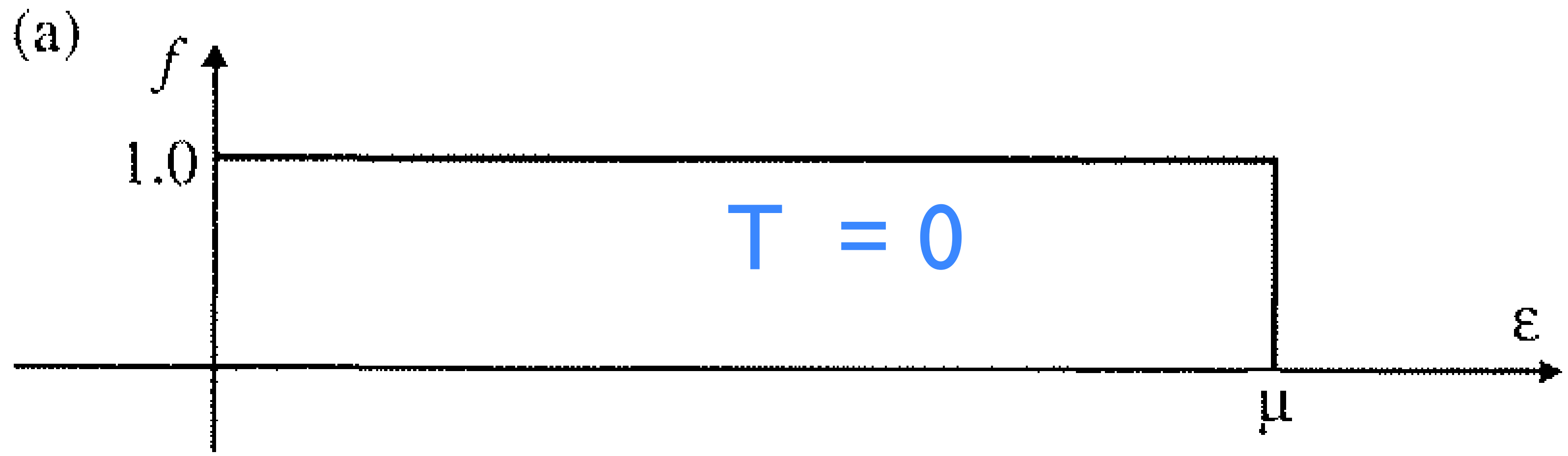
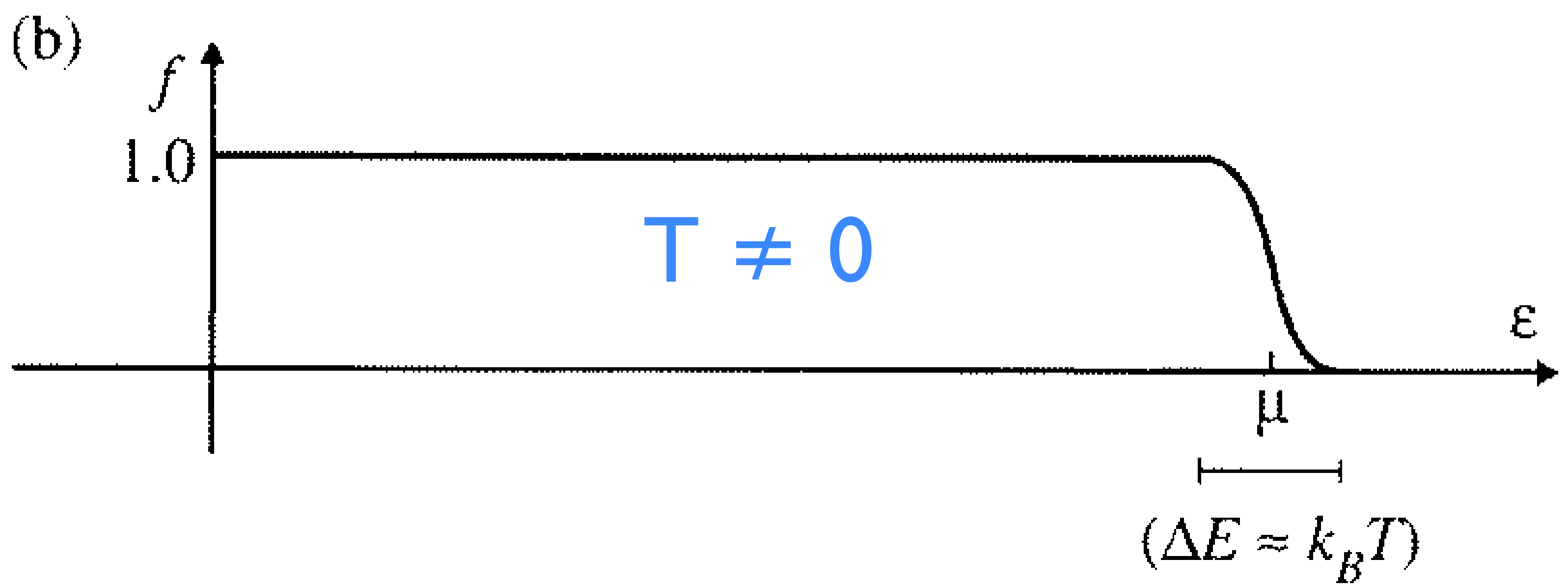
F-D distribution function

$$f(E) = \frac{1}{e^{\frac{E-\mu}{k_B T}} + 1}$$

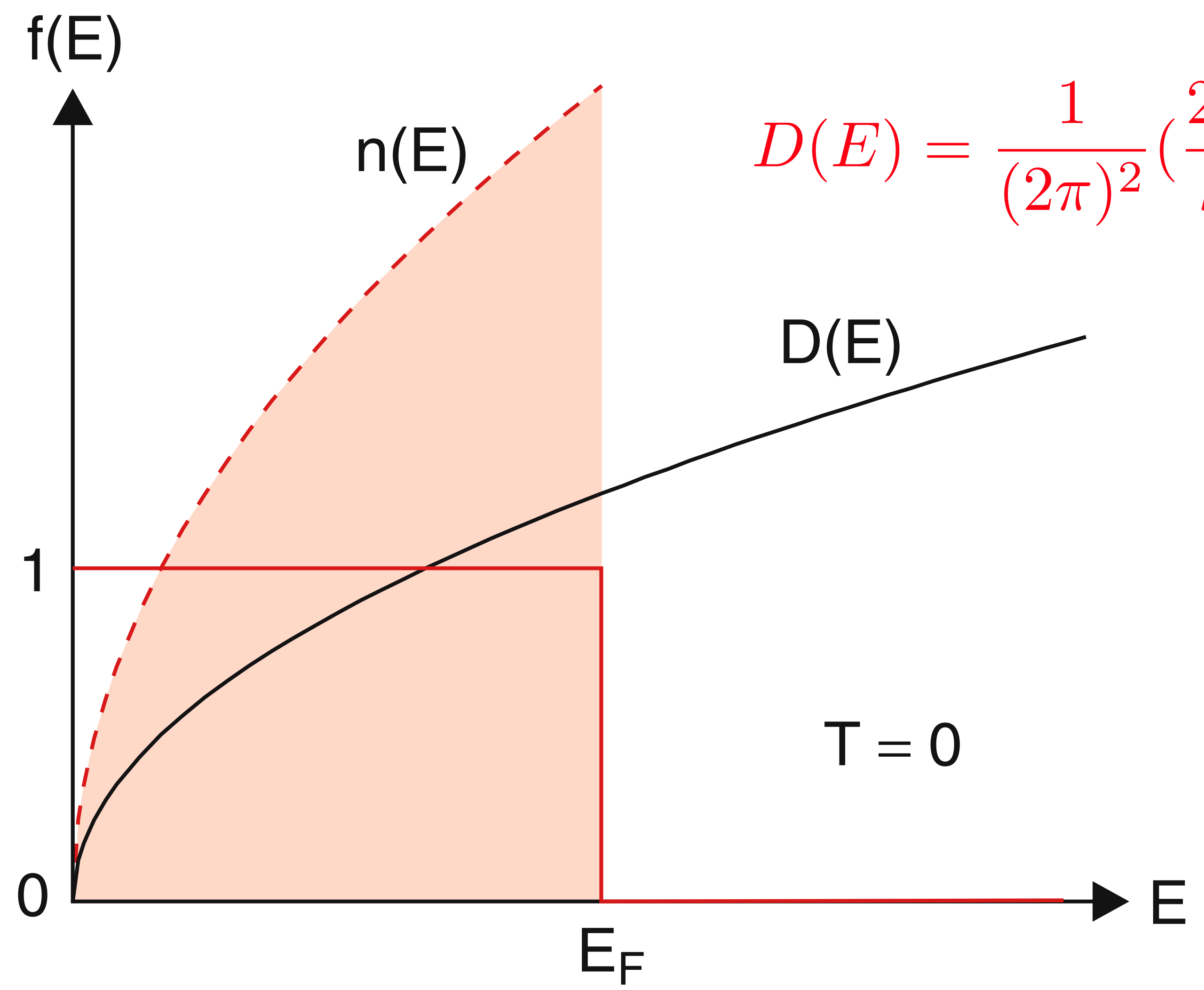




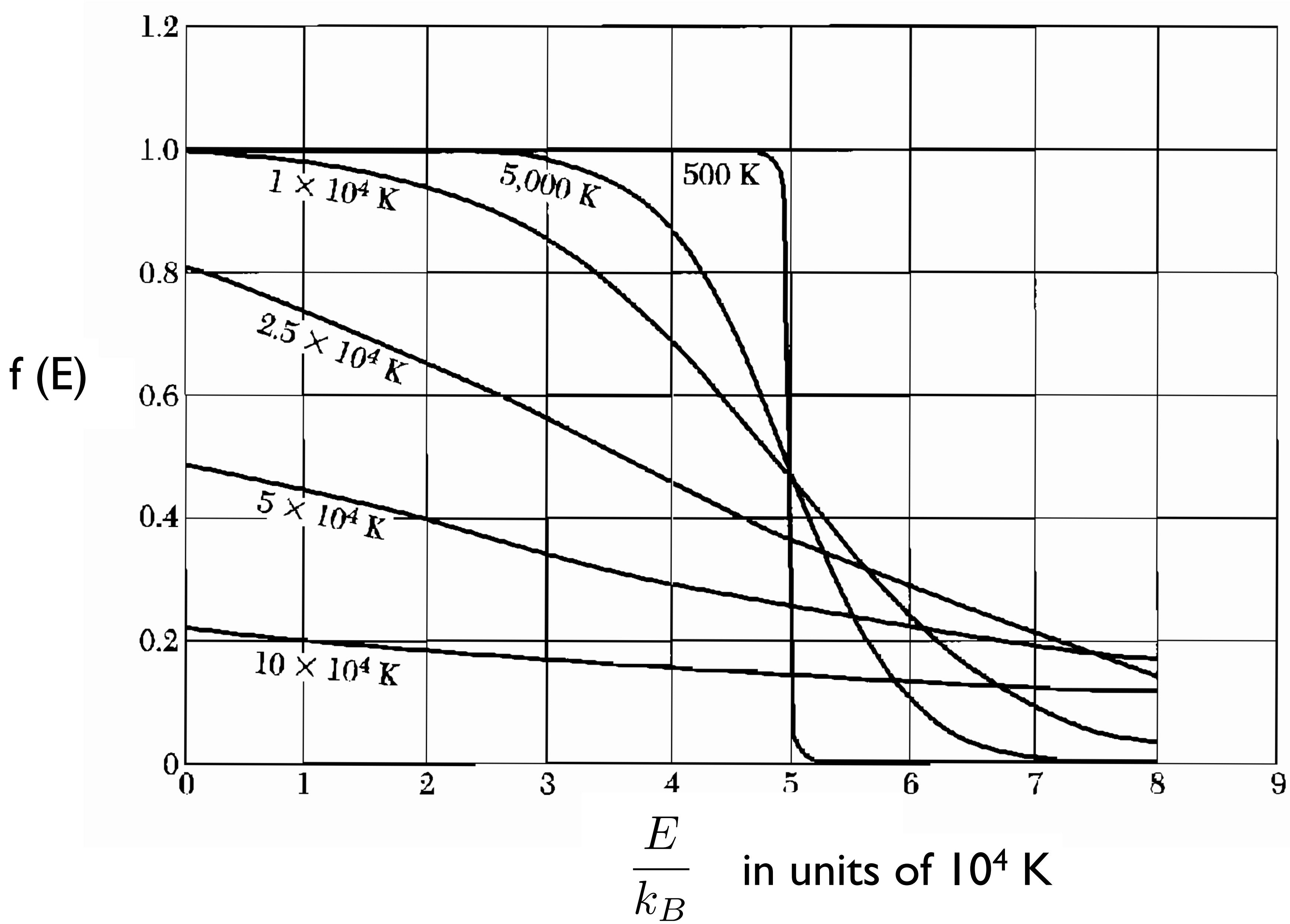
Density of states, F-D distribution function, etc..

$$f(E) = \frac{1}{e^{\frac{E-\mu}{k_B T}} + 1}$$

$$D(E) = \frac{1}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{2}{3}} E^{\frac{1}{2}}$$



T- dependence of F-D distribution function



Lecture 4

Electronic heat capacity

At T=0, states up to E_F are all filled up

Electronic energy at T=0 and at any T are:

$$U(0) = \int ED(E)\mathrm{dE} = \int_0^{\mathrm{E_F}} \mathrm{ED(E)dE}$$

$$\boxed{U(0) = \frac{E_F^{\frac{5}{2}}}{5\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}}$$

$$U(T) = \int_0^{\infty} E \cdot D(E) \cdot f(E,T)\mathrm{dE}$$

$$\Longrightarrow U(T) = \frac{1}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \underbrace{\int_0^{\infty} \frac{E^{\frac{3}{2}}}{e^{\frac{E-\mu}{k_B T}}+1}\mathrm{dE}}$$

No general analytical solution for this integral

Electronic heat capacity

$$\Longrightarrow U(T) = \frac{1}{(2\pi)^2}(\frac{2m}{\hbar^2})^{\frac{3}{2}} \int_0^\infty \frac{E^{\frac{3}{2}}}{e^{\frac{E-\mu}{k_B T}} + 1} \mathrm{dE}$$

Asymptotic form exists.

For any practical temperature (T),

$$E_F >> k_B T \;\; (E_F \sim 10000\,\mathrm{K})$$

$$\therefore \mu >> k_B T$$

$$U(T) = \frac{2}{5}\mu^{\frac{5}{2}}\left[1 + \frac{5}{8}(\frac{\pi k_B T}{\mu})^2\right]\frac{1}{(2\pi)^2}(\frac{2m}{\hbar^2})^{\frac{3}{2}}$$

Electronic heat capacity

$$U(T) = \frac{2}{5}\mu^{\frac{5}{2}}\left[1 + \frac{5}{8}\left(\frac{\pi k_B T}{\mu}\right)^2\right]\frac{1}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}$$

μ is T-dependent

$$n = \int_0^\infty \cancel{E}\; D(E)\; f(E,T)\,\mathrm{dE} \qquad = \text{constant}$$

$$n = \frac{1}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \int_0^\infty \frac{E^{\frac{1}{2}}}{e^{\frac{E-\mu}{k_B T}} + 1}\,\mathrm{dE}$$

$$\mu \approx E_F\left[1 - \frac{\pi^2}{12}\left(\frac{k_B T}{\mu}\right)^2\right]$$

Electronic heat capacity

$$\mu \approx E_F \left[1 - \frac{\pi^2}{12}(\frac{k_B T}{\mu})^2\right]$$

$$U(T) \approx \frac{2}{5} E_F^{\frac{5}{2}} \left[1 + \frac{5}{12}(\frac{\pi k_B T}{\mu})^2\right] \frac{1}{(2\pi)^2}(\frac{2m}{\hbar^2})^{\frac{3}{2}}$$

With $\mu \to E_F$

$$U(T) = U(0) + \frac{n\pi^2 k_B^2 T^2}{E_F}$$

Electronic heat capacity

$$U(T) = U(0) + \frac{n\pi^2 k_B^2 T^2}{E_F}$$

$$U(0) = \frac{E_F^{\frac{5}{2}}}{5\pi^2}(\frac{2m}{\hbar^2})^{\frac{3}{2}}$$

$$C_{electronic} = \frac{\partial U}{\partial T} = \frac{1}{2}\pi^2 n \frac{k_B^2 T}{E_F}$$

Classical result: $C_v = \frac{3}{2} n k_B$

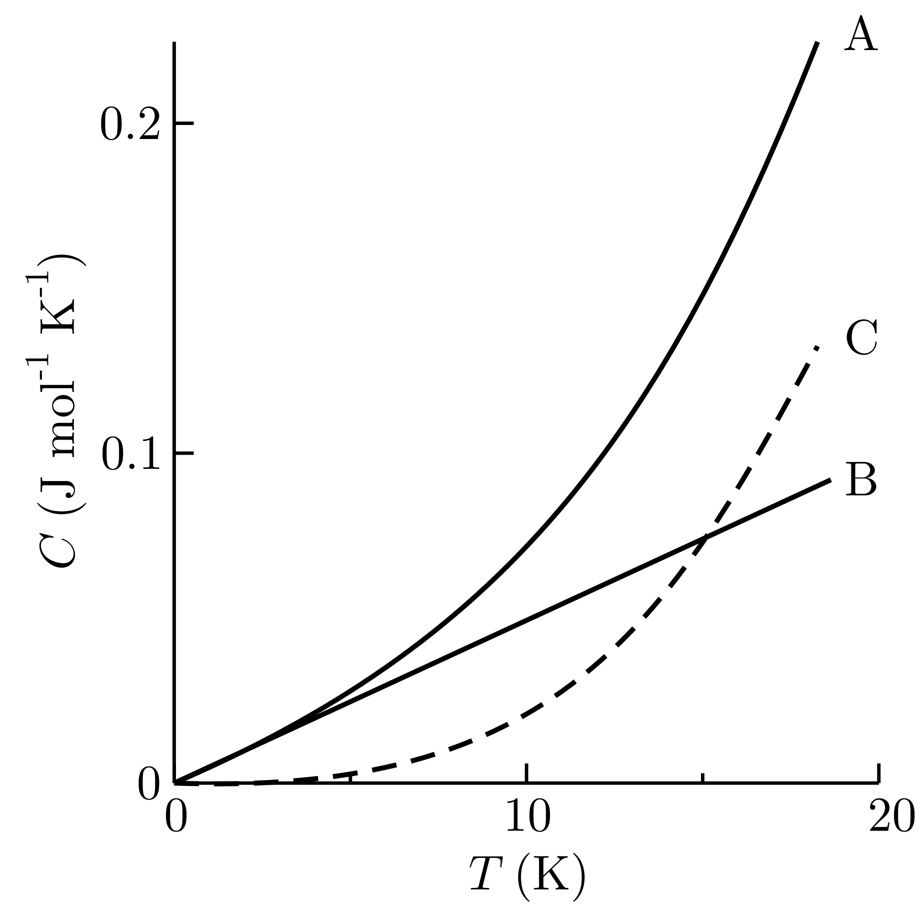
Failure of Drude's model

Drude's results
(equipartition of energy)

$$C = \frac{3}{2} n k_B$$

Sp. heat is T-independent

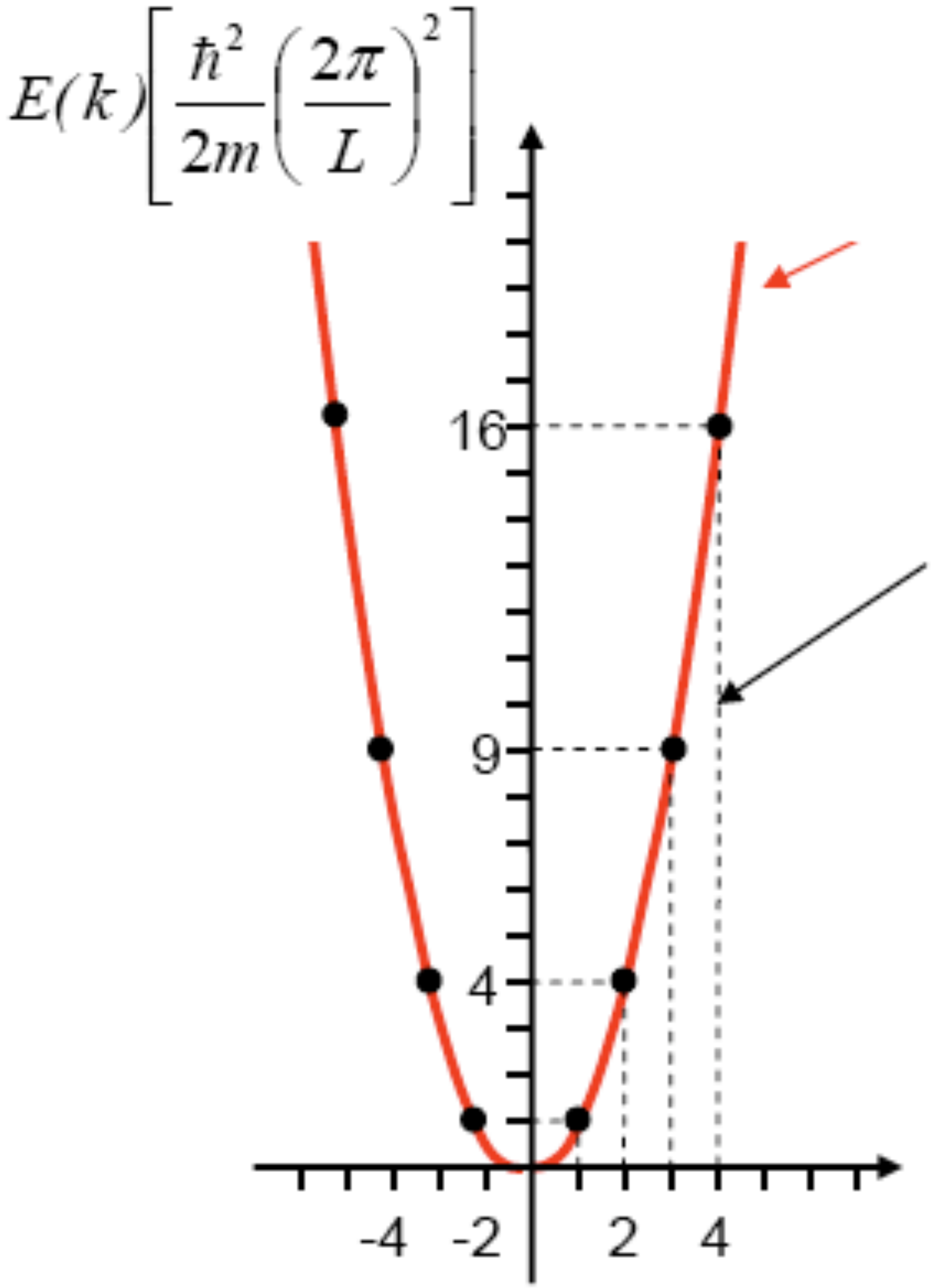
Sp. heat of metals have **two** components



$$C_V = \gamma T + \alpha T^3$$

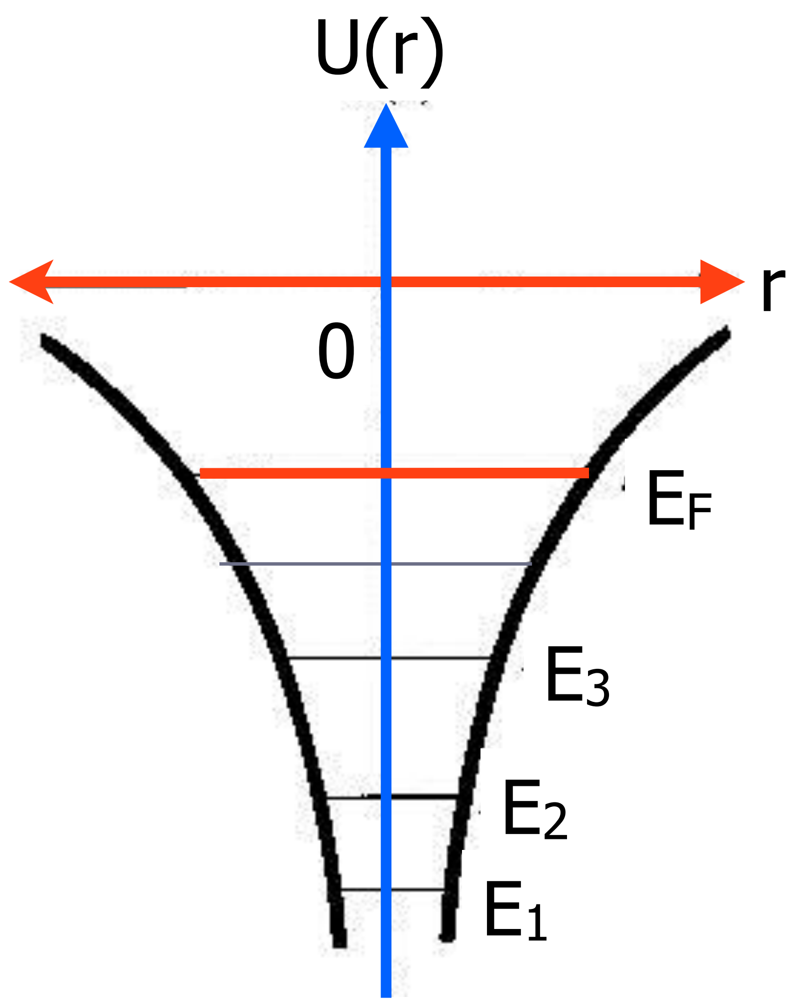
Electrons Phonons

Ref.: G. Duyckaerts, Physica **6,** 817 (1939).



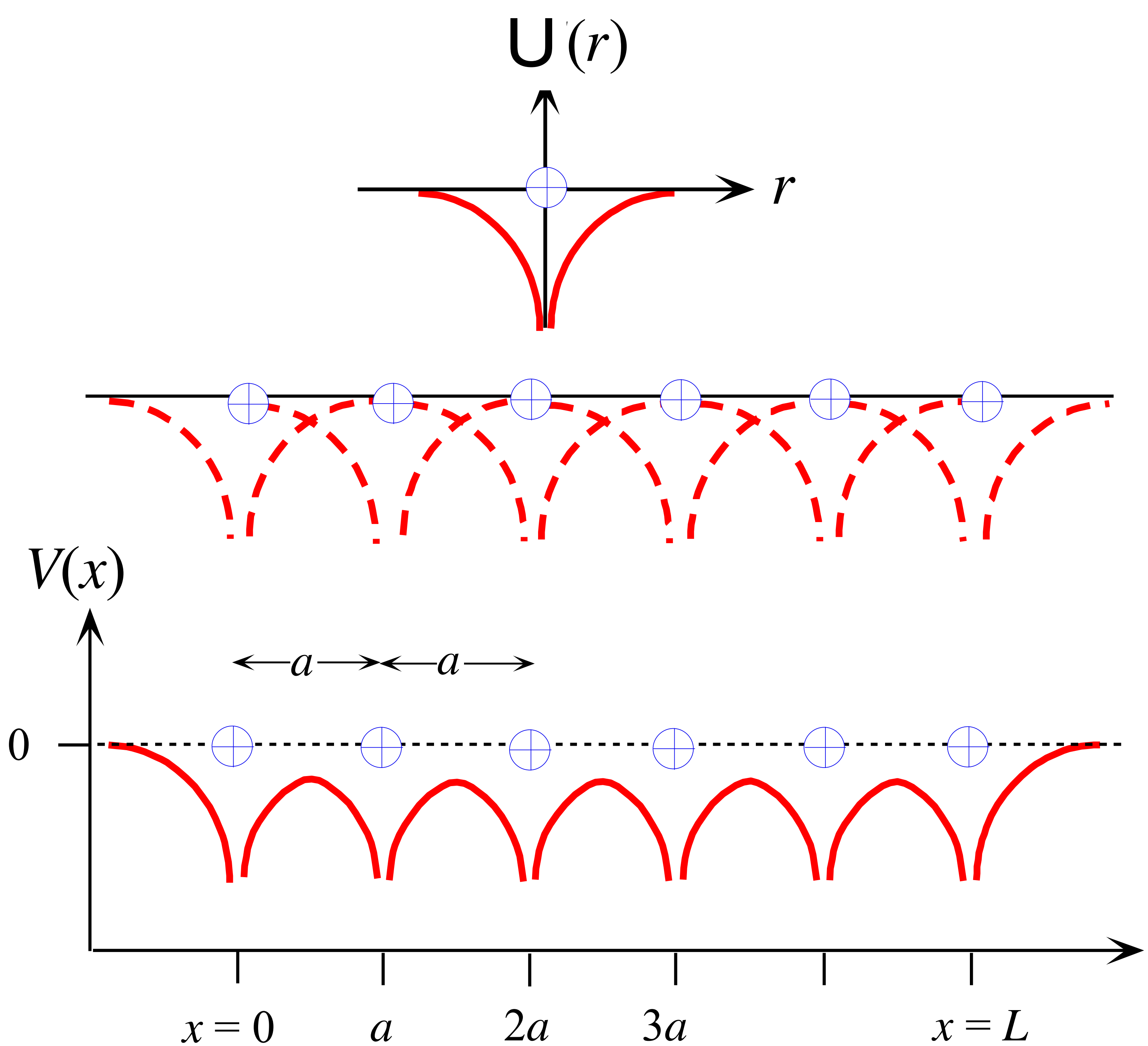
$$k_x = 2\pi/L$$

Potential energy for an isolated atom (e.g., hydrogen atom)



$$U(r) = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}$$

Potential energy for a multiple atoms (periodically placed)



Kronig-Penney simplification of 1D potential