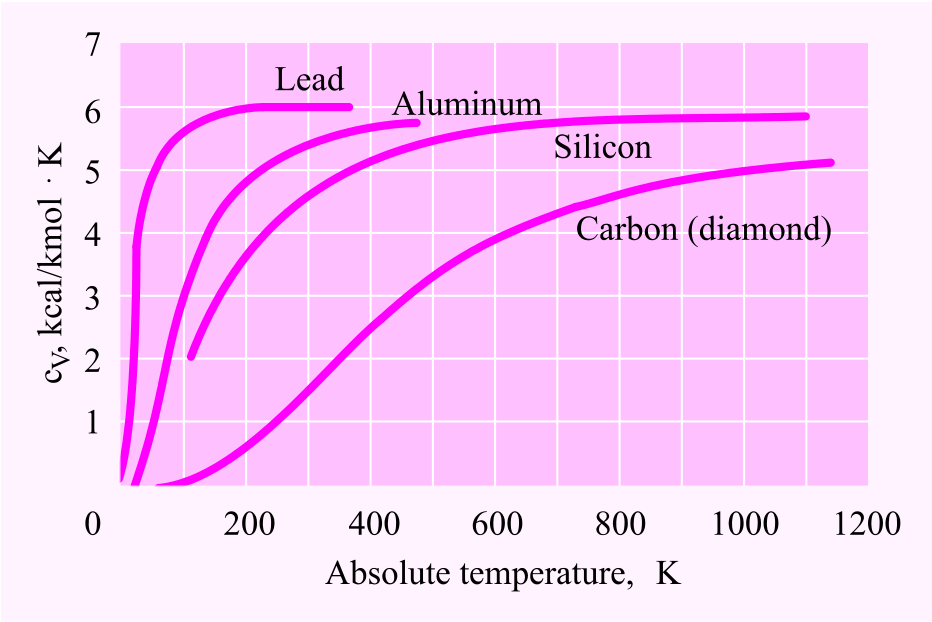
Specific Heat of Solids



$E = 3N_0 k_B T = 3RT$

internal energy of 1kilomole of soild

N_0 : Avogadro's number

$$c_V = \left(\frac{dE}{dT} \right)_V$$

$$c_V = \frac{d(3RT)}{dT} = 3R$$ Dulong-Petit law

Einstein's Theory of Specific Heat of Solids

$$\bar{\varepsilon} = \frac{h\nu}{e^{h\nu/k_BT} - 1}$$

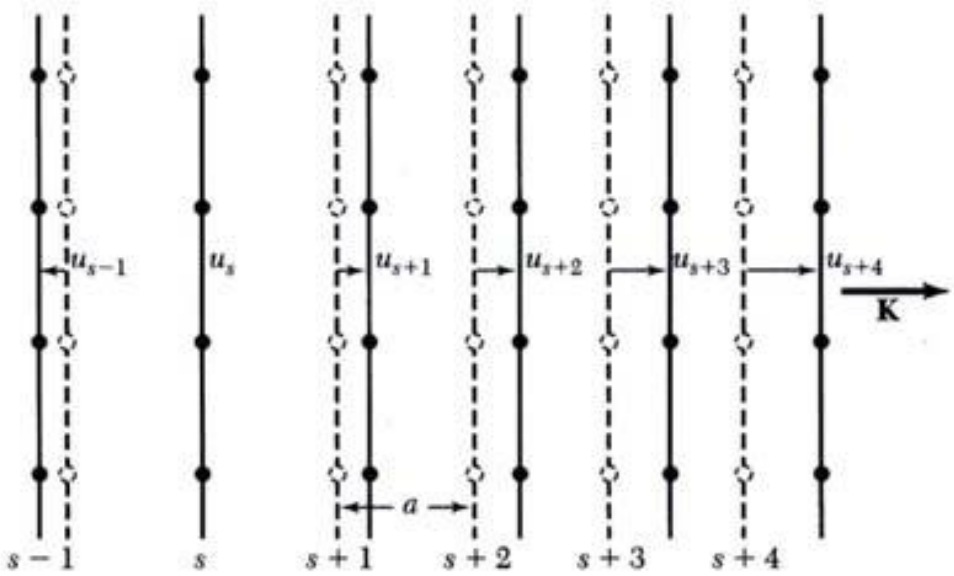
$$E = 3N_0\bar{\varepsilon}$$

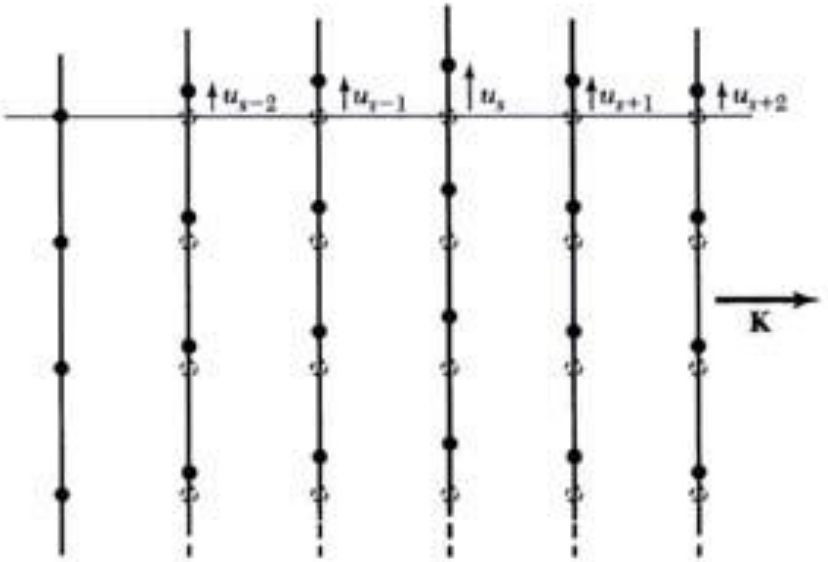
$$c_V = \left(\frac{dE}{dT}\right)_V = 3R\left(\frac{h\nu}{k_BT}\right)^2 \frac{e^{h\nu/k_BT}}{\left(e^{h\nu/k_BT} - 1\right)^2}$$

Coupled harmonic oscillators

Phonons

Phonons





$$F_s = C(u_{s+1} - u_s) + C(u_{s-1} - u_s)$$

$$M\frac{d^2u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s)$$

$$-M\omega^2 u_s = C(u_{s+1} + u_{s-1} - 2u_s)$$

C. Kittel, *Introduction to Solid State Physics*, 8th ed., John Wiley & Sons, 2005.

Phonons

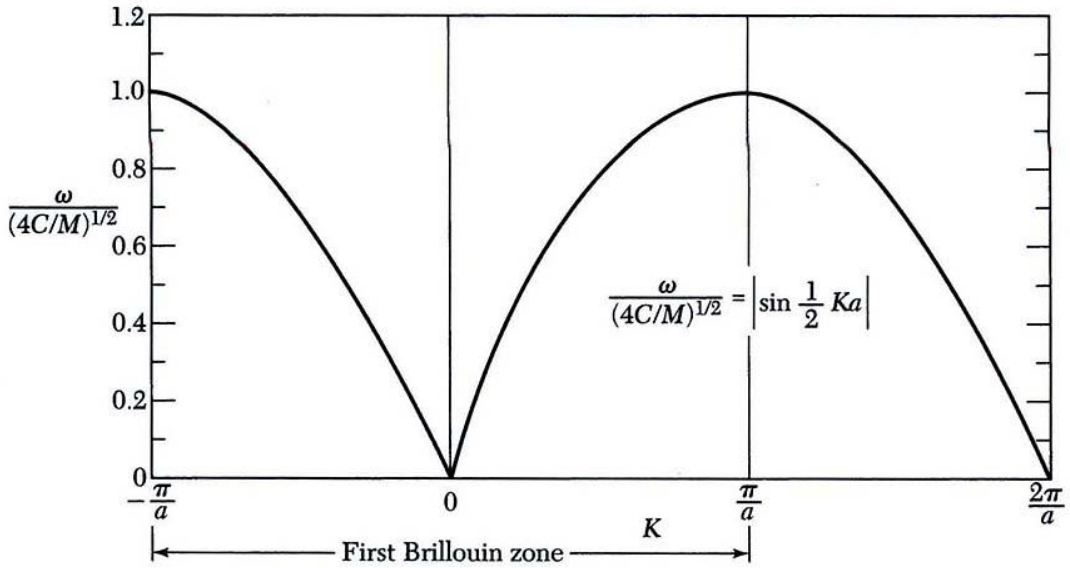
$$u_{s\pm1} = u\exp(isKa)\exp(\pm iKa)$$

$$-\omega^2 Mu\exp(isKa) = Cu\{\exp[i(s+1)Ka] + \exp[i(s-1)Ka] - 2\exp(isKa)\}$$

$$\omega^2 M = -C[\exp(iKa) + \exp(-iKa) - 2]$$

$$\omega^2 = (2C/M)(1 - \cos Ka)$$

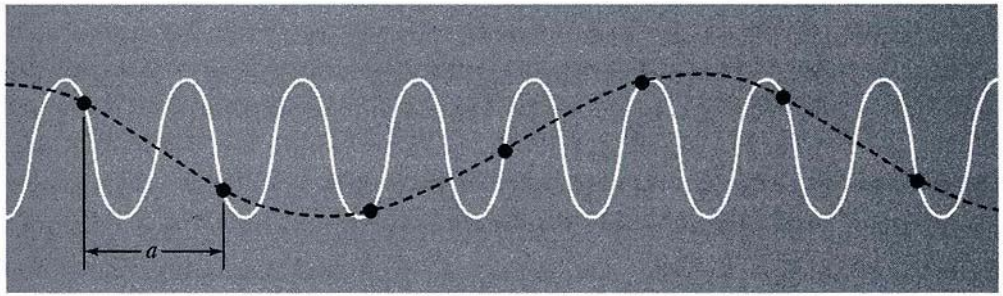
$$\omega^2 = (4C/M)\sin^2 \tfrac{1}{2}Ka \;; \qquad \omega = (4C/M)^{1/2}\left|\sin \tfrac{1}{2}Ka\right|$$



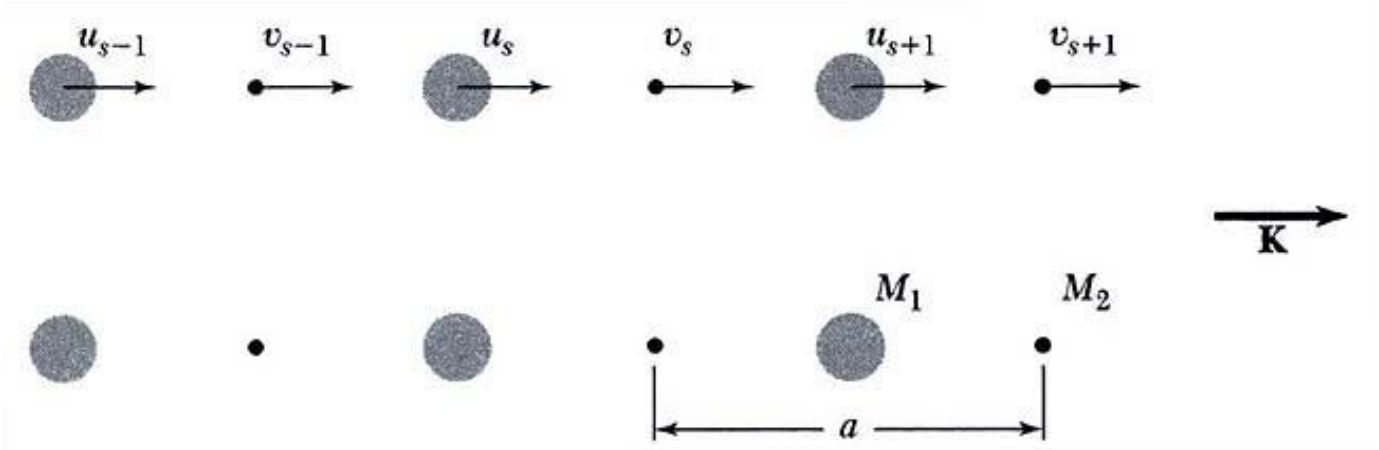
Phonons

$$\frac{u_{s+1}}{u_s} = \frac{u \exp[i(s+1)Ka]}{u \exp(isKa)} = \exp(iKa)$$

$$u_{s+1}/u_s = \exp(iKa) \equiv \exp(i2\pi n) \exp[i(Ka - 2\pi n)] \equiv \exp(iK'a)$$



Phonons – Two Atoms per Primitive Basis

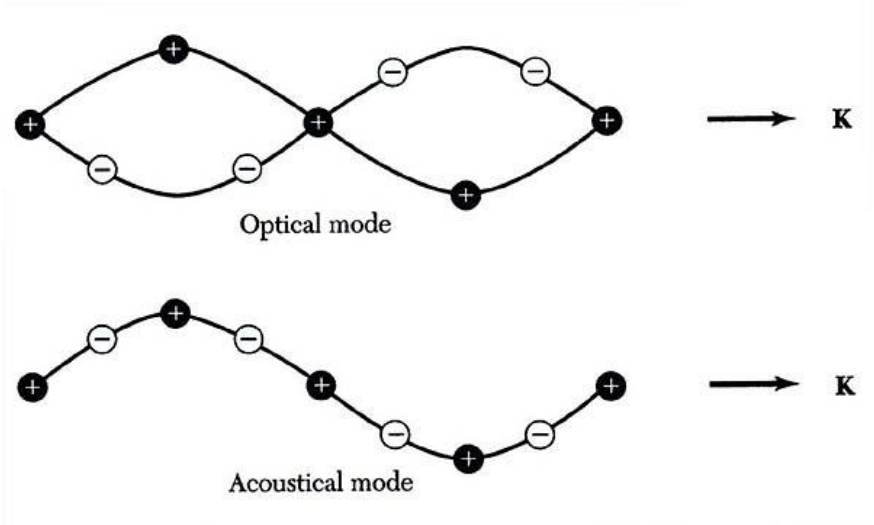


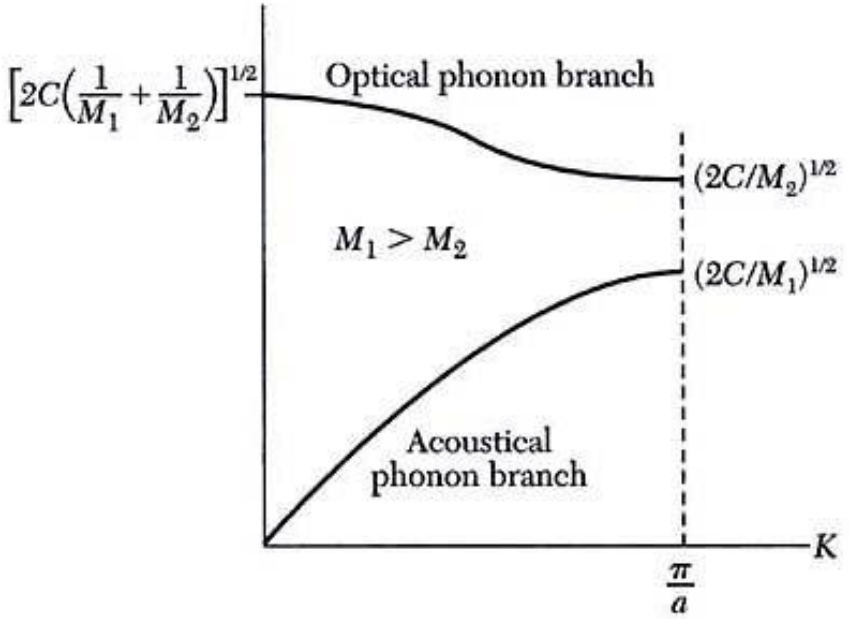
$$M_1 \frac{d^2 u_s}{dt^2} = C(v_s + v_{s-1} - 2u_s) \ ;$$

$$M_2 \frac{d^2 v_s}{dt^2} = C(u_{s+1} + u_s - 2v_s) \ .$$

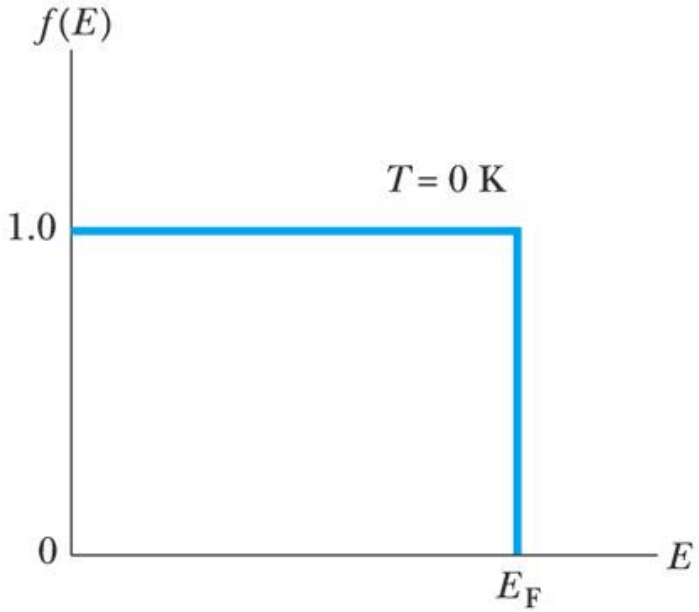
$$u_s = u \exp(isKa) \exp(-i\omega t) \ ; \qquad v_2 = v \exp(isKa) \exp(-i\omega t)$$

Phonons – Two Atoms per Primitive Basis

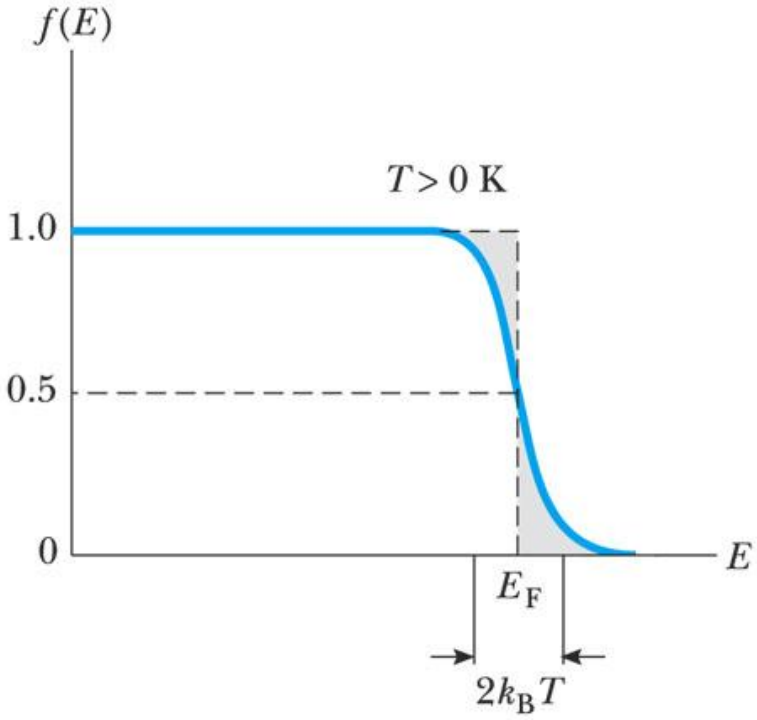




Fermi-Dirac Distribution



(a)



(b)

Density of States in 3D Structure (Metal)

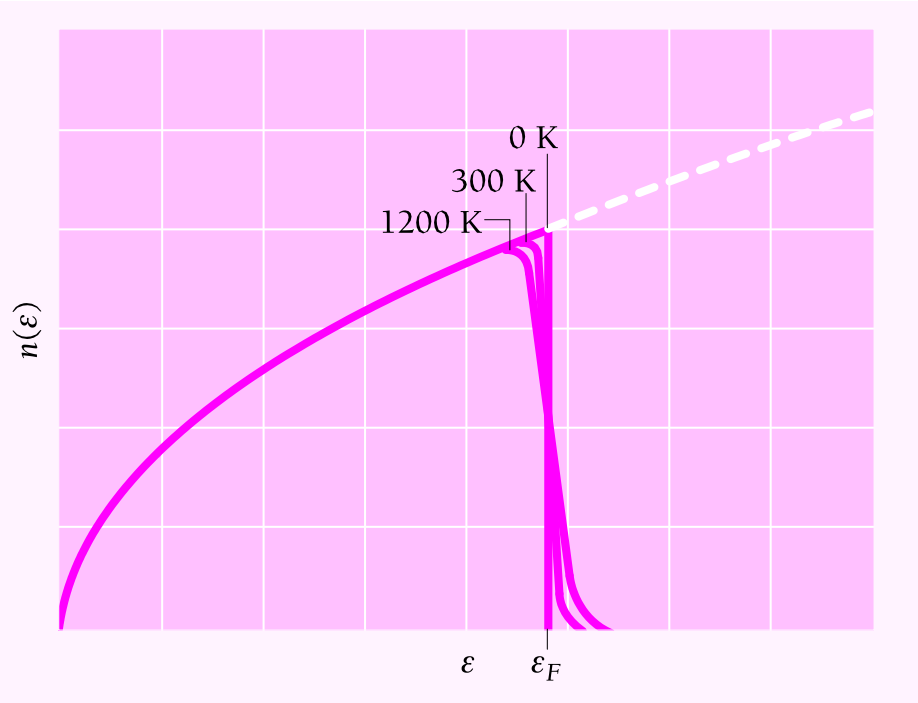
$$g(E)dE = D\sqrt{E}dE$$

$$D = \frac{8\sqrt{2}\pi m^{3/2}}{h^3}$$

$$n(E)dE = \frac{D\sqrt{E}dE}{e^{(E-E_F)/k_BT}+1}$$

$$\frac{N}{V} = \int_0^\infty n(E)dE = D\int_0^\infty \frac{\sqrt{E}dE}{e^{(E-E_F)/k_BT}+1}$$

Fermi Energy in Metal



$$\text{At } T = 0K$$

$$\frac{N}{V} = D\int_0^{E_F} \sqrt{E}\,dE = \frac{2}{3}DE_F^{3/2}$$

$$E_F(0) = \frac{h^2}{2m}\left(\frac{3N}{8\pi V}\right)^{2/3}$$

표 9.2 페르미 에너지 eV

금속		페르미 에너지, eV
Lithium	Li	4.72
Sodium	Na	3.12
Aluminum	Al	11.8
Potassium	K	2.14
Cesium	Cs	1.53
Copper	Cu	7.04
Zinc	Zn	11.0
Silver	Ag	5.51
Gold	Au	5.54