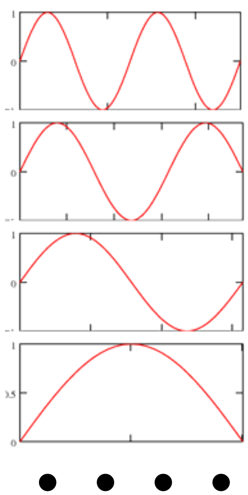
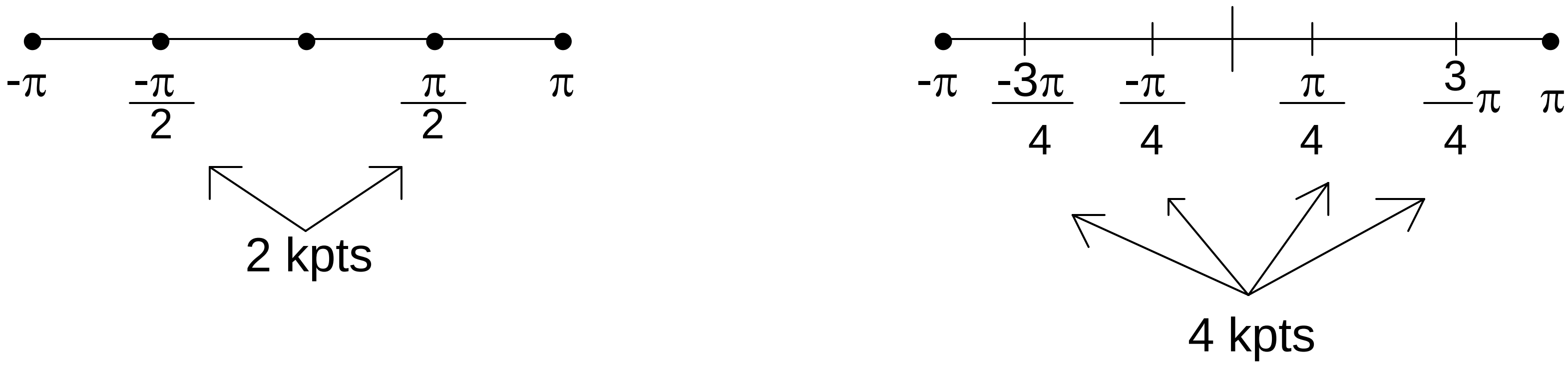
Chain of 4 atoms

	0	a	2a	3a
$\sin\frac{4\pi}{5a}x$	0.58	-0.95	0.95	-0.58
$\sin\frac{3\pi}{5a}x$	0.95	-0.58	-0.58	0.95
$\sin\frac{2\pi}{5a}x$	0.95	0.58	-0.58	-0.95
$\sin\frac{1\bullet\pi}{5a}x$	0.58	0.95	0.95	0.58



Notice similarity of the above wavefunctions to those for the particle-in-the-box problem.

Gaussian uses the range (-π, π), where the 1/L has been suppressed.



$$\Delta = \frac{\pi}{N}, \quad k_n = \left(n - \frac{N}{2}\right)\Delta,$$ where N = # kpoints, n = integer

The most commonly used scheme is that of Monkhurst-Pack, which eliminates points that are redundant by symmetry and adjusts the weights on the remaining points accordingly.

Direct lattice a_1, a_2, a_3

Reciprocal lattice vectors b_1, b_2, b_3

$$b_i = 2\pi \frac{a_j \mathrm{x} a_k}{(a_1 \mathrm{x} a_2)\bullet a_3}, \quad \text{i, j, k are a cyclic permutation of 1, 2, 3}$$

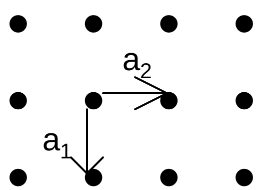
$a_1 x a_2 \bullet a_3$ = volume of the primitive cell.

The first Brillouin zone is the smallest polyhedr0n confined by planes perpendicularly bisecting the reciprocal lattice vectors

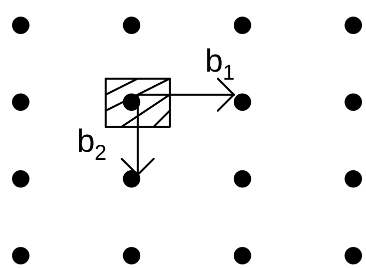
$b_i \bullet a_i = 1$

$$T_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3,$$

{h, k, l} = Miller indices



r space



shaded region = 1^{st} BZ

Bloch's theorem

if V(x + a) = (V(x)

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

free particle: $u_k(x)$ = constant

$$k_x = \ell_x \frac{2\pi}{L_x},\ k_y = \ell_y \frac{2\pi}{L_y},\ k_z = \ell_z \frac{2\pi}{L_z}$$

ℓ_x, ℓ_y, ℓ_z are integers

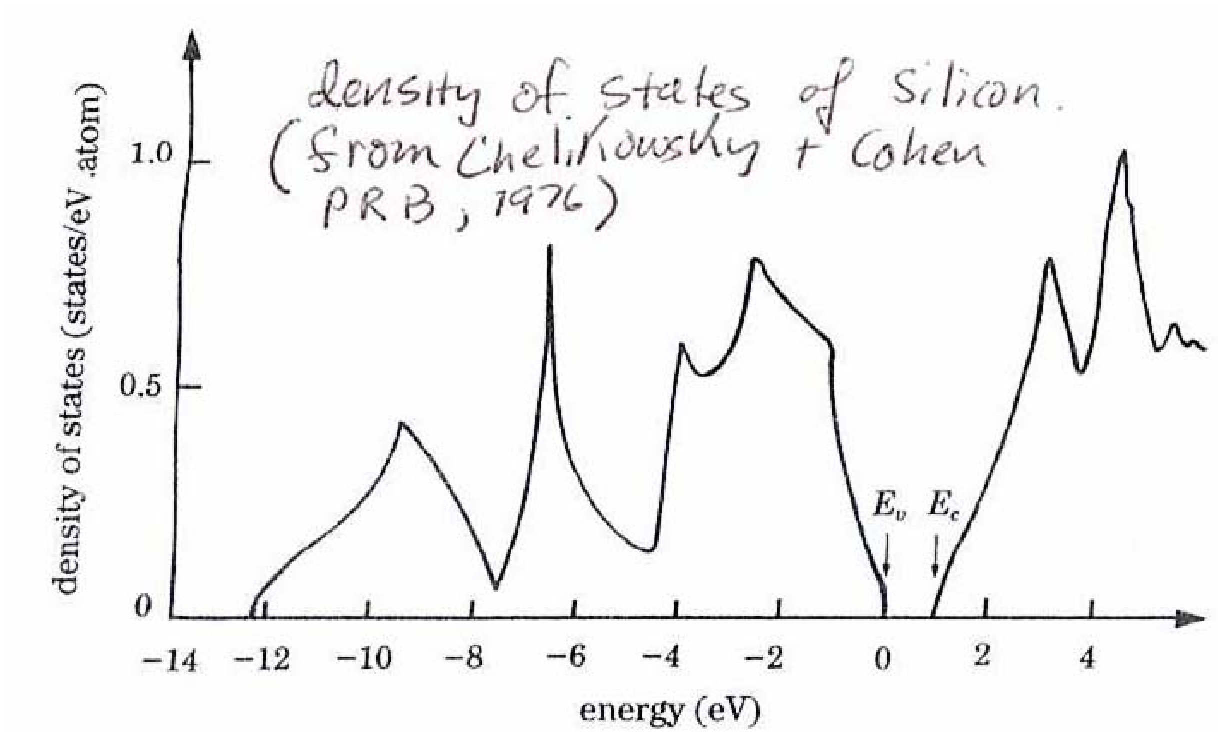
# of states in volume d^3k = $$n(k)d^3k = 2\frac{L_x L_y L_z}{(2\pi)^3} d^3k$$

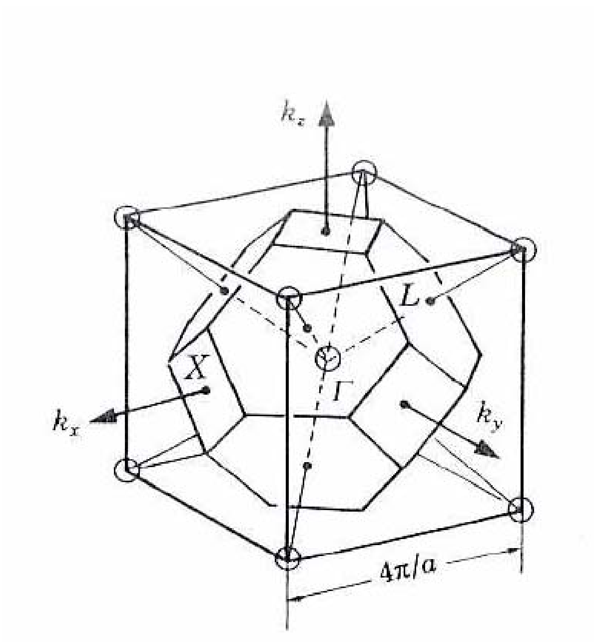
$$dN = n(E)dE = \int_{\delta V(E)} n(k)d^3k$$

↑

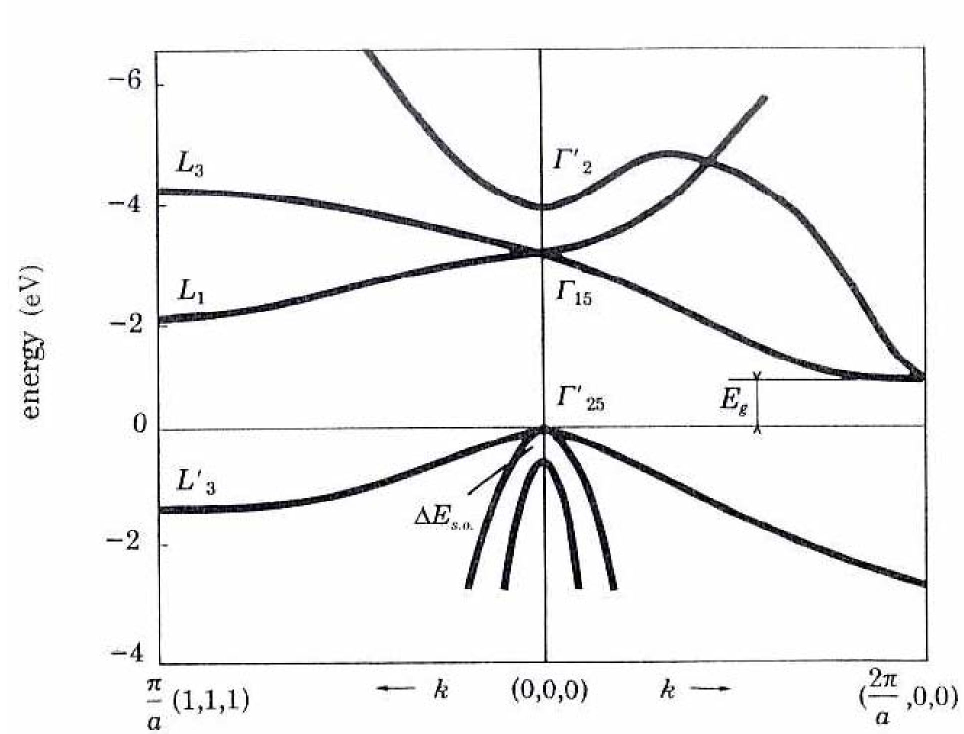
volume between constant energy surfaces
S(E), S(E + dE)

for a free electron $$n(E) = 4\pi \left(\frac{L}{h} \right)^3 (2m)^{3/2} \sqrt{E}$$





reciprocal lattice of
silicon (from Sapoval & Hermann,
<u>Physics of Semiconductors</u>,
Springer



Band structure of silicon
(from Sapoval & Hermann)