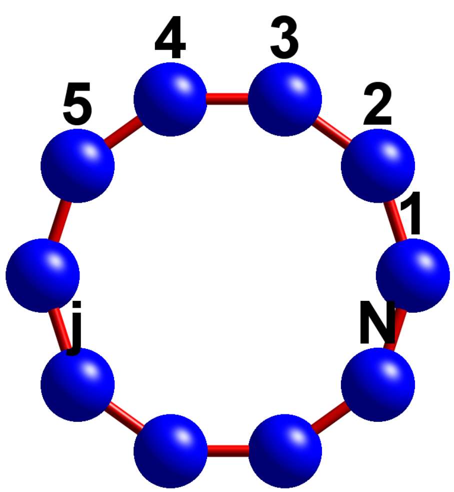
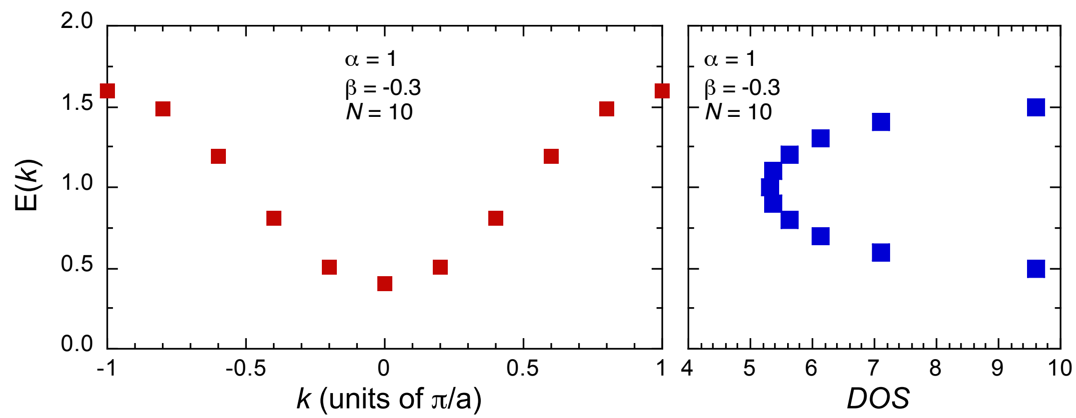
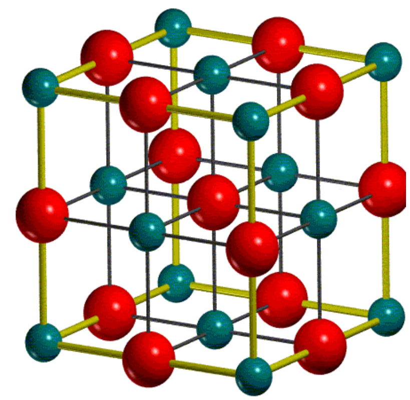
PH575 Spring 2019

Lecture #10
Density of states
Sutton Ch. 3 p 55, Ch.4 pp 88-92

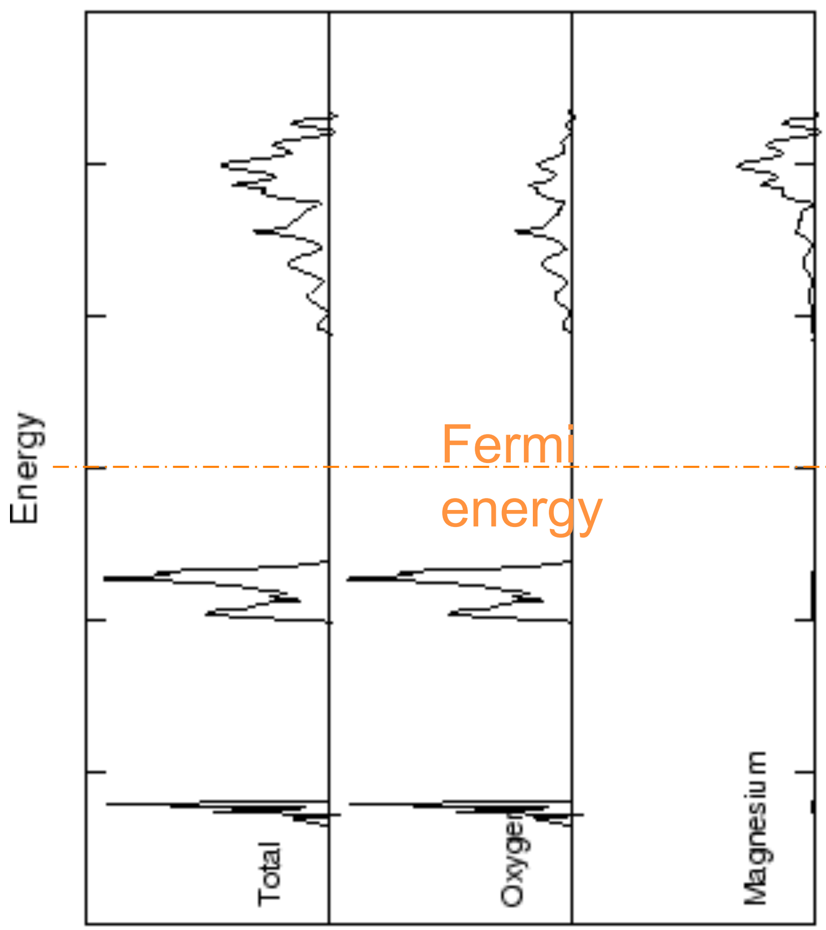




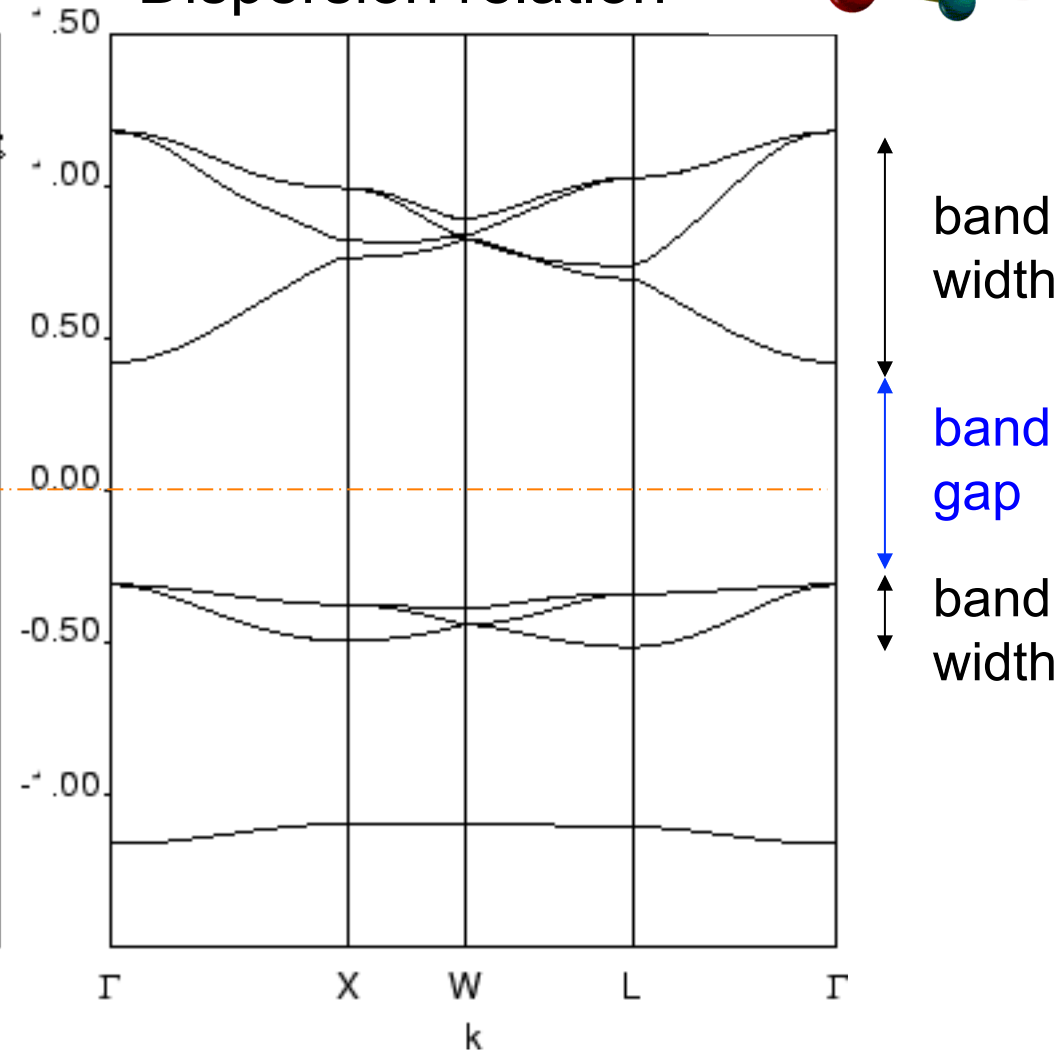
MgO - an ionic crystal



Density of states



Dispersion relation



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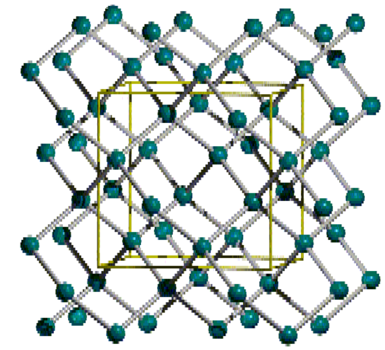
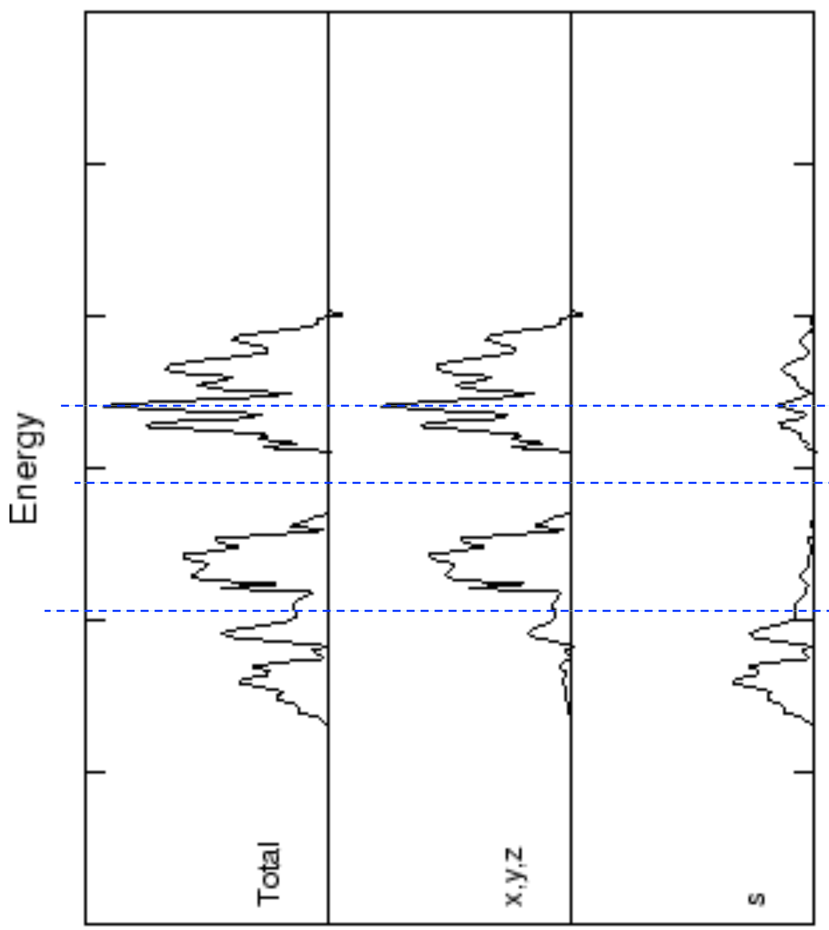
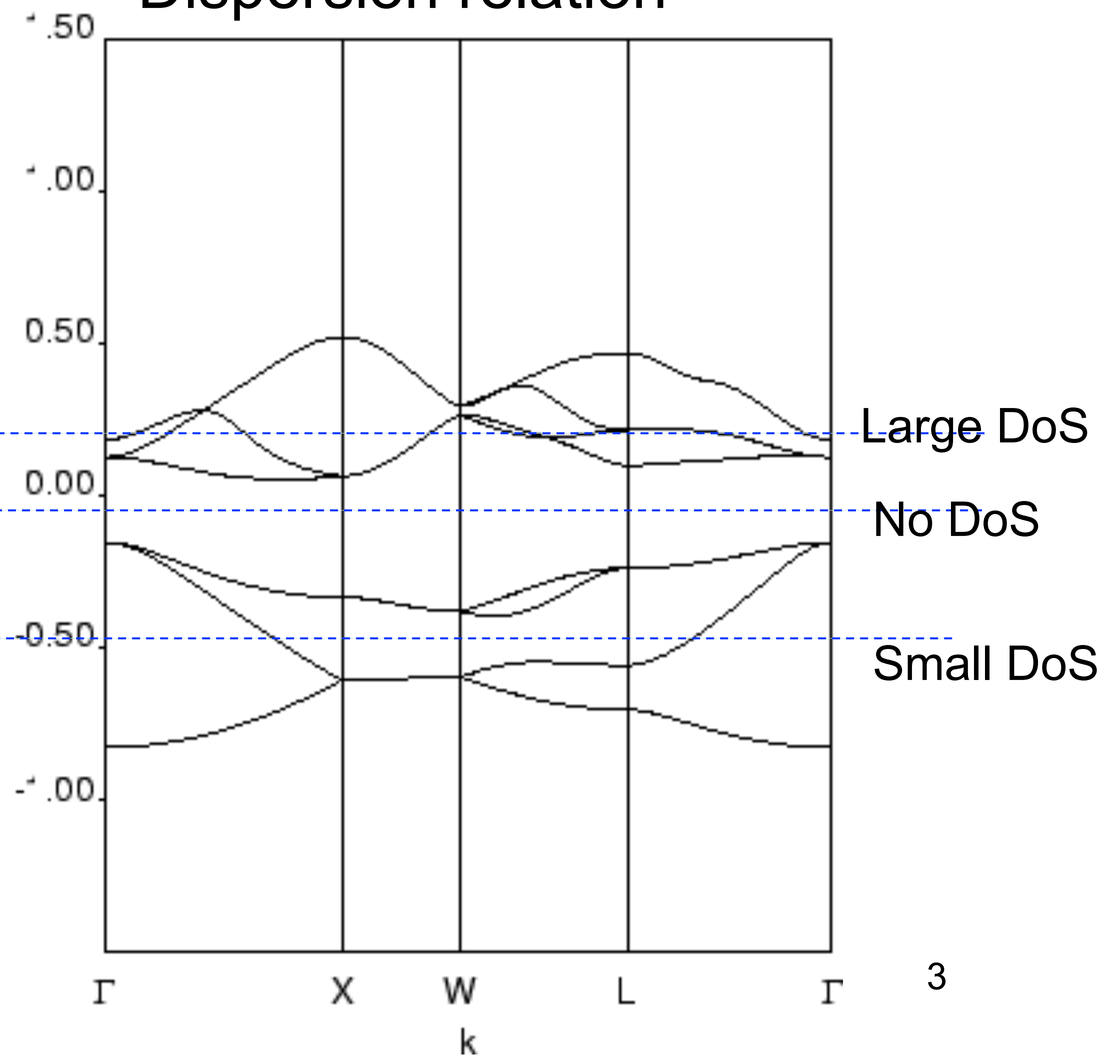
Si - a covalent crystal



Density of states



Dispersion relation



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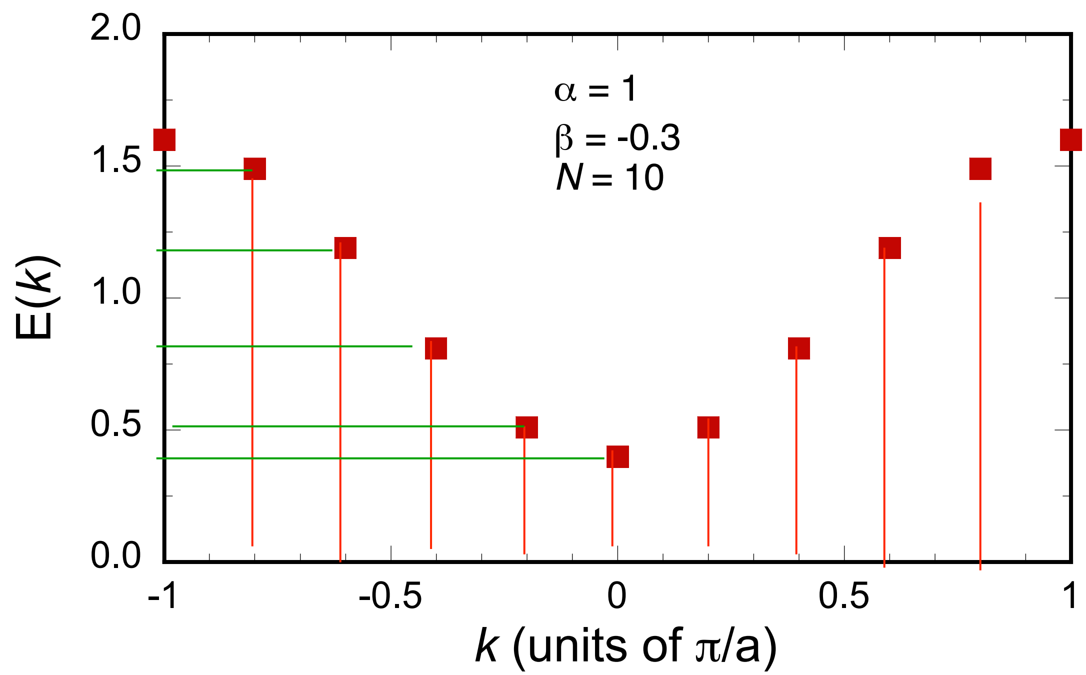
Density of states:
Very important concept in solid state systems.
Properties of a system heavily influenced by the number of states per unit energy interval.
e.g. absorption of light, tunneling current,



How densely are states packed along *k* axis?
Spacing is uniform in *k*!

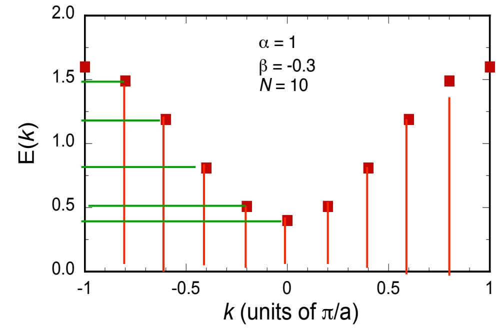
$$D_k(k)dk = dS$$

dS = number of states in a small interval

$$D_k(k) = \frac{N}{2\pi / a} = \frac{L}{2\pi}$$

D(k) = density of states in *k* space – or number of states per unit *k*. It is a constant (independent of *k*) because the states are evenly spaced in *k* space

Define the density of states (per unit energy) as *D(E)*, sometimes written as $D_E(E)$ to remind us that it's a number per unit energy.



$$D_E(E) = \frac{dS}{dE} = \frac{\#\text{ states in energy interval } dE}{\text{energy interval } dE}$$

$$D_E(E) = \underbrace{2}_{\pm k}\frac{dS}{dk}\frac{dk}{dE} = 2D(k)\frac{1}{\dfrac{dE}{dk}}$$

Uniform Na/2π

From dispersion relation *E*(*k*)

We know density in k-space and we know E(k)!
Note – we have not considered spin of electron.

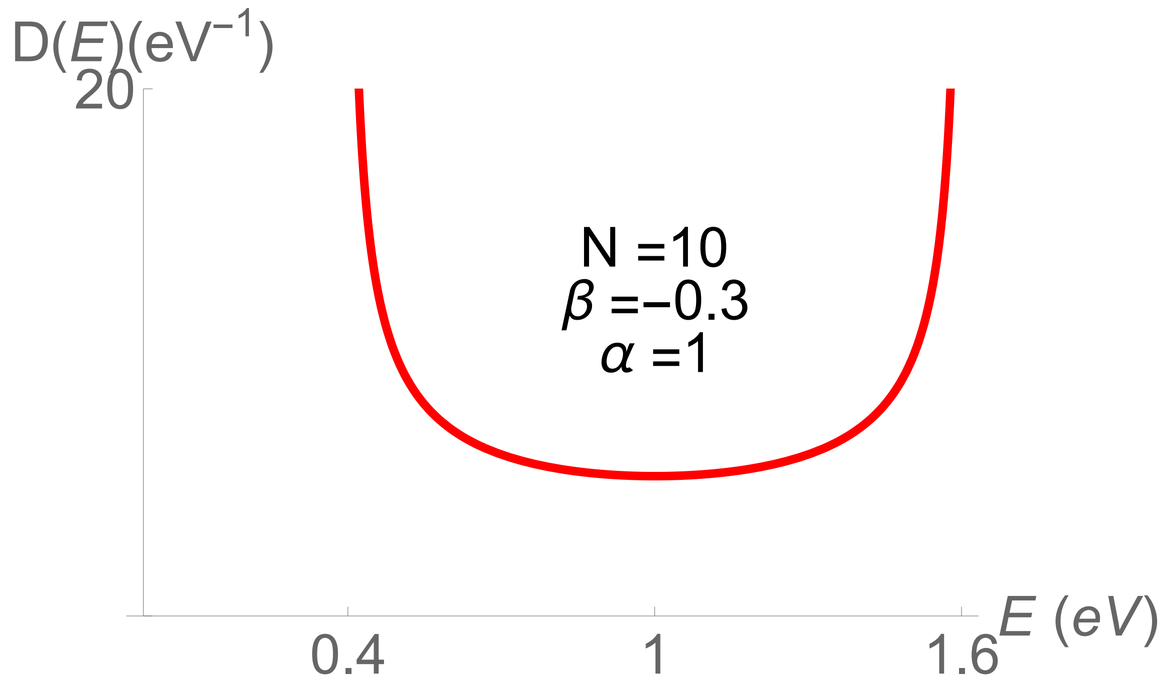
$$E(k) = \alpha + 2\beta\cos(ka)$$

$$\cos(ka) = \frac{E-\alpha}{2\beta}$$

$$\left|\frac{dE}{dk}\right| = 2\beta a\sin(ka)$$

$$= a\sqrt{4\beta^2 - (E-\alpha)^2}$$

$$D_k(k) = \frac{L}{2\pi}$$



$$D_E(E) = D_k(k)\left|\frac{dk}{dE}\right| = \frac{N}{\pi}\frac{1}{\sqrt{4\beta^2 - (E-\alpha)^2}}$$

If we include the spin of the electron, then for every k, there are 2 states - one for each spin, so we would multiply the above by 2. The plot of D(E) is above.

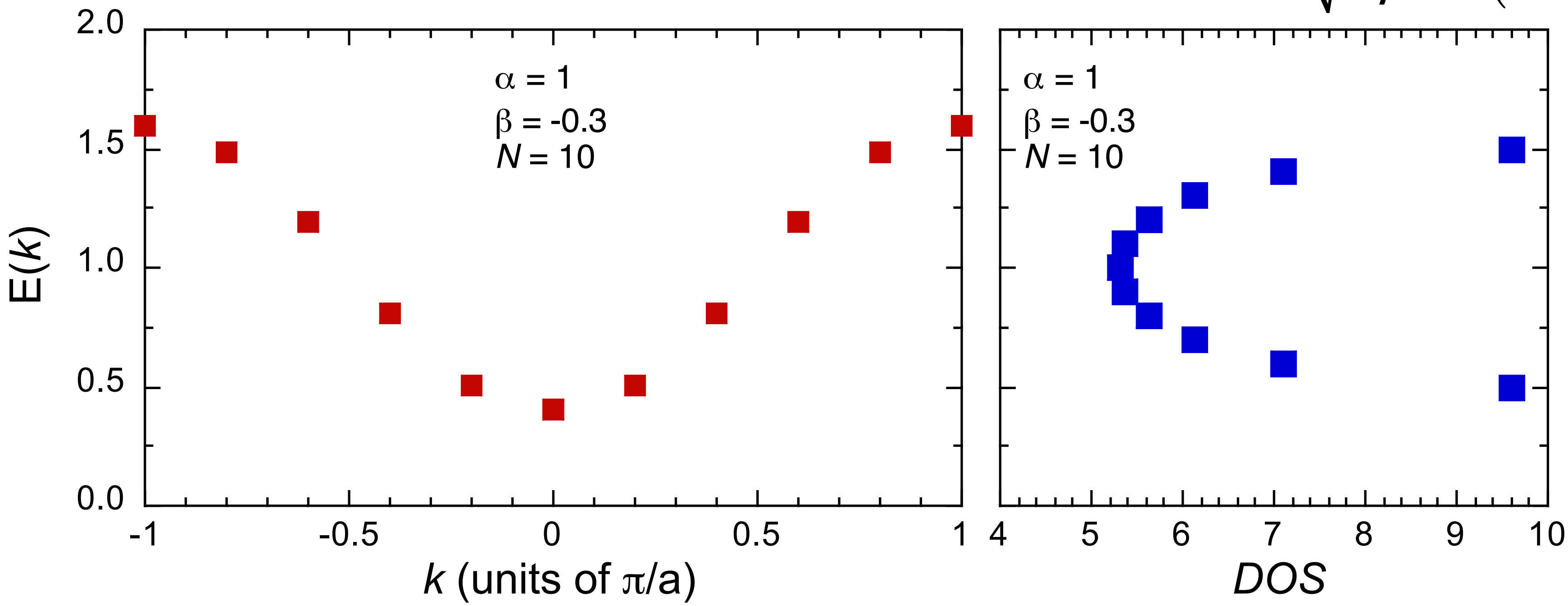
SUMMARY – Linear, infinite, homonuclear chain

Dispersion relation

$$E(k) = \alpha + 2\beta\cos(ka)$$

Density of States

$$D_{E,nospin}(E) = \frac{N}{\pi}\frac{1}{\sqrt{4\beta^2 - (E-\alpha)^2}}$$



Bandwidth: 4β

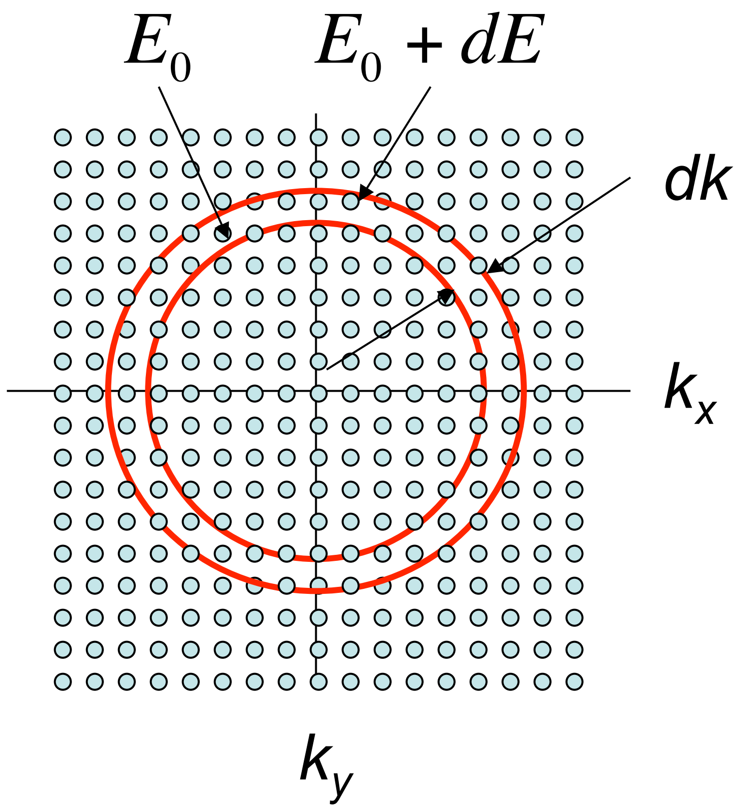
$$k = \frac{2\pi}{\lambda} = \frac{m}{N}\frac{2\pi}{a}$$

2-D Density of states:

$$dS = D_k(\vec{k}) \times \text{ area of } k\text{-space} \qquad \text{area} = 2\pi k dk$$

$$D_k\left(\vec{k}\right) = \frac{N_x}{\frac{2\pi}{a}} \frac{N_y}{\frac{2\pi}{a}} = \frac{N_x N_y a^2}{\left(2\pi\right)^2}$$

$$k^2 = k_x^2 + k_y^2$$



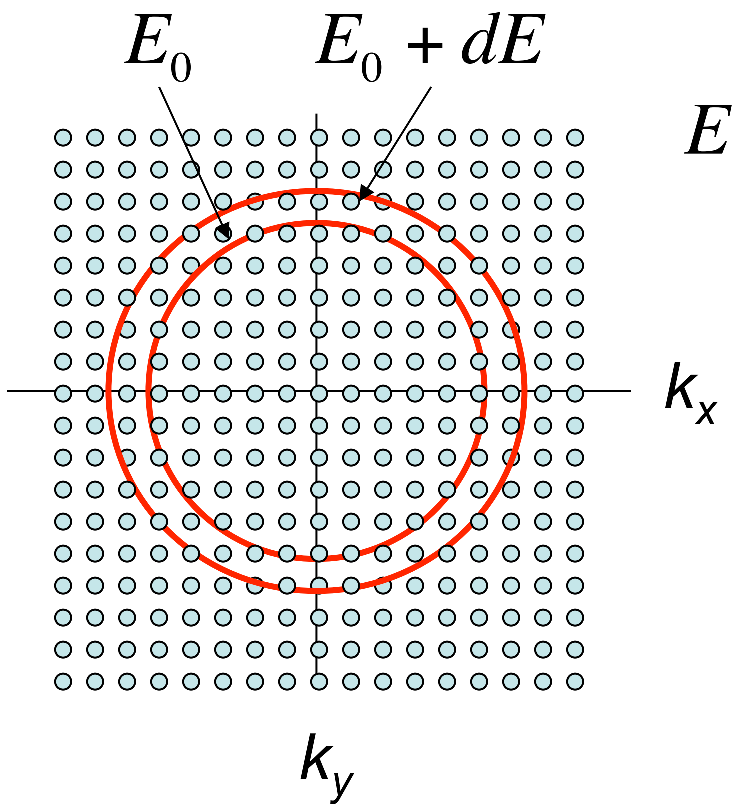
$$D_E\left(E\right) dE = D_k(k) 2\pi k dk$$

$$D_E\left(E\right) = \frac{N_x N_y a^2}{\left(2\pi\right)^2} 2\pi k \frac{dk}{dE}$$

2-D Density of states:

$$D_E(E) = \frac{N_x N_y a^2}{(2\pi)^2} 2\pi k \frac{dk}{dE}$$

Special case when *E* depends only on the magnitude of **k**, e.g. when band is parabolic or free-particle-like:



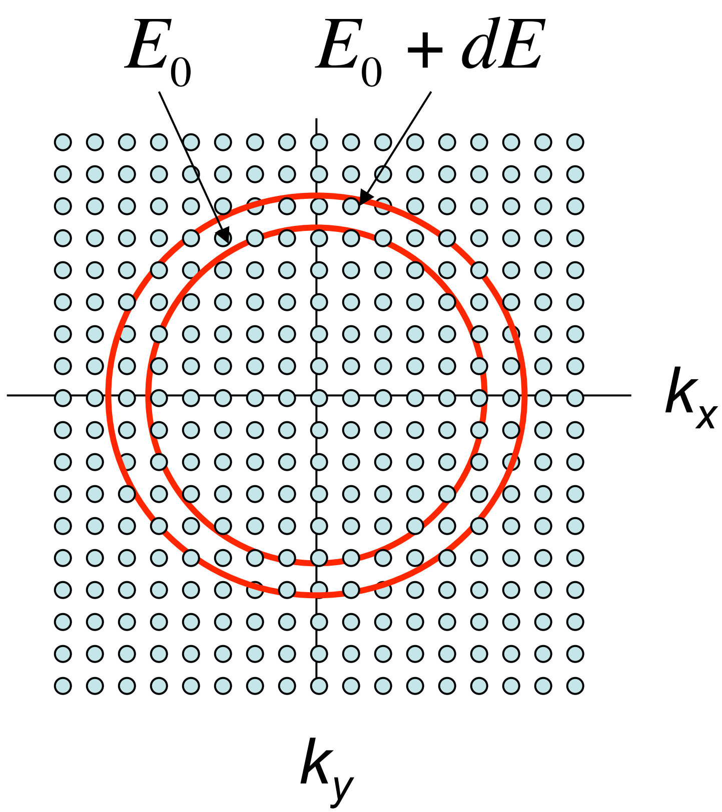
$$E(k) = \alpha + \frac{\hbar^2 k^2}{2m^*} \qquad k = \sqrt{\frac{2m^*(E-\alpha)}{\hbar^2}}$$

$$\frac{dk}{dE} = \frac{d}{dE}\sqrt{\frac{2m^*(E-\alpha)}{\hbar^2}} = \frac{1}{2}\sqrt{\frac{2m^*}{\hbar^2(E-\alpha)}}$$

$$D_E(E) = \frac{m^* L^2}{2\pi\hbar^2}$$

2-D Density of states for parabolic bands (no spin)

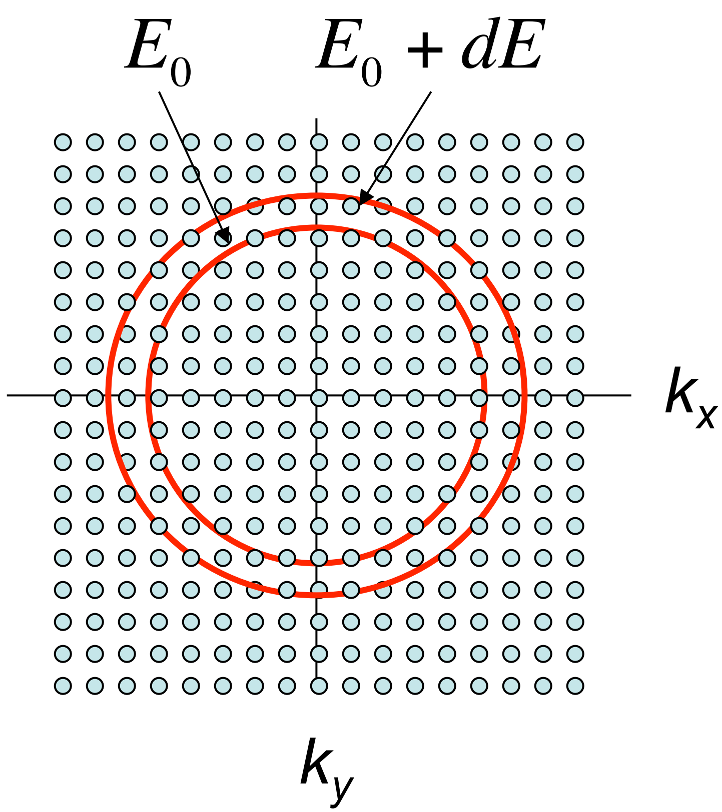
$$D_E(E) = \frac{m^* L^2}{2\pi\hbar^2}$$



D(*E*)is constant! As *E* increases, the number of states at that energy increases in proportion! If spin is considered, we must multiply by 2. (*cf* Sutton 7.15 – careful of h and hbar)

3-D Density of states:

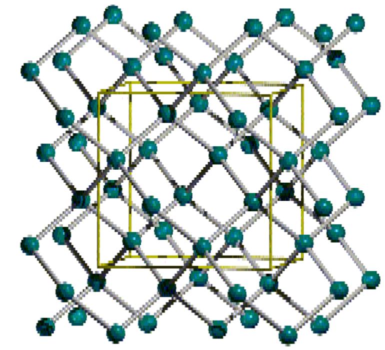
Rotate this in your imagination to get 3D picture! You extend 2D->3D (hwk). See Sutton Eqn 7.17



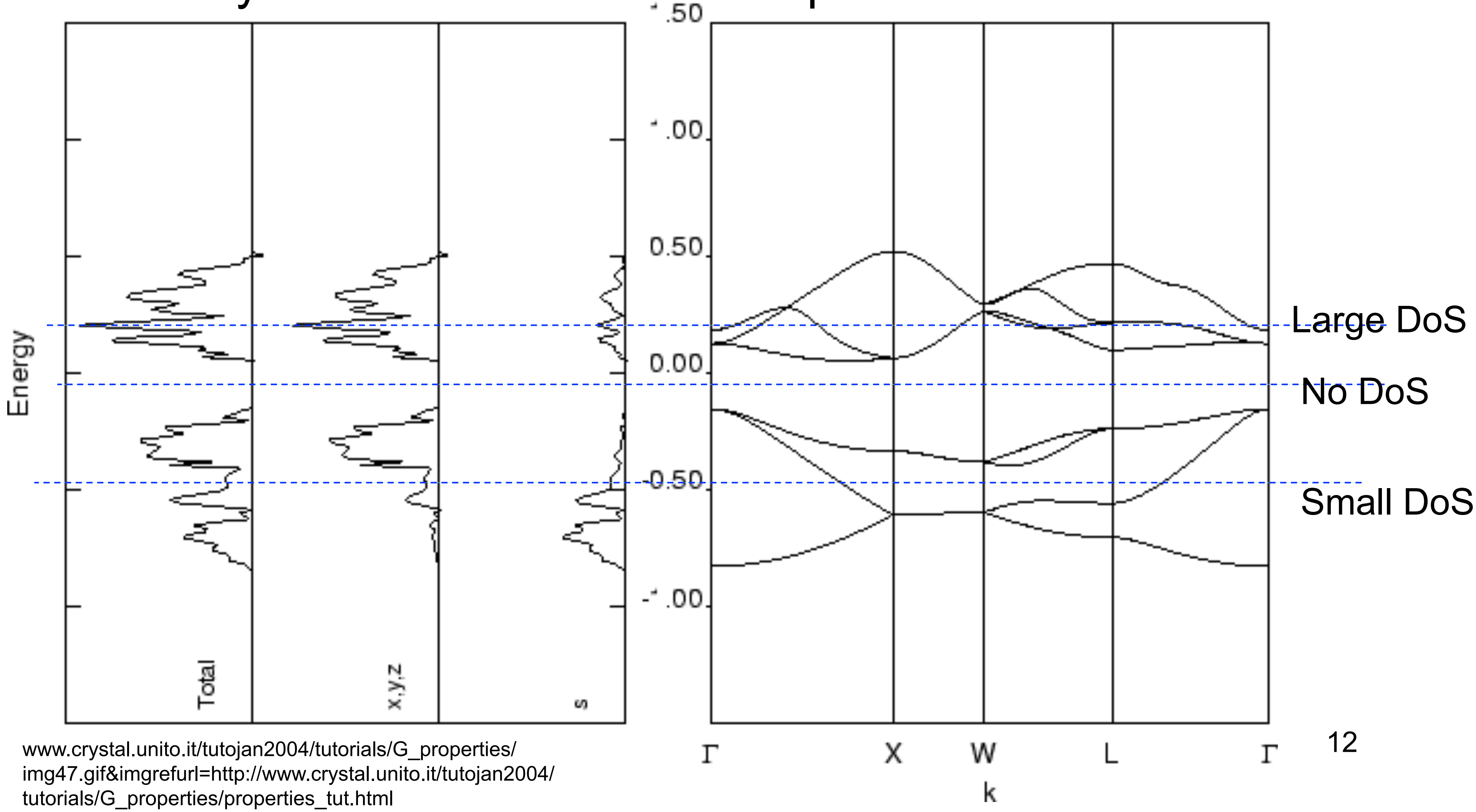
FYI General case of non-circular constant energy surfaces

$$D(E_0) = \left(\frac{a}{2\pi}\right)^3 \int_{E=E_0} \frac{dS(k)}{\left|\nabla_k E(k)\right|}$$

Si - a covalent crystal



Density of states | Dispersion relation



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