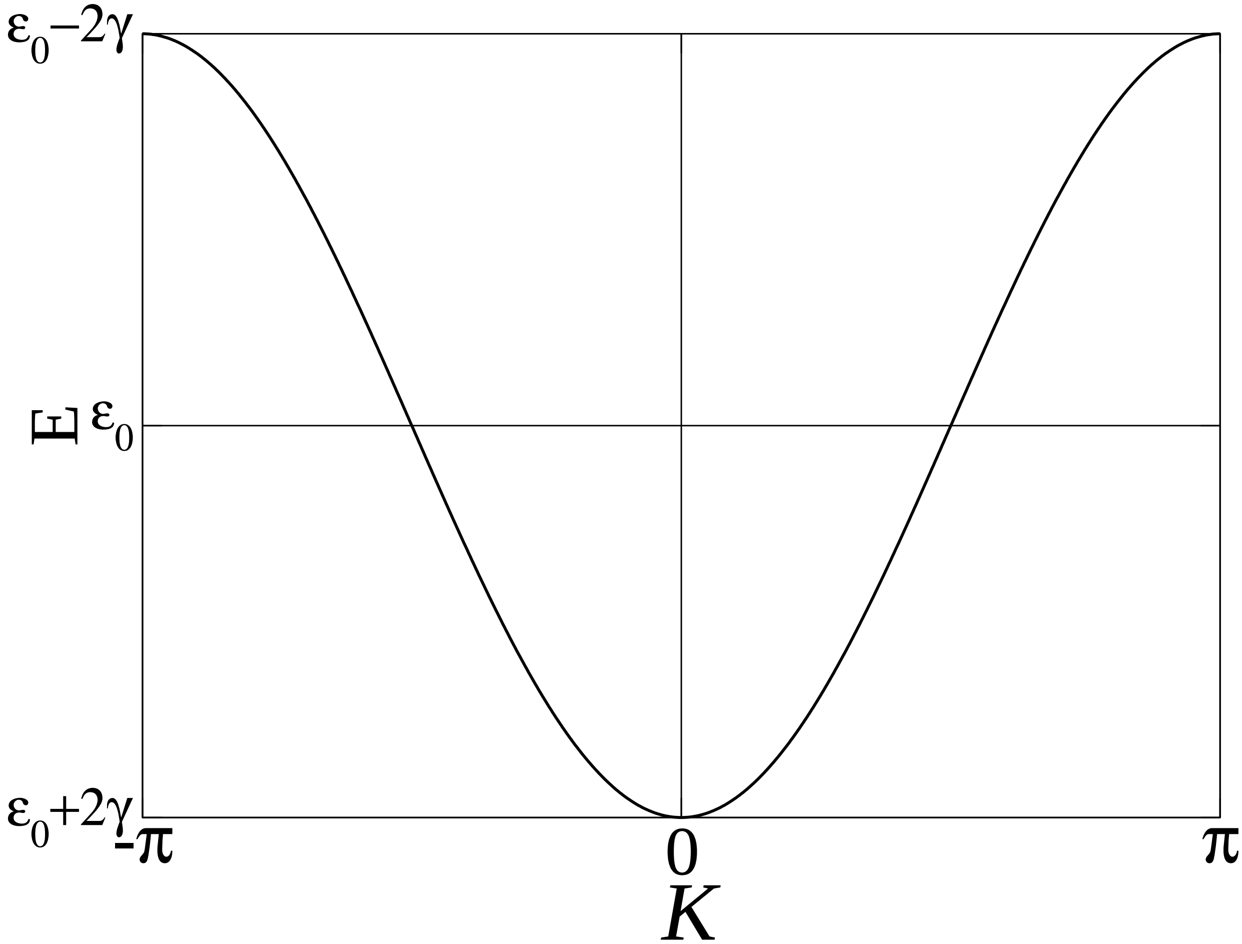
and the eigenvalues

$$E_m = \epsilon_0 + 2\gamma\cos\left(\frac{2\pi m}{N}\right)$$



Again take the limit $N \to \infty$

$$E_m \to E_K = \epsilon_0 + 2\gamma \cos K \quad \text{with} \quad 0 \le K < 2\pi$$



A few important points:

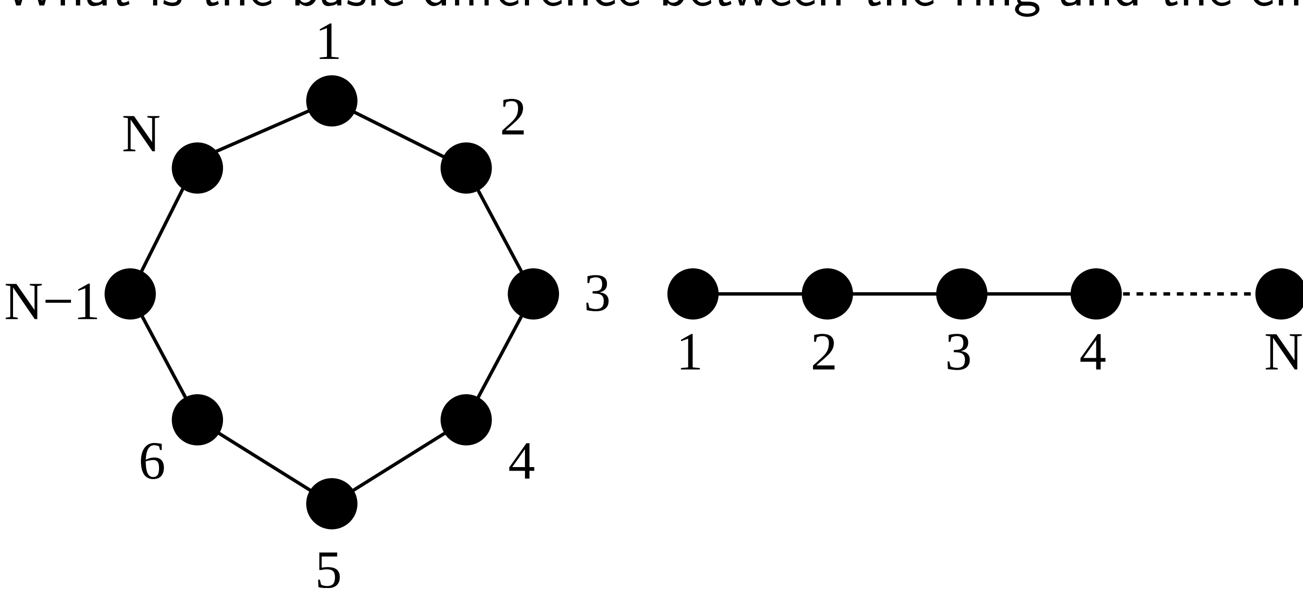
- Why the molecular state $|\psi\rangle$ has 1) real coefficients for the chain and 2) complex for the ring?

  If you solve the time-dependent Schrödinger equation you will find states of the form

$$|\psi_m(t)\rangle = \sum_j^N \frac{1}{\sqrt{N}} \mathrm{e}^{i(Kj+E_m/\hbar t)}|j\rangle$$

- Why the dispersion relation has the symmetry $K \rightarrow -K$

- What is the basic difference between the ring and the chain?



The Bloch's Theorem

All we have done so far is based on the *guess* that

$$\psi_j = \mathrm{e}^{iKj}$$

This is the most general solution of our problem, as it is demonstrated by the Bloch's Theorem.

The Bloch's Theorem

The eigenstates $\psi(\vec{r})$ of a one-particle Hamiltonian $H(\vec{r}) = H(\vec{r}+\vec{T})$, where $\vec{T}$ is a generic vector, can be chosen to be a plane-wave times a function with the same periodicity of the Hamiltonian:

$$\psi(\vec{r}) = u(\vec{r})\mathrm{e}^{i\vec{k}\cdot\vec{r}} \quad \text{where} \quad u(\vec{r}+\vec{T}) = u(\vec{r})$$

What does it mean? ... is it what we have done?

Consider again the ring (topologically is equivalent to the infinite chain).

All atoms in the ring are equivalent → All observables must be invariant for translation along the ring.

> Note:
> This does not mean that the molecular state $|\psi\rangle$ is invariant!!

Consider for example the probability to find an electron at x

$$|\psi(x)|^2 = |\psi(x+n)|^2$$

This means

$$\psi(x+n) = \mathrm{e}^{i\phi_n}\psi(x)$$

Now express the wavefunctions $\psi(x) = \langle x|\psi\rangle$ in term of atomic orbital $\langle x|j\rangle$

$$\psi(x) = \sum_j^N \psi_j \langle x|j\rangle$$

$$\psi(x+n) = \sum_j^N \psi_j \langle x+n|j\rangle = \sum_j^N \psi_j \langle x|j-n\rangle = \sum_j^N \psi_{j+n} \langle x|j\rangle$$

our condition becomes

$$\mathrm{e}^{i\phi_n} \sum_j^N \psi_j \langle x|j\rangle = \sum_j^N \psi_{j+n} \langle x|j\rangle$$

therefore we need

$$\psi_{j+n}/\psi_j = \mathrm{e}^{i\phi_n}$$

which gives

$$\boxed{\psi_j = A\mathrm{e}^{iKj}}$$

Then

$$\psi(x+n) = \mathrm{e}^{iKn}\psi(x)$$

It follows immediately that

$$\psi(x) = \mathrm{e}^{iKx}u(x) \quad \text{with} \quad u(x+j) = u(x)$$

How do we use this result?

The dispersion can be easily written:

The molecular state is:

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_j^N \mathrm{e}^{iKj} |j\rangle$$

Then the Schrödinger equation:

$$\sum_j^N \mathrm{e}^{iKj} H|j\rangle = E \sum_j^N \mathrm{e}^{iKj} |j\rangle$$

now multiply by $\langle l|$

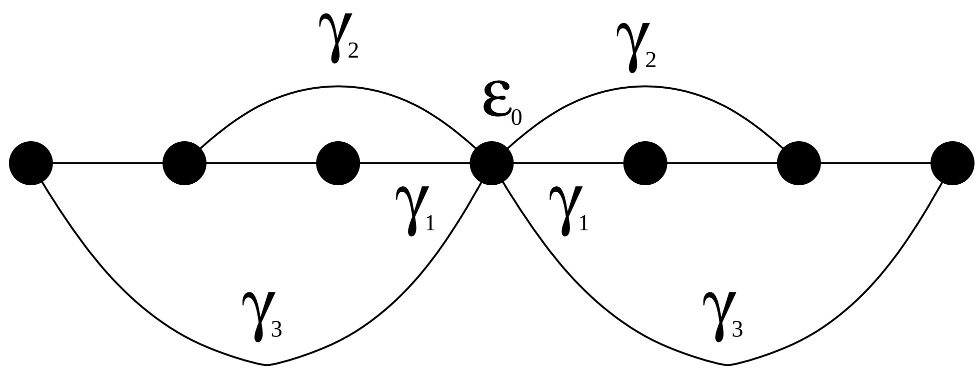
$$\sum_j^N \mathrm{e}^{iKj} \langle l|H|j\rangle = E \sum_j^N \mathrm{e}^{iKj} \langle l|j\rangle$$

Since $\langle l|j\rangle = \delta_{lj}$

$$E_K = \sum_j^N \mathrm{e}^{iK(j-l)} \langle l|H|j\rangle$$

Example:

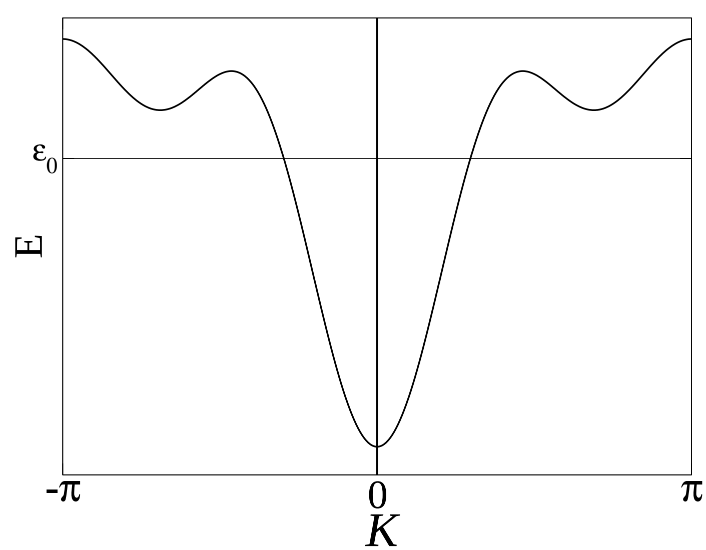
Consider the linear chain where now also second and third nearest neighbors hopping integrals are not zero (γ_2, γ_3):



$$E_K = \sum_{j}^{N} \mathrm{e}^{iK(j-l)} \langle l|H|j\rangle =$$

$$= \epsilon_0 + \gamma_1(\mathrm{e}^{iK} + \mathrm{e}^{-iK}) + \gamma_2(\mathrm{e}^{2iK} + \mathrm{e}^{-2iK}) + \gamma_3(\mathrm{e}^{3iK} + \mathrm{e}^{-3iK}) =$$

$$= \epsilon_0 + 2\gamma_1 \cos K + 2\gamma_2 \cos 2K + 2\gamma_3 \cos 3K$$



k-space

K labels all possible energies $E_K \rightarrow$ it is the band "quantum number"

For the ring

$$-\pi < K < \pi$$

Suppose the atom in the ring are separated by a distance a. Then the phase factor of the Bloch's Theorem is:

$$\mathrm{e}^{imak}$$

where now k is the band "quantum number" and

$$-\pi/a < k < \pi/a$$

We say that k spans the k-space.

The *Brillouin zone* is the region of k space in which all eigenstates of the ring may be labeled uniquely.