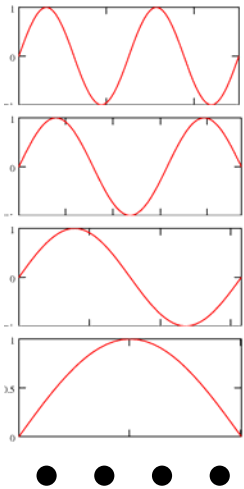


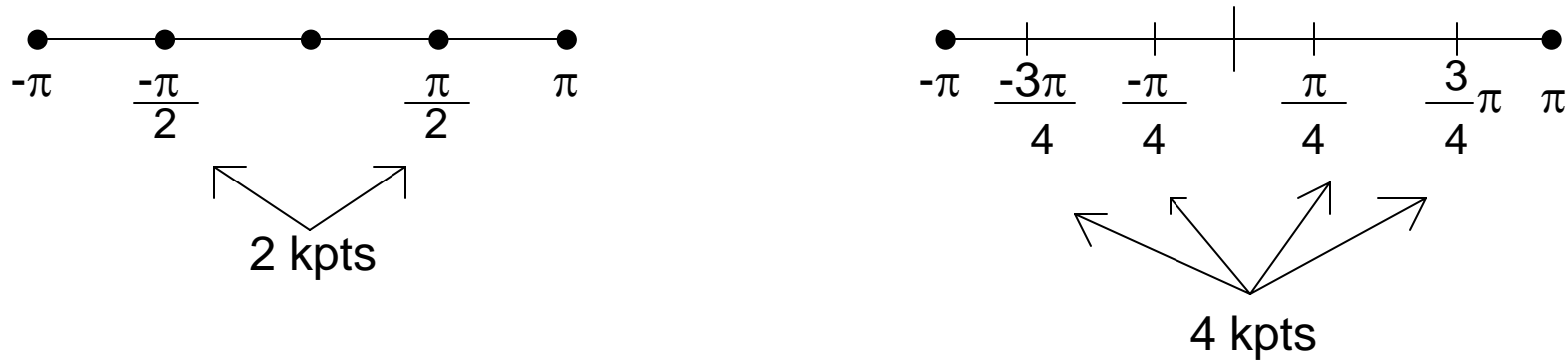
## Chain of 4 atoms

	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
$\sin \frac{1\cdot\pi}{5a} x$	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  $(-\pi, \pi)$ , where the  $1/L$  has been suppressed.



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

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

Direct lattice  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$

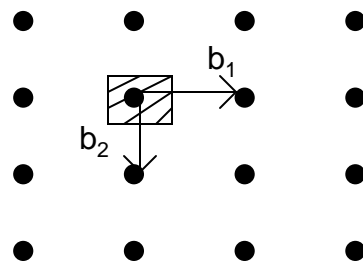
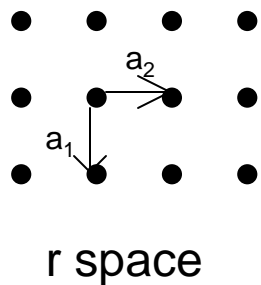
Reciprocal lattice vectors  $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$

$$\mathbf{b}_i = 2\pi \frac{\mathbf{a}_j \times \mathbf{a}_k}{(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3}, \quad i, j, k \text{ are a cyclic permutation of } 1, 2, 3$$

$\mathbf{a}_1 \times \mathbf{a}_2 \cdot \mathbf{a}_3 = \text{volume of the primitive cell.}$

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

$$\mathbf{b}_i \cdot \mathbf{a}_i = 1 \quad T_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3, \quad \{h, k, l\} = \text{Miller indices}$$



shaded region =  
1<sup>st</sup> BZ

## Bloch's theorem

$$\text{if } V(x + a) = V(x)$$

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

free particle:  $u_k(x) = \text{constant}$

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

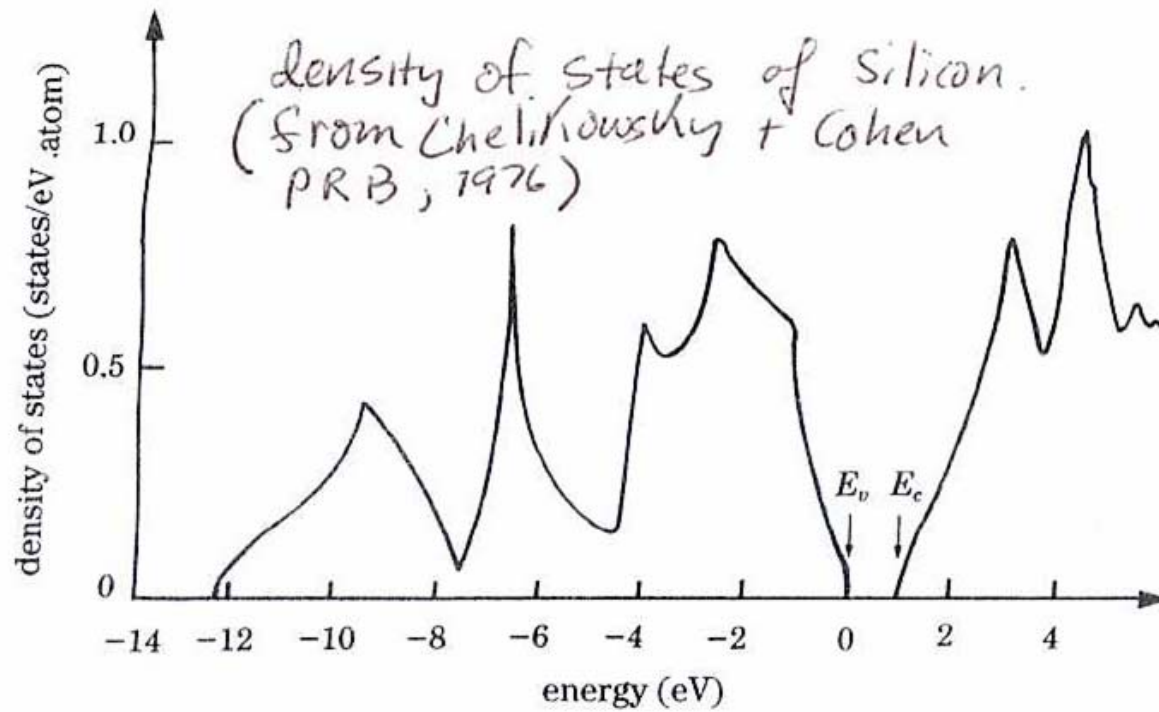
$$\# \text{ of states in volume } d^3k = n(k)d^3k = 2 \frac{L_x L_y L_z}{(2\pi)^3} d^3k$$

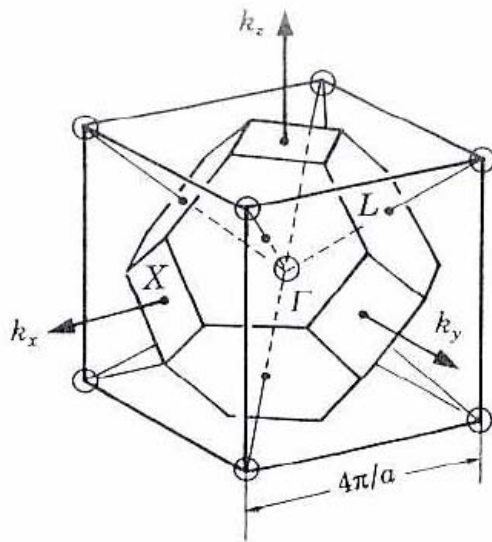
$$dN = n(E)dE = \int_{\delta V(E)} n(k)d^3k$$

↑

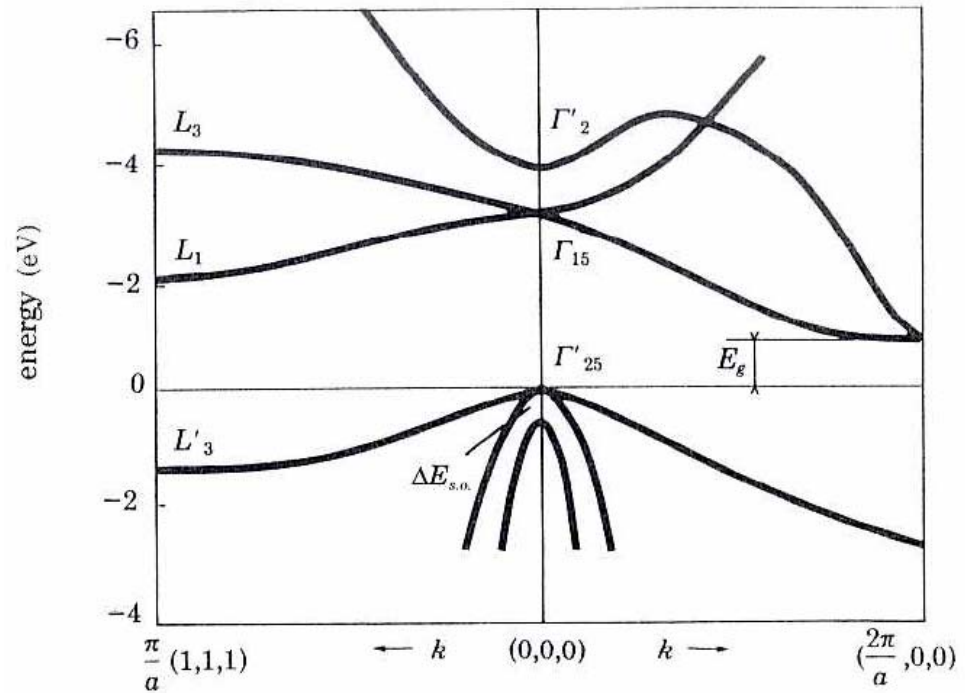
volume between constant energy surfaces  
 $S(E), S(E + dE)$

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, Physics of Semiconductors, Springer)



Band structure of silicon (from Sapoval & Hermann)