روش یا تقریب تنگ- بست چیست؟

قضیه بلوخ چیست؟

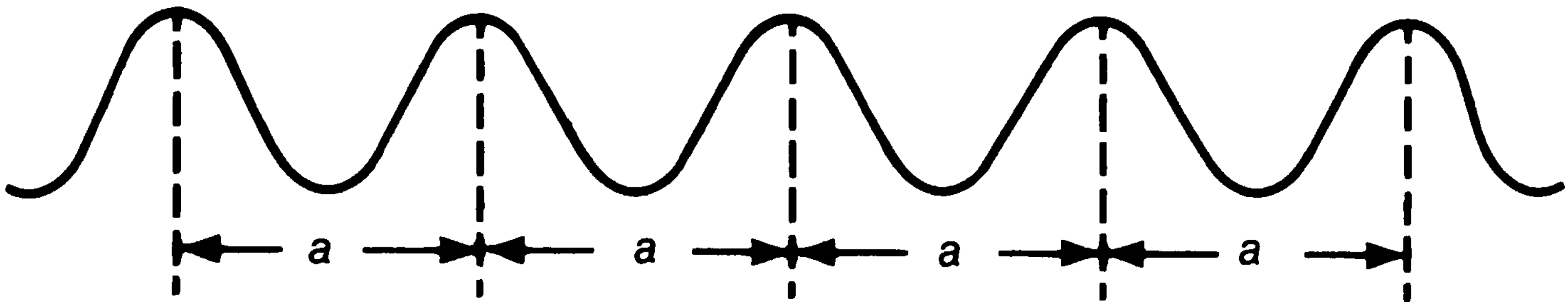
آیا تقریب تنگ- بست سبب شکافتگی ترازها می شود؟

آیا بین روش تنگ- بست و قضیه بلوخ ارتباطی وجود دارد؟

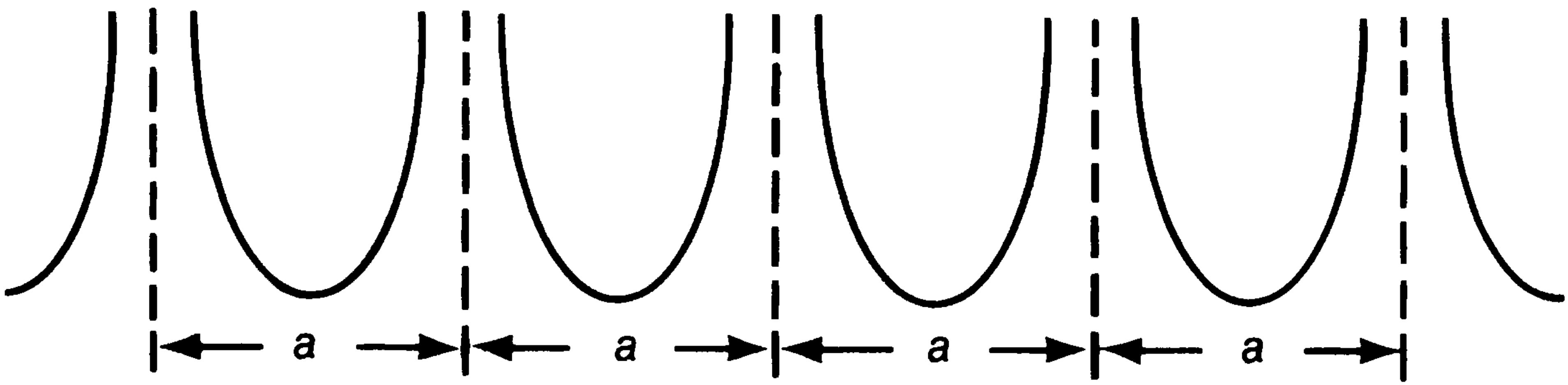
آیا قضیه بلوخ مستقل از روش تنگ- بست است؟

LATTICE TRANSLATION AS A DISCRETE SYMMETRY

Consider a periodic potential in one dimension, where $V(x \pm a) = V(x)$, as depicted in the following Figure.



Periodic potential in one dimension with periodicity a



The periodic potential when the barrier height between two adjacent lattice sites becomes infinite.

Realistically, we may consider the motion of an electron in a chain of regularly spaced positive ions.

In general, the Hamiltonian is not invariant under a translation represented by $\tau(l)$ with l arbitrary, where $\tau(l)$ has the property (see Section 1.6)

$$\tau^{\dagger}(l)\,x\,\tau(l) = x + l \qquad \tau(l)|x'\rangle = |x' + l\rangle$$

However, when l coincides with the lattice spacing a, we do have

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

Because the kinetic-energy part of the Hamiltonian H is invariant under the translation with any displacement, the entire Hamiltonian satisfies

$$\tau^{\dagger}(a) H \tau(a) = H.$$

Because $\tau(l)$ is unitary, we have [from the above equation)]

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

so the Hamiltonian and $\tau(l)$ can be simultaneously diagonalized.

Although $\tau(l)$ is unitary, it is not Hermitian, so we expect the eigenvalue to be a complex number of modulus 1.

Before we determine the eigenkets and eigenvalues of $\tau(l)$ and examine their physical significance, it is instructive to look at a special case of periodic potential when the barrier height between two adjacent lattice sites is made to go to infinity, as in Figure 4.6b.

What is the ground state for the potential of Figure 4.6b?

Clearly, a state in which the particle is completely localized in one of the lattice sites can be a candidate for the ground state.

To be specific let us assume that the particle is localized at the nth site and denote the corresponding ket by |n>.

This is an energy eigenket with energy eigenvalue E_0, namely, $H|n\rangle = E_0|n\rangle$.

Its wave function $\langle x'|n\rangle$ is finite only in the nth site.

However, we note that a similar state localized at some other site also has the same energy E_0, so actually there are denumerably infinite ground states n, where n runs from $-\infty$ to ∞.

Now $|n\rangle$ is obviously not an eigenket of the lattice-translation operator, because when the lattice-translation operator is applied to it, we obtain $|n + 1\rangle$:

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

So despite the fact that $\tau(a)$ commutes with H, $|n\rangle$—which is an eigenket of H—is not an eigenket of $\tau(a)$.

This is quite consistent with our earlier theorem on symmetry because we have an infinite fold degeneracy.

When there is such degeneracy, the symmetry of the world need not be the symmetry of energy eigenkets.

Our task is to find a simultaneous eigenket of H and $\tau(a)$.

Here we may recall how we handled a somewhat similar situation with the symmetrical double-well potential of the previous section.

We noted that even though neither |R> nor |L> is an eigenket of π, we could easily form a symmetrical and an antisymmetrical combination of |R> and |L> that are parity eigenkets.

The case is analogous here.

Let us specifically form a linear combination

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

where θ is a real parameter with $-\pi \leq \theta \leq \pi$.

We assert that $|\theta\rangle$ is a simultaneous eigenket of H and $\tau(a)$.

That it is an H eigenket is obvious because |n> is an energy eigenket with eigenvalue E_0, independent of n.

To show that it is also an eigenket of the lattice translation operator we apply $\tau(a)$ as follows:

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

Note that this simultaneous eigenket of H and $\tau(a)$ is parameterized by a continuous parameter θ.

Furthermore, the energy eigenvalue E_0 is independent of θ.

Let us now return to the more realistic situation of Figure 4.6a, where the barrier between two adjacent lattice sites is not infinitely high.

We can construct a localized ket $|n\rangle$ just as before with the property $\tau(a)|n\rangle = |n+1\rangle$.

However, this time we expect that there is some leakage possible into neighboring lattice sites due to quantum-mechanical tunneling.

In other words, the wave function $\langle x'|n\rangle$ has a tail extending to sites other than the nth site.

The diagonal elements of H in the $\{|n\rangle\}$ basis are all equal because of translation invariance, that is,

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

independent of n, as before.

However we suspect that H is not completely diagonal in the $\{|n\rangle\}$ basis due to leakage.

Now, suppose the barriers between adjacent sites are high (but not infinite).

We then expect matrix elements of H between distant sites to be completely negligible.

Let us assume that the only nondiagonal elements of importance connect immediate neighbors.

That is,

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

In solid-state physics this assumption is known as the tight-binding approximation.

Let us define

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

Clearly, Δ is again independent of n due to translation invariance of the Hamiltonian.

To the extent that $|n\rangle$ and $|n'\rangle$ are orthogonal when $n \neq n'$, we obtain

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

Note that $|n\rangle$ is no longer an energy eigenket.

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

$$\begin{aligned}&\langle n+1|H|n\rangle \\ &= E_0\langle n+1|n\rangle - \Delta\langle n+1|n+1\rangle \\ &- \Delta\langle n+1|n-1\rangle = -\Delta\end{aligned}$$

$$\begin{aligned}&\langle n-1|H|n\rangle \\ &= E_0\langle n-1|n\rangle - \Delta\langle n-1|n+1\rangle \\ &- \Delta\langle n-1|n-1\rangle = -\Delta\end{aligned}$$

As we have done with the potential of Figure 4.6b, let us form a linear combination

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

Clearly, θ is an eigenket of translation operator $\tau(a)$ because the steps in $\tau(a)|\theta\rangle = e^{-i\theta}|\theta\rangle$ still hold:

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

A natural question is, is $|\theta\rangle$ an energy eigenket?

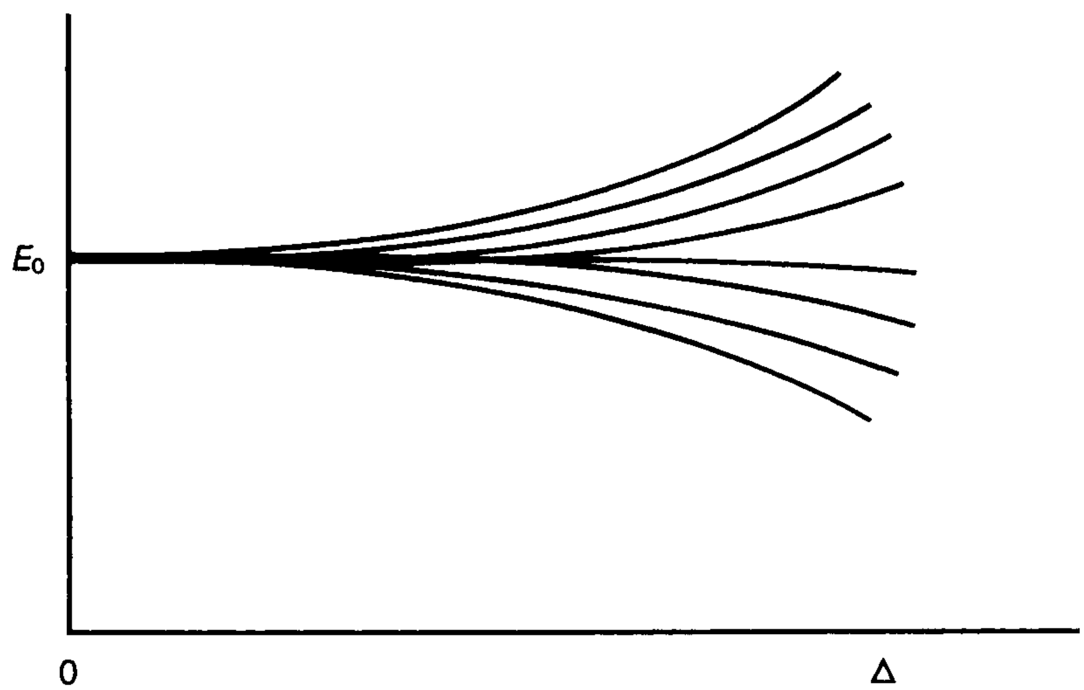
To answer this question, we apply H:

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

The big difference between this and the previous situation is that the energy eigenvalue now depends on the continuous real parameter θ.

The degeneracy is lifted as Δ becomes finite, and we have a continuous distribution of energy eigenvalues between E_0 -2 Δ and E_0+2 Δ.

See following figure, where we visualize how the energy levels start forming a continuous energy band as Δ is increased from zero.



To see the physical meaning of the parameter θ let us study the wave function $\langle x'|\theta\rangle$.

For the wave function of the lattice-translated state $\tau(a)|\theta\rangle$, we obtain

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

by letting $\tau(a)$ act on <x'|.

But we can also let $\tau(a)$ operate on $|\theta\rangle$ and use $\tau(a)|\theta\rangle = e^{-i\theta}|\theta\rangle$.

Thus,

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

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

We solve this equation by setting

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

with $\theta = ka$, where $u_k(x')$ is a periodic function with period a, as we can easily verify by explicit substitutions, namely,

$$e^{ik(x'-a)}u_k(x'-a) = e^{ikx'}u_k(x')e^{-ika}$$

Thus we get the important condition known as **Bloch's theorem**:

The wave function of $|\theta\rangle$, which is an eigenket of $\tau(a)$, can be written as a plane wave $e^{ikx'}$ times a periodic function with periodicity a.

Notice that the only fact we used was that $|\theta\rangle$ is an eigenket of $\tau(a)$ with eigenvalue $e^{-i\theta}$ [see $\tau(a)|\theta\rangle = e^{-i\theta}|\theta\rangle$].

In particular, the theorem holds even if the tight-binding approximation $\langle n'|H|n\rangle \neq 0$ *only if* $n' = n$ *or* $n' = n \pm 1$ breaks down.

We are now in a position to interpret our earlier result $H\sum e^{in\theta}|n\rangle = (E_0 - 2\Delta cos\theta)\sum e^{in\theta}|n\rangle$ for $|\theta\rangle$ given by $|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle$.

We know that the wave function is a plane wave characterized by the propagation wave vector k modulated by a periodic function $u_k(x')$ [see $\langle x'|\theta\rangle = e^{ikx'}u_k(x')$].

As θ varies from $-\pi$ to π, the wave vector k varies from $-\frac{\pi}{a}$ to $\frac{\pi}{a}$.

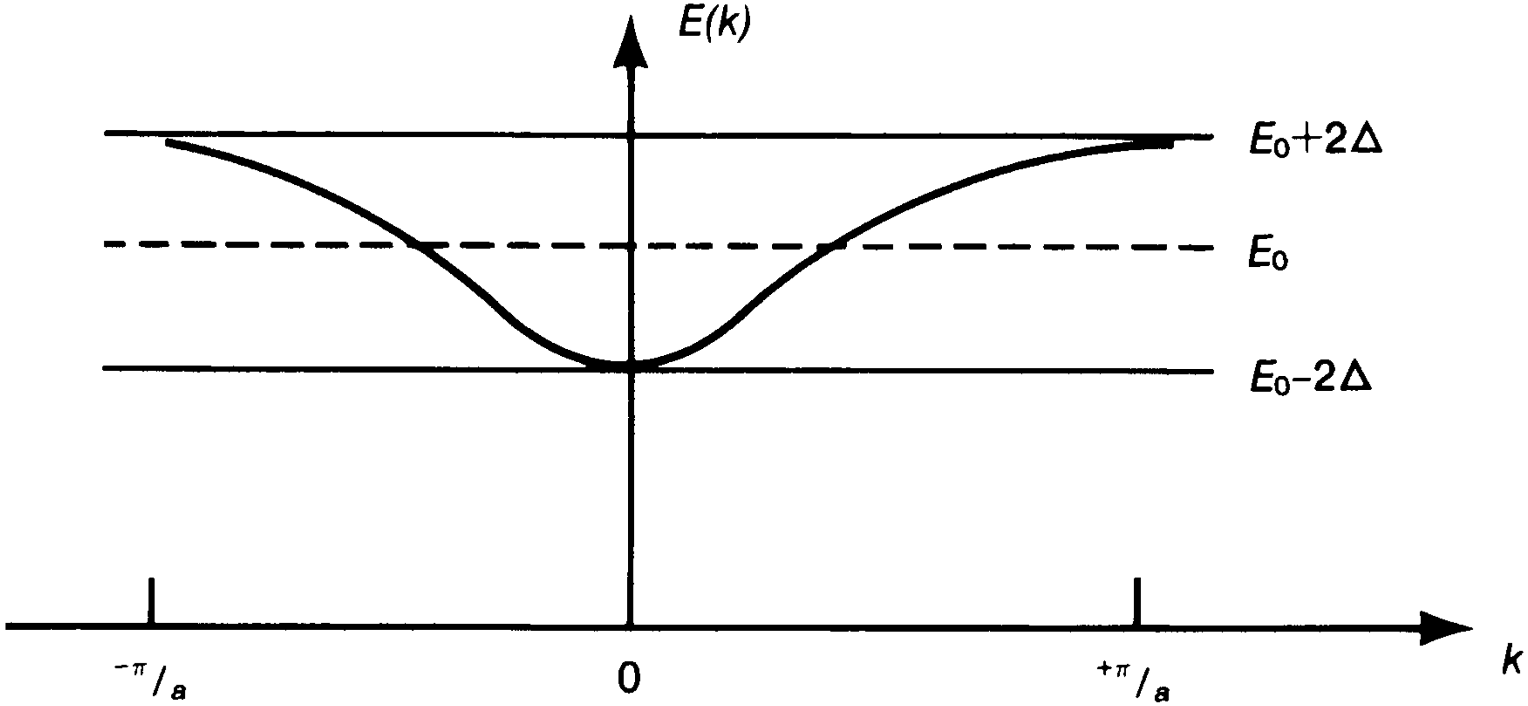
The energy eigenvalue E now depends on k as follows:

$$E(k) = E_0 - 2\Delta \cos ka$$

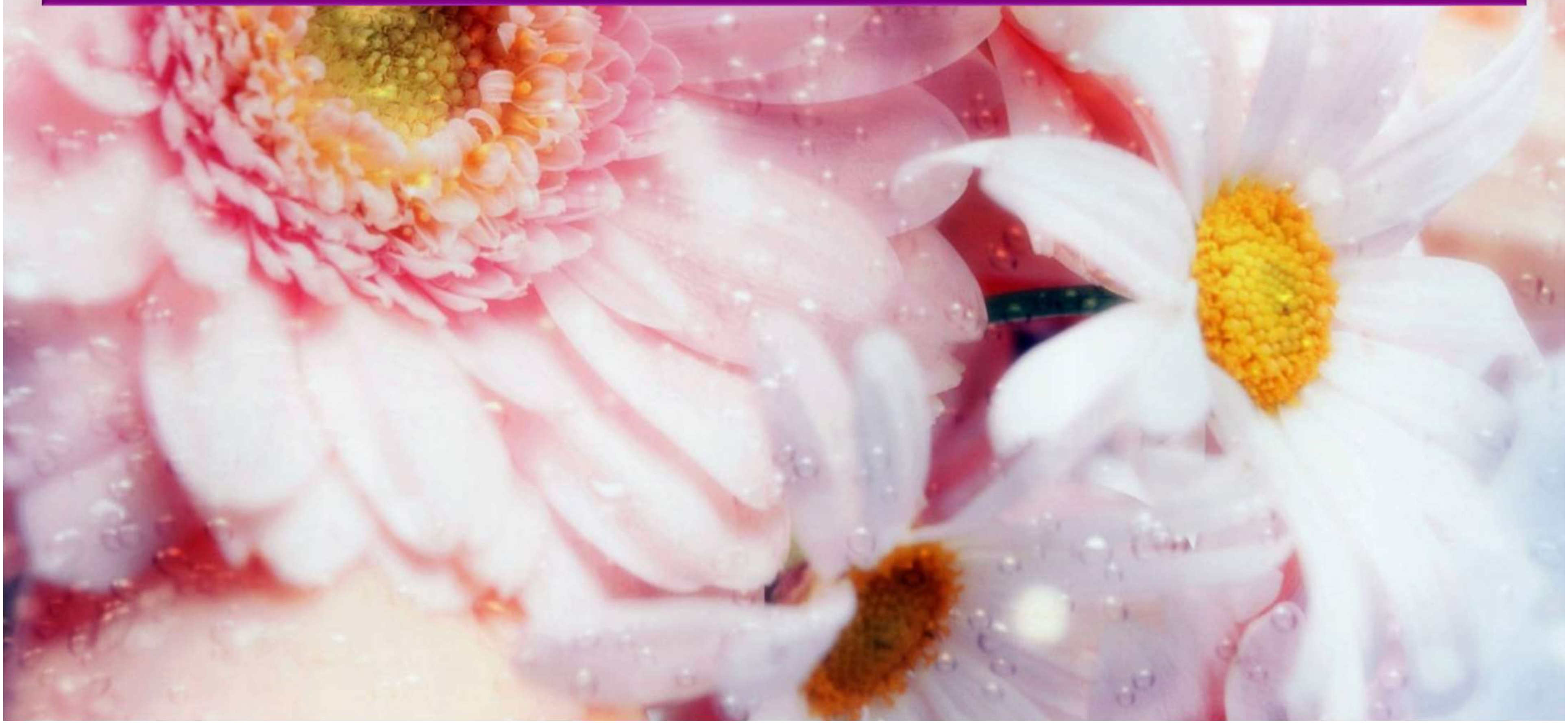
Notice that this energy eigenvalue equation is independent of the detailed shape of the potential as long as the tight-binding approximation is valid.

Note also that there is a cutoff in the wave vector k of the Bloch wave function $\langle x'|\theta\rangle = e^{ikx'}u_k(x')$ given by $|k| = \frac{\pi}{a}$.

Equation $E(k) = E_0 - 2\Delta coska$ defines a dispersion curve, as shown in the following Figure.



As a result of tunneling, the denumerably infinitefold degeneracy is now completely lifted, and the allowed energy values form a continuous band between $\boldsymbol{E_0 - 2\Delta}$ and $\boldsymbol{E_0 + 2\Delta}$, known as the **Brillouin zone**.



So far we have considered only one particle moving in a periodic potential. In a more realistic situation we must look at many electrons moving in such a potential. Actually the electrons satisfy the Pauli exclusion principle, as we will discuss more systematically in Chapter 6, and they start filling the band. In this way, the main qualitative features of metals, semiconductors, and the like can be understood as a consequence of translation invariance supplemented by the exclusion principle.

The reader may have noted the similarity between the symmetrical double-well problem of Section 4.2 and the periodic potential of this section. Comparing Figures 4.3 and 4.6, we note that they can be regarded as opposite extremes (two versus infinite) of potentials with a finite number of troughs.