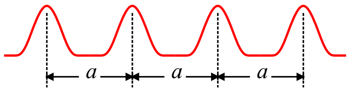
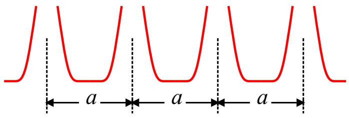
Lattice translations

We consider a particle in the one dimensional periodic potential

$$V(x \pm a) = V(x).$$



(a)



(b)

The Hamiltonian of the system is not in general invariant under translations

$$\tau^\dagger(l) x \tau(l) = x + l, \quad \tau(l)|x'\rangle = |x' + l\rangle.$$

However, when l is exactly equal to the period of the lattice a we have

$$\tau^\dagger(a) V(x) \tau(a) = V(x + a) = V(x).$$

Because the operator corresponding to the kinetic energy in the Hamiltonian is translationally invariant the whole Hamiltonian H satisfies the condition

$$\tau^\dagger(a) H \tau(a) = H,$$

which, due to the unitarity of the translation operator can be written as

$$[H, \tau(a)] = 0.$$

The operators H and $\tau(a)$ have thus common eigenstates.
Note The operator $\tau(a)$ is unitary and hence its eigenvalues need not be real.
Let us suppose that the potential barrier between the lattice points is infinitely high. Let $|n\rangle$ be the state localized in the lattice cell n, i.e.

$$\langle x'|n\rangle \neq 0 \text{ only if } x' \approx na.$$

Obviously $|n\rangle$ is a stationary state. Because all lattice cells are exactly alike we must have

$$H|n\rangle = E_0|n\rangle, \ \forall n.$$

Thus the system has countably infinite number of ground states $|n\rangle$, $n = -\infty, \ldots, \infty$.
Now

$$\tau(a)|n\rangle = |n + 1\rangle,$$

so the state $|n\rangle$ is not an eigenstate of the translation $\tau(a)$.
Let's try

$$|\theta\rangle \equiv \sum_{-\infty}^{\infty} e^{in\theta}|n\rangle,$$

where θ is a real parameter and

$$-\pi \leq \theta \leq \pi.$$

Obviously we have

$$H|\theta\rangle = E_0|\theta\rangle.$$

Furthermore we get

$$\begin{aligned} \tau(a)|\theta\rangle &= \sum_{n=-\infty}^{\infty} e^{in\theta}|n+1\rangle = \sum_{n=-\infty}^{\infty} e^{i(n-1)\theta}|n\rangle \\ &= e^{-i\theta}|\theta\rangle. \end{aligned}$$

Thus every state corresponding to a value of the continuous parameter θ has the same energy, i.e. the ground state of the system infinitely degenerate.
Let us suppose further that

- $|n\rangle$ is a state localized at the point n so that
$$\tau(a)|n\rangle = |n + 1\rangle,$$
- $\langle x'|n\rangle \neq 0$ (but small), when $|x' - na| > a$.

Due to the translation symmetry the diagonal elements of the Hamiltonian H in the base $\{|n\rangle\}$ are all equal to eachother:

$$\langle n|H|n\rangle = E_0.$$

Let us suppose now that

$$\langle n'|H|n\rangle \neq 0 \text{ only if } n' = n \text{ or } n' = n \pm 1.$$

We are dealing with the so called *tight binding approximation.*
When we define

$$\Delta = -\langle n \pm 1|H|n\rangle,$$

we can write

$$H|n\rangle = E_0|n\rangle - \Delta|n + 1\rangle - \Delta|n - 1\rangle,$$

where we have exploited the orthonormality of the basis $\{|n\rangle\}$. Thus the state $|n\rangle$ is not an energy eigen state.
Let us look again at the trial

$$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle.$$

Like before we have

$$\tau(a)|\theta\rangle = e^{-i\theta}|\theta\rangle.$$

Furthermore

$$\begin{aligned} &H \sum e^{in\theta}|n\rangle \\ &\quad = E_0 \sum e^{in\theta}|n\rangle - \Delta \sum e^{in\theta}|n+1\rangle \\ &\qquad -\Delta \sum e^{in\theta}|n-1\rangle \\ &\quad = E_0 \sum e^{in\theta}|n\rangle - \Delta \sum (e^{in\theta - i\theta} + e^{in\theta + i\theta})|n\rangle \\ &\quad = (E_0 - 2\Delta\cos\theta) \sum e^{in\theta}|n\rangle. \end{aligned}$$

The earlier degeneracy will be lifted if $\Delta \neq 0$ and

$$E_0 - 2\Delta \leq E \leq E_0 + 2\Delta.$$

Bloch's theorem
Let us consider the wave function $\langle x'|\theta\rangle$. In the translated state $\tau(a)|\theta\rangle$ the wave function is

$$\langle x'|\tau(a)|\theta\rangle = \langle x' - a|\theta\rangle$$

when the operator $\tau(a)$ acts on left. When it acts on right we get

$$\langle x'|\tau(a)|\theta\rangle = e^{-i\theta}\langle x'|\theta\rangle,$$

so we have

$$\langle x' - a|\theta\rangle = \langle x'|\theta\rangle e^{-i\theta}.$$

This equation can be solved by substituting

$$\langle x'|\theta\rangle = e^{ikx'}u_k(x'),$$

when $\theta = ka$ and $u_k(x')$ is a periodic function with the period a.
We have derived a theorem known as the *Bloch theorem*:
Theorem 1 *The wave function of the eigenstate $|\theta\rangle$ of the translation operator $\tau(a)$ can be written as the procuct of the plane wave $e^{ikx'}$ and a function with the period a.*
Note When deriving the theorem we exploited only the fact that $|\theta\rangle$ an eigenstate of the operator $\tau(a)$ belonging to the eigenvalue $e^{i\theta}$. Thus it is valid for all periodic systems (whether the tight binding approximation holds or not)
With the help of the Bloch theorem the dispersion relation of the energy in the tight binding model can be written as

$$E(k) = E_0 - 2\Delta\cos ka,\ -\frac{\pi}{a} \le k \le \frac{\pi}{a}.$$

This continuum of the energies is known as the *Brillouin zone*.