Bloch's Theorem in 1D and the Kronig–Penney Model

1. Periodic potentials and Fourier expansion

We consider a 1D crystal with a periodic potential

$$V(x+a) = V(x). \tag{1}$$

It can be expanded as a Fourier series over reciprocal lattice vectors $G = 2\pi n/a$:

$$V(x) = \sum_G V_G e^{iGx}. \tag{2}$$

2. Action of H on a plane wave

For a free electron, eigenstates are plane waves e^{ikx}. When acted on by $H = -\frac{\hbar^2}{2m}\partial_x^2 + V(x)$, the kinetic term preserves k, while the potential term couples it to plane waves with $k+G$. Thus,

$$He^{ikx} \in \text{span}\{e^{i(k+G)x}\}, \tag{3}$$

which is a closed subspace S_k.

3. Subspaces and the Brillouin zone

Each k defines a distinct subspace S_k. However, k and $k+G$ belong to the same subspace, so it suffices to take k within the range $-\pi/a \leq k \leq \pi/a$. This interval defines the **first Brillouin zone (1BZ)**. Any wavevector can be written as $k_{\text{1BZ}} + G$.

4. Bloch form of eigenstates

Because H is block-diagonal in these subspaces, its eigenfunctions can be written as linear combinations of plane waves $e^{i(k+G)x}$. Factoring out e^{ikx} leads to Bloch's theorem:

$$\psi_k(x) = e^{ikx}u_k(x), \qquad u_k(x+a) = u_k(x). \tag{4}$$

Thus eigenstates are travelling waves modulated by a periodic function.

5. Symmetry in 1D

In 1D, the Schr"odinger equation is a second-order ODE, so for each energy there are only two independent solutions. Together with time-reversal/inversion symmetry,

$$E(k) = E(-k), \tag{5}$$

this implies that there can be no additional degeneracy at a fixed k. Therefore, in 1D bands cannot cross.

6. Location of extrema

Because $E(k) = E(-k)$, the derivative dE/dk vanishes at $k = 0$ (the Γ point). At the zone edge $k = \pm\pi/a$, Bragg reflection couples $\pm k$ states into standing waves with zero group velocity. Therefore extrema occur only at Γ and at the zone boundary.

7. Free electron bands and folding

If $V = 0$, the dispersion is free-electron-like:

$$E(k) = \frac{\hbar^2 k^2}{2m}. \tag{6}$$

Folding into the first Brillouin zone produces overlapping parabolas. At the zone boundary, different plane waves become degenerate.

8. Periodic potential and gap opening

A periodic potential couples states differing by reciprocal lattice vectors. At the zone boundary, plane waves $e^{\pm i\pi x/a}$ are degenerate. The potential couples them, leading to standing waves:

$$\cos(\pi x/a), \quad \sin(\pi x/a). \tag{7}$$

One has density maxima on the ions, the other has nodes on the ions, so their energies split. This opens a band gap.

9. Two-level picture at the boundary

Near $k = \pi/a$, the subspace spanned by $e^{i\pi x/a}$ and $e^{-i\pi x/a}$ leads to a 2×2 Hamiltonian

$$H = \begin{pmatrix} E_0 & V_G \\ V_G^* & E_0 \end{pmatrix}, \tag{8}$$

where $E_0 = \hbar^2(\pi/a)^2/2m$ is the free-electron energy and V_G is the Fourier component of the potential. Diagonalization yields

$$E = E_0 \pm |V_G|, \tag{9}$$

so a gap $2|V_G|$ opens at the zone boundary.

10. Finite system size and allowed k values

So far we treated the system as infinite, which makes k continuous in the first Brillouin zone. In a real sample of finite length L, there are only

$$M = \frac{L}{a} \tag{10}$$

unit cells.

Imposing Born–von Karman boundary conditions, $\psi(x+L) = \psi(x)$, restricts the allowed values of k to

$$k = \frac{2\pi m}{L}, \qquad m = -\frac{M}{2}, \ldots, +\frac{M}{2} - 1. \tag{11}$$

Thus within the first Brillouin zone $[-\pi/a, \pi/a]$ there are exactly M distinct k-points, equal to the number of unit cells. Each energy band therefore contains M states.

This connects the crystal momentum picture to counting of quantum states: the number of states per band equals the number of unit cells in the crystal.

11. Kronig–Penney model

A concrete solvable model is the 1D Kronig–Penney potential: a periodic array of rectangular barriers (well width w, barrier width b, height V_0). The dispersion relation is

$$\cos(ka) = \cos(qw)\cosh(\beta b) + \frac{\beta^2 - q^2}{2q\beta}\sin(qw)\sinh(\beta b), \tag{12}$$

with $a = w + b$, $q = \sqrt{2mE}/\hbar$, and $\beta = \sqrt{2m(V_0 - E)}/\hbar$.

This transcendental equation defines the allowed energies $E(k)$. Gaps appear naturally at the Brillouin zone edges, and the dependence on w, b, and V_0 provides clear physical intuition: larger barriers or wider spacing flatten bands and widen gaps.

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Summary: Bloch's theorem ensures eigenstates are plane waves modulated by a periodic function. In 1D, symmetry constrains bands to be even functions of k, forbids crossings, and places extrema only at Γ and zone edges. The periodic potential opens gaps at the zone boundaries, which can be seen explicitly in both the simple two-level picture and the exactly solvable Kronig–Penney model. For a finite crystal of length L, the number of allowed k values per band equals the number of unit cells $M = L/a$.