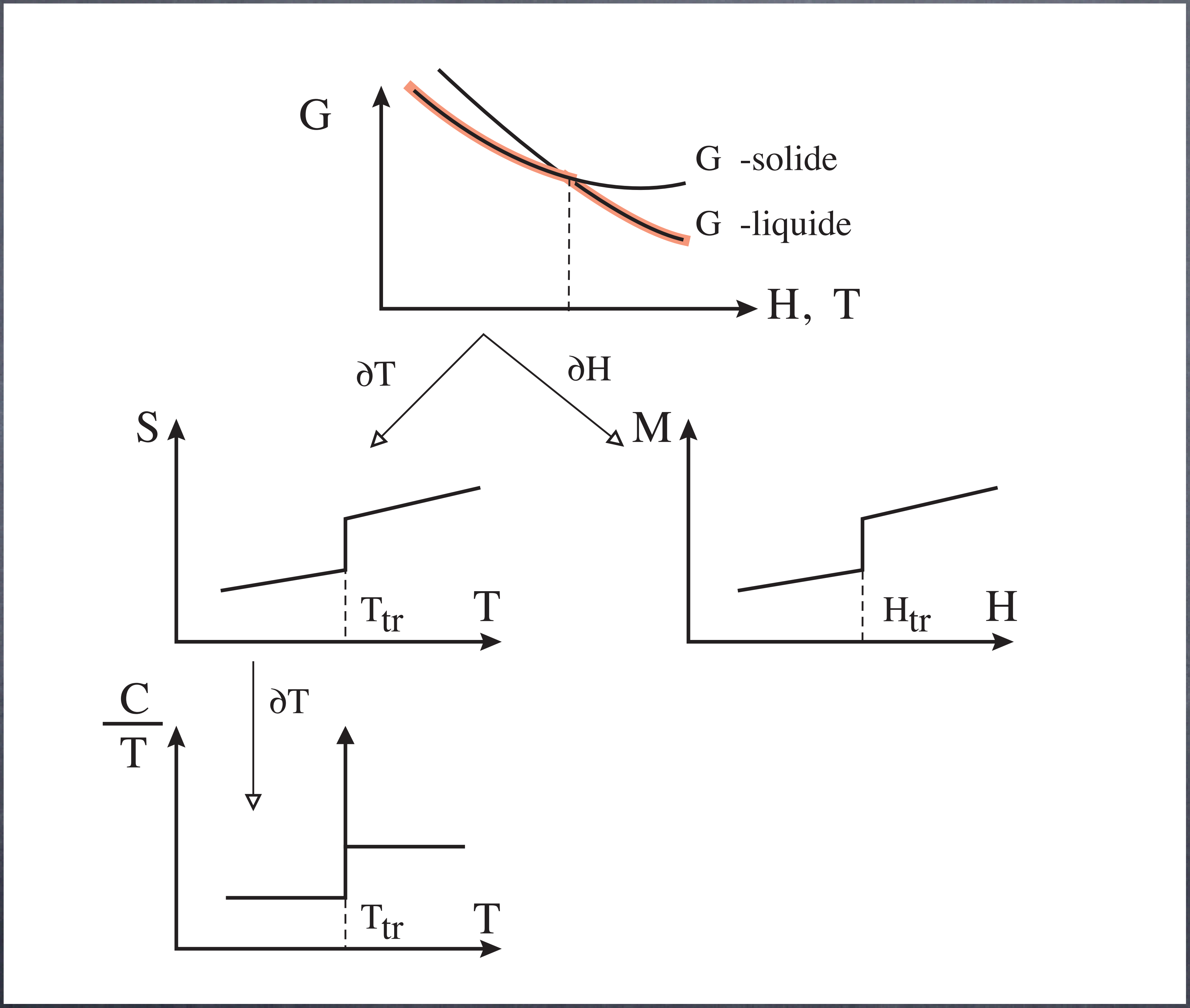
Phase transitions: 1^{st}-2^{nd} order

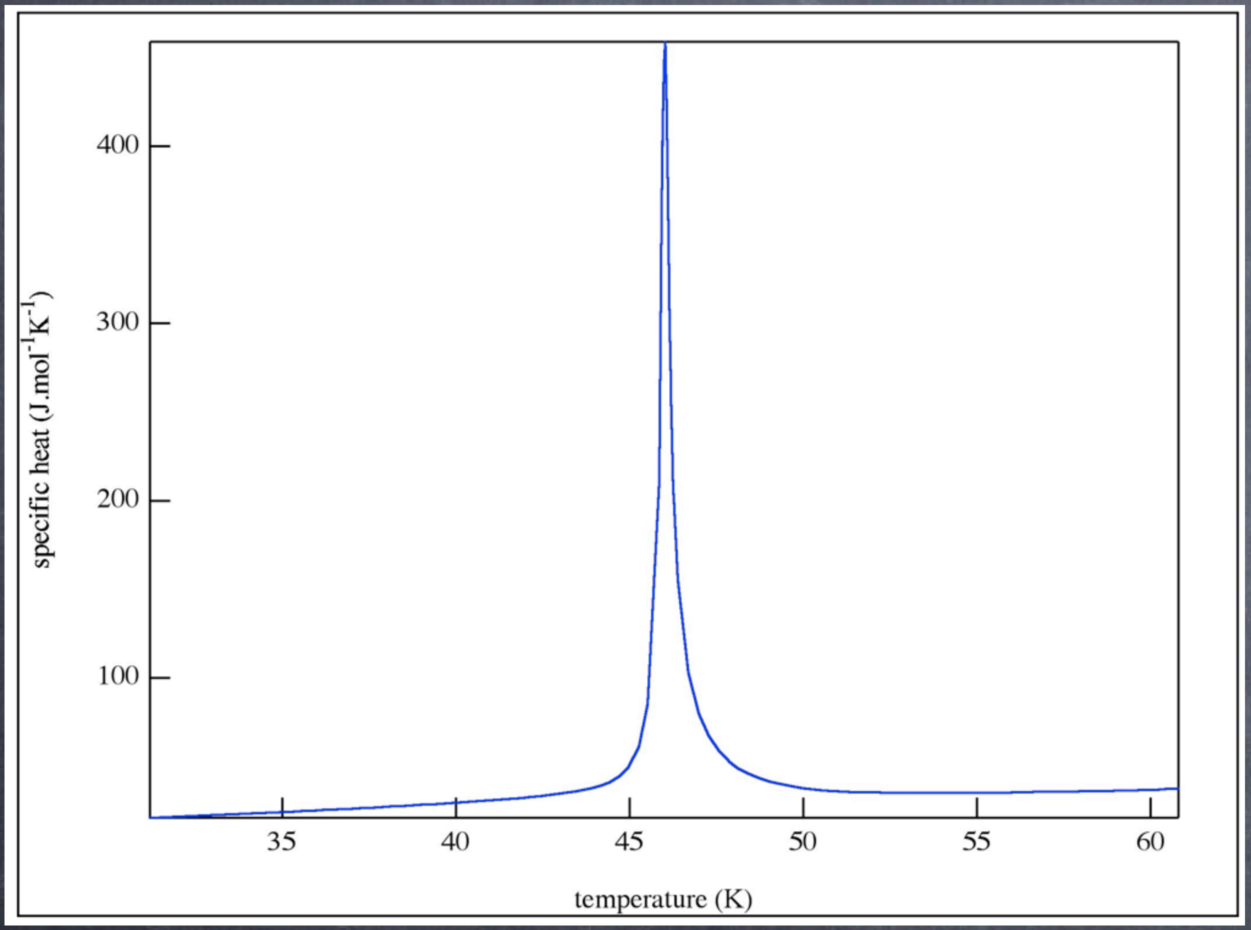
- definitions, Ehrenfest classification
- Transition superfluide λ ?
- fluctuations vs broadening
- renormalization group, scaling, divergence of ξ
- Ginzburg - Landau description, order parameter
- 1^{st}order transitions : no prediction ! hysteresis
- 2^{nd} order transitions : $C_{OD=0} < C_{OD\neq 0}$

Ehrenfest : 1st order



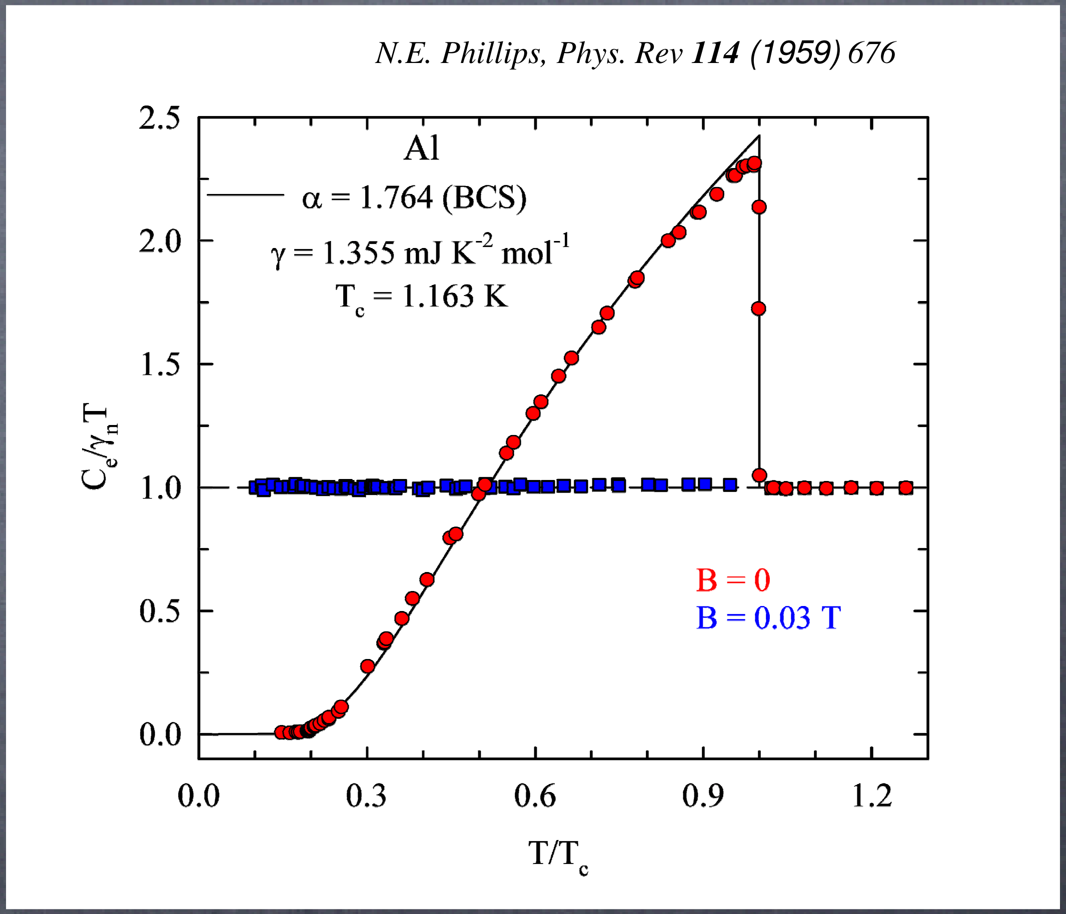
Examples

$AuCrS_2$: Pyrochlore



1st order structural +Antiferomagnetic

Al : Metal



mean-field 2nd order superconducting

Clausius-Clapeyron

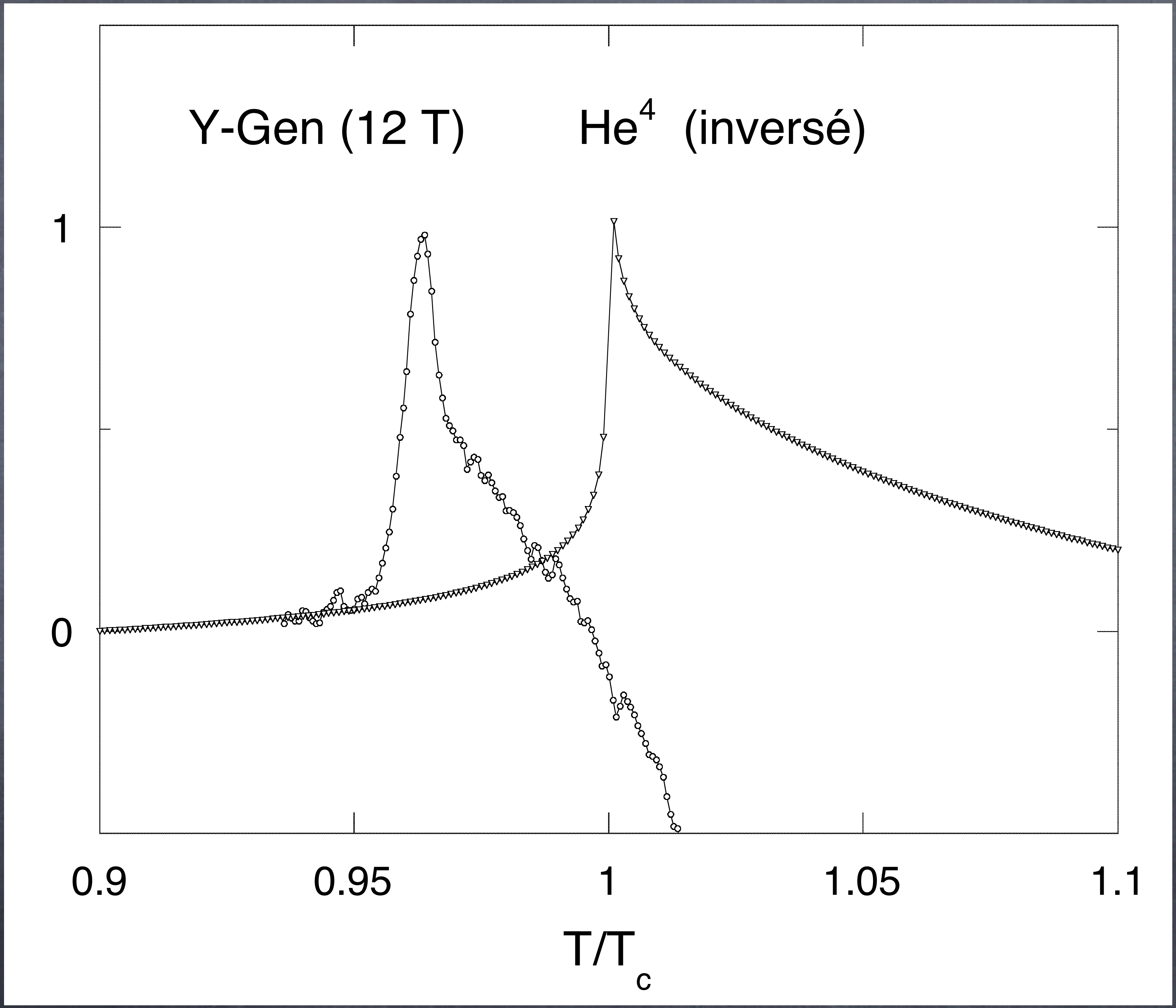
- demonstrate 1st order : $\Delta S = -\Delta M \, dH/dT$

  $$\Delta S = L/T = \Delta V \, dp/dT$$

- 2nd order : $\Delta(C/T) = \Delta(\partial V/\partial T) \, dp/dT$

  or $\Delta(C/T) = -\Delta(\partial M/\partial T) \, dH/dT$

1st or 2nd ?



REAL world fluctuations = broadening !!

- definitions, Ehrenfest classification
- Transition superfluide λ ?
- fluctuations vs broadening

qualitatively, a broad 1^{st} order = sharp 2^{nd} with fluctuations

Clausius-Clapeyron ALWAYS true !

- $\Delta S = -\Delta M \, dH/dT$

  $\Delta S = L/T = \Delta V \, dp/dT$

- doesn't prove the order of the transition
- just check for consistent measurements
- even true out of equilibrium (Prigogine)
- in fact often 1st order with hysteresis

Phase transitions: 1st-2nd order

- Ginzburg - Landau description, order parameter
- renormalization group, scaling, divergence of ξ

$$\frac{F}{V} = \frac{k_B T}{V_{coh}} = \frac{k_B T}{\xi^{-\nu}} \qquad \xi = (1 - \frac{T}{T_c})^{-\nu}$$

$$\tfrac{c}{T} = k_B \tau^{-\alpha} \text{ and } \alpha = 2 - d\nu$$

- 1st order transitions : no prediction !
  hysteresis
- 2nd order transitions : $C_{OD=0} < C_{OD\neq 0}$

Summary : Phase transitions

- definitions, Ehrenfest classification
- Transition superfluide λ ?
- fluctuations vs broadening
- renormalization group, scaling, divergence of ξ
- Ginzburg - Landau description, order parameter
- 1st order transitions : no prediction ! hysteresis
- 2nd order transitions : $C_{OD=0} < C_{OD\neq 0}$

PHONONS

Total energy of phonons : sum over each phonon

$E_{ph}(T) = \Sigma_{ph}\, h\omega_{ph}.n_{BE}(T, h\omega_{ph}) + E_{ph}(0)$

phonon energy

Bose-Einstein distribution

$$n_{BE}(T,\hbar\omega_{ph}) = \frac{1}{e^{\hbar\omega_{ph}/(K_BT)}-1}$$

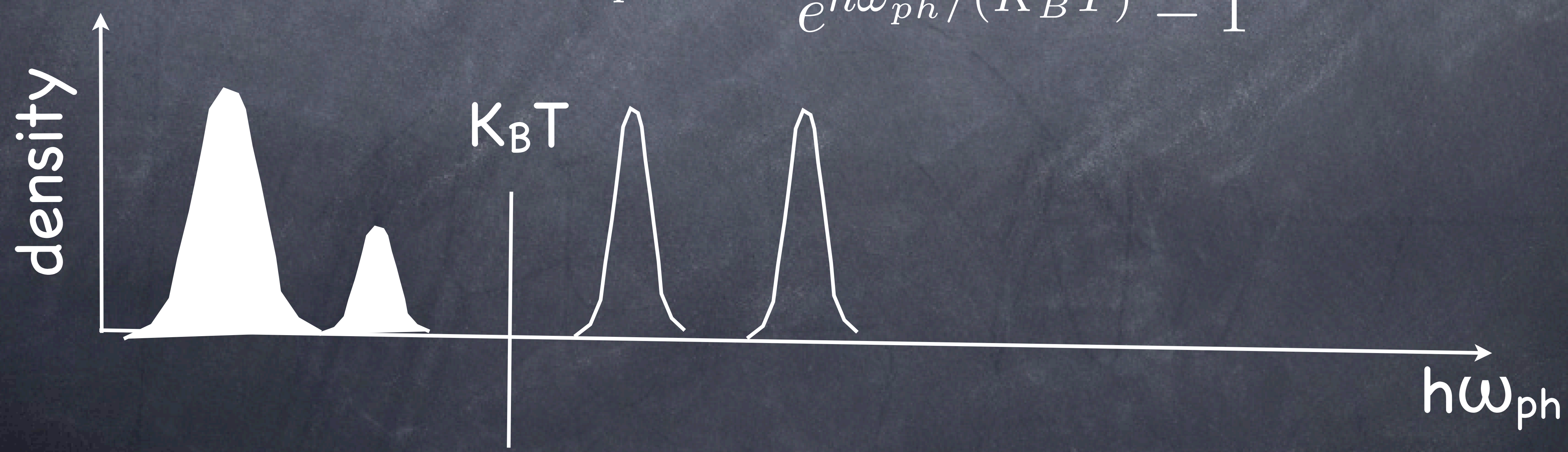
$E_{ph}(0)$: zero point energy

PHONONS

Bose-Einstein distribution

ALL phonons with energy smaller or on the order of $k_B T$ will contribute

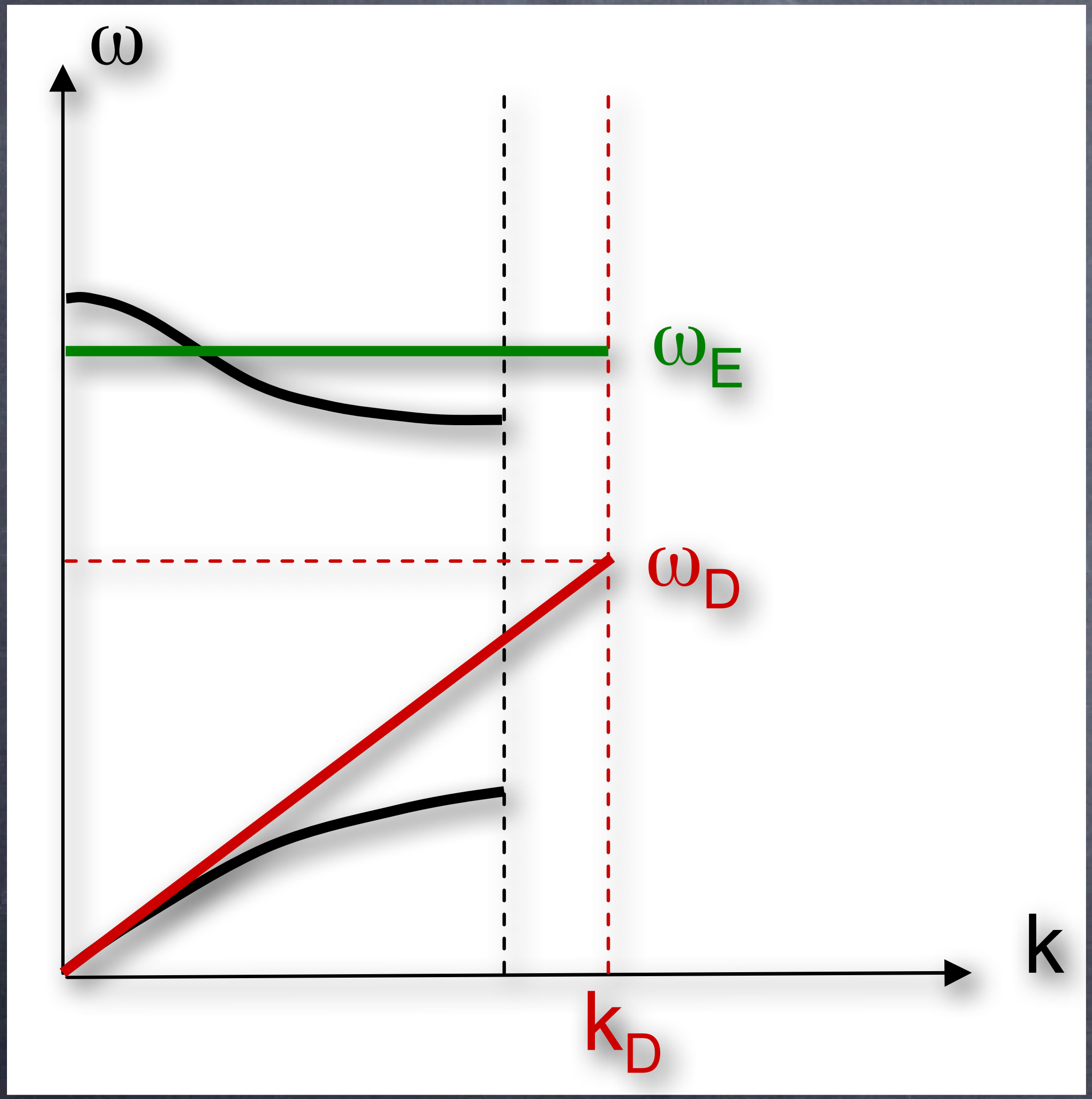
$$n_{BE}(T, \hbar\omega_{ph}) = \frac{1}{e^{\hbar\omega_{ph}/(K_B T)} - 1}$$



PHONONS

How to count phonons ? ... 2 models.

$$E_{ph}(T) = \boxed{\Sigma_{ph}} h\omega_{ph}.n_{BE}(T, h\omega_{ph})$$

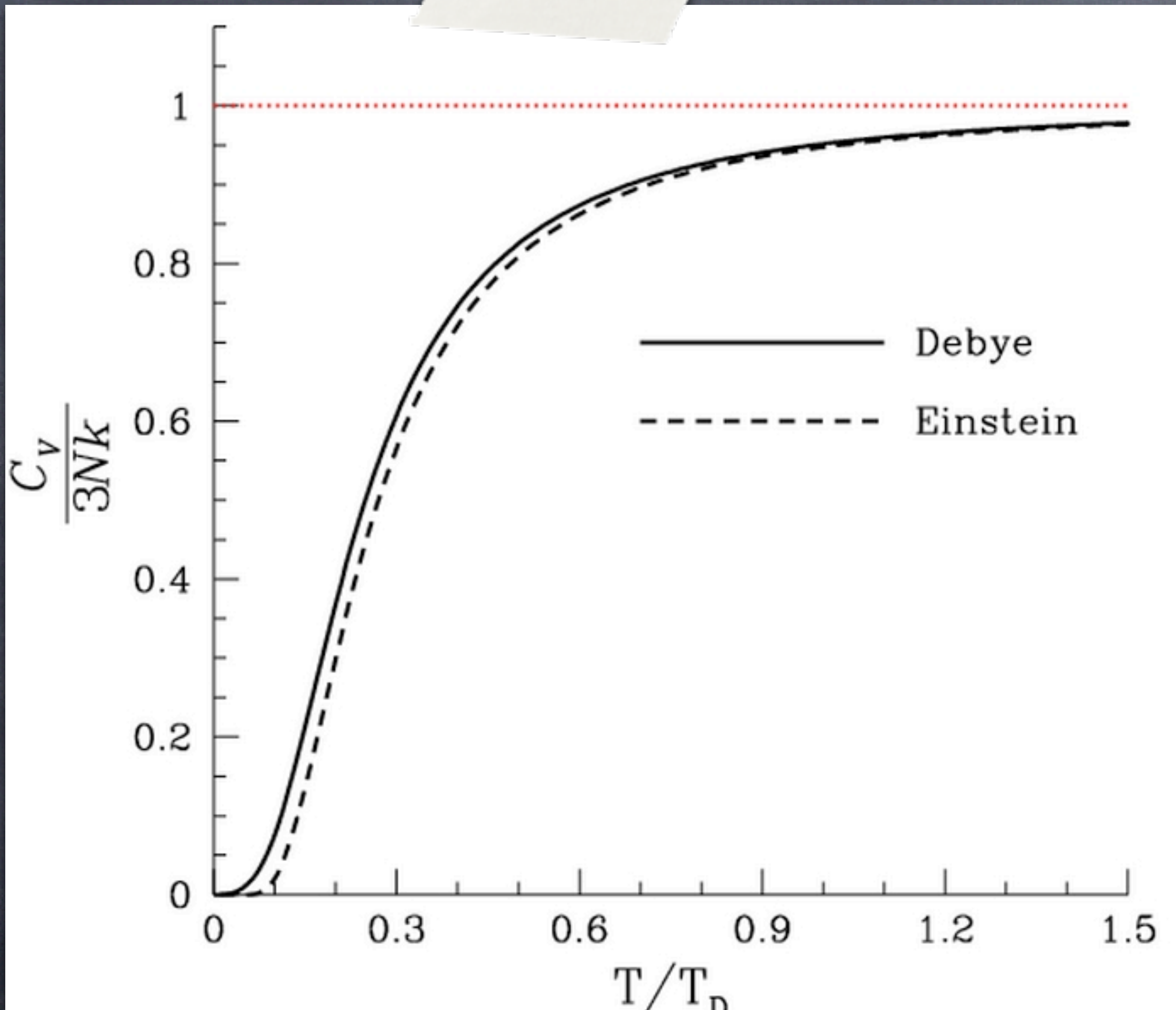


- $\boxed{\text{Einstein : } \omega_{ph} = \text{cte}}$
- $\boxed{\text{Debye : } \omega_{ph} = v_{son} \,.\, K}$

⇒ different densities of state

cf Kittel or Aschroft

LES PHONONS



source : Wiki

- $T \to \infty$: $C = 3NK_B$
- $T \ll \theta_D$: Debye
  $C = cte\ (T/\theta_D)^3$
  où $\theta_D \propto v_{sound}$
- $T \gg \theta_D$: Einstein

The deconvolution is not unique
knowing C(T)
calculating phonons ??

PHONONS

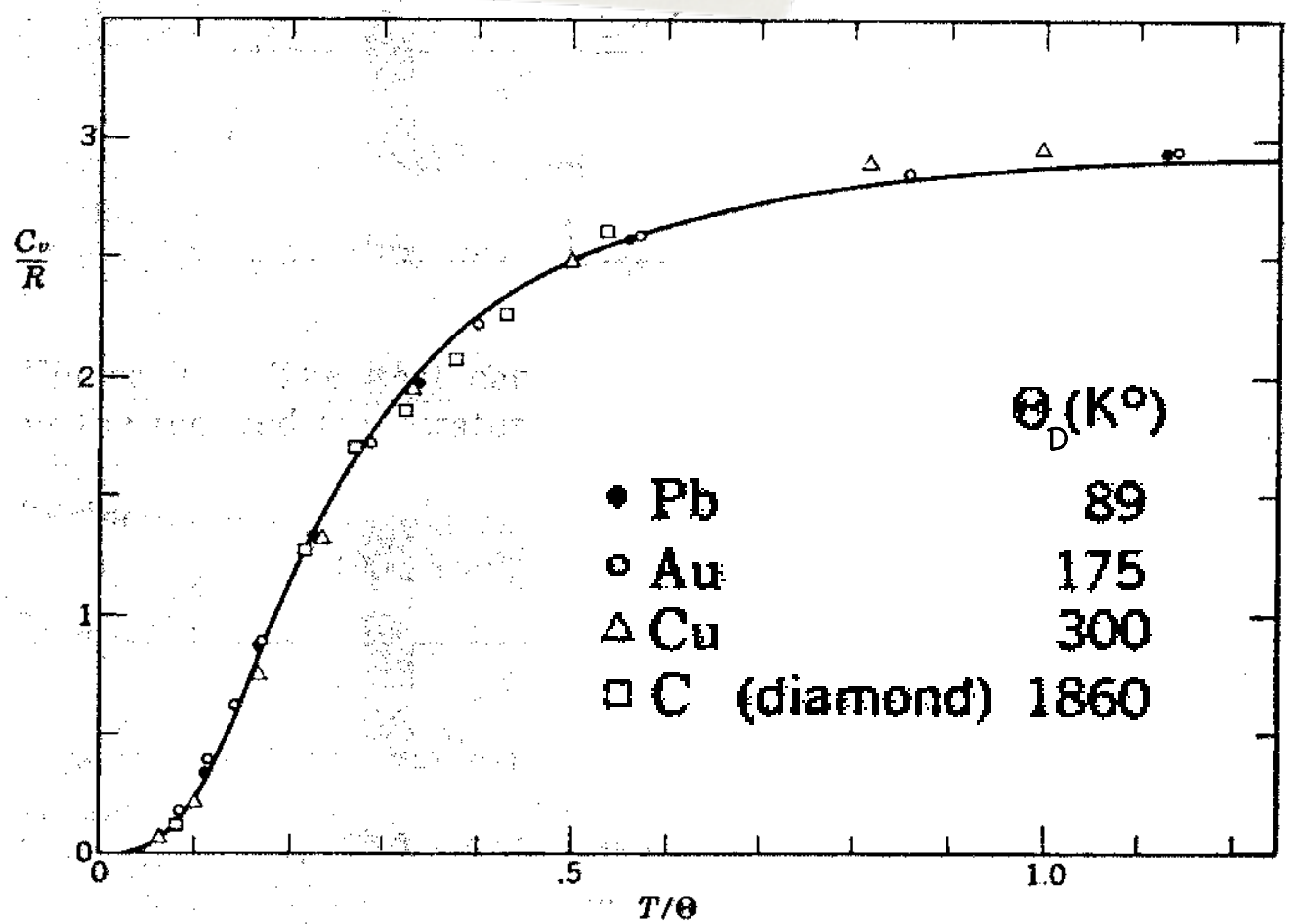


Figure 7.3. The heat capacity over the universal gas constant *vs* the reduced temperature for lead, gold, copper, and diamond. The solid curve is the Debye theoretical curve. (R. B. Leighton, "Principles of Modern Physics," New York, McGraw-Hill Book Co., Inc., 1957, by permission)

Lead, gold, copper, diamond :

Debye is a good approx!!

- $T \to \infty$: $C = 3NK_B$
- $T \ll \theta_D$: Debye

$C = cte\,(T/\theta_D)^3$

où $\theta_D \propto v_{sound}$

à $T \ll \theta_D$ en $J.K^{-1}.mol^{-1}$

$$c_v = \frac{2\Pi^2}{5}\aleph_A k_B\left(\frac{k_B T}{\hbar v_{son}}\right)^3$$

ELECTRONS

electronic energy = somme for each electron

$$E_e(T) = \sum_e \varepsilon . n_{FD}(T,\varepsilon)$$

energy of electron

Fermi-Dirac distribution

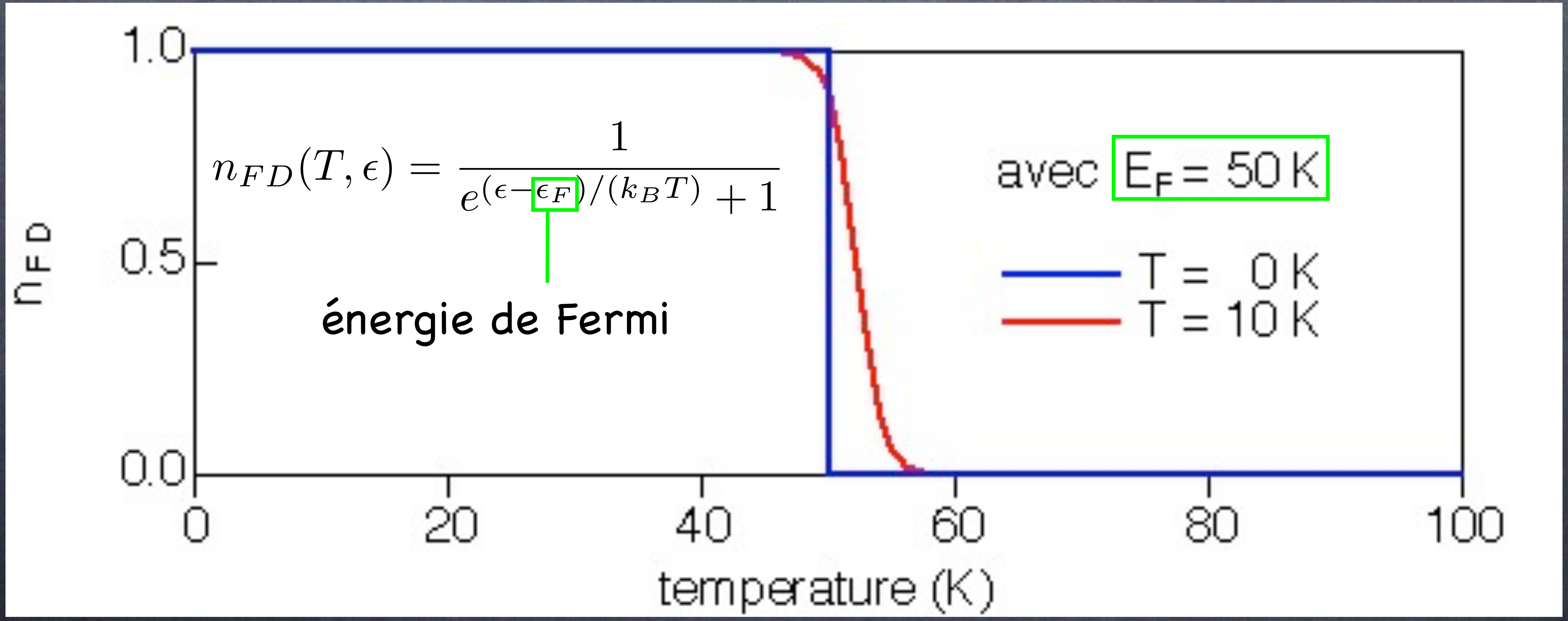
$$n_{FD}(T,\epsilon) = \frac{1}{e^{(\epsilon - \boxed{\epsilon_F})/(k_B T)} + 1}$$

Fermi energy

ELECTRONS

Fermi-Dirac distribution

Only electrons about Fermi energy will contribute to the specific heat (derivative of n_{FD}).



ELECTRONS

electron counting ?

density of states at E_F : $D(E_F)$

with $k_B T_F = E_F$ in $J.K^{-1}.mol^{-1}$

$$C_e = \frac{\Pi^2 \aleph_A k_B}{2} \cdot \frac{T}{T_F}$$

NB : $T_F > 10^4$ K

$C_e = \gamma T$

ELECTRONS

the density of states : $D(E_F)$

is related to the effective mass m^*

$$\Downarrow$$

$C_e = \gamma T$

et $\gamma \; \alpha \; m^*$

$\boxed{\text{probing electronic correlations}}$

EXAMPLE : METAL

Metal : $\boxed{\text{electrons}}$ + $\boxed{\text{phonons}}$

for $T \ll \theta_D$ (Cu : 300K, Pb : 90K ..)

$$C = \boxed{\gamma\, T} + \boxed{A\, T^3}$$

dominates at low temperature

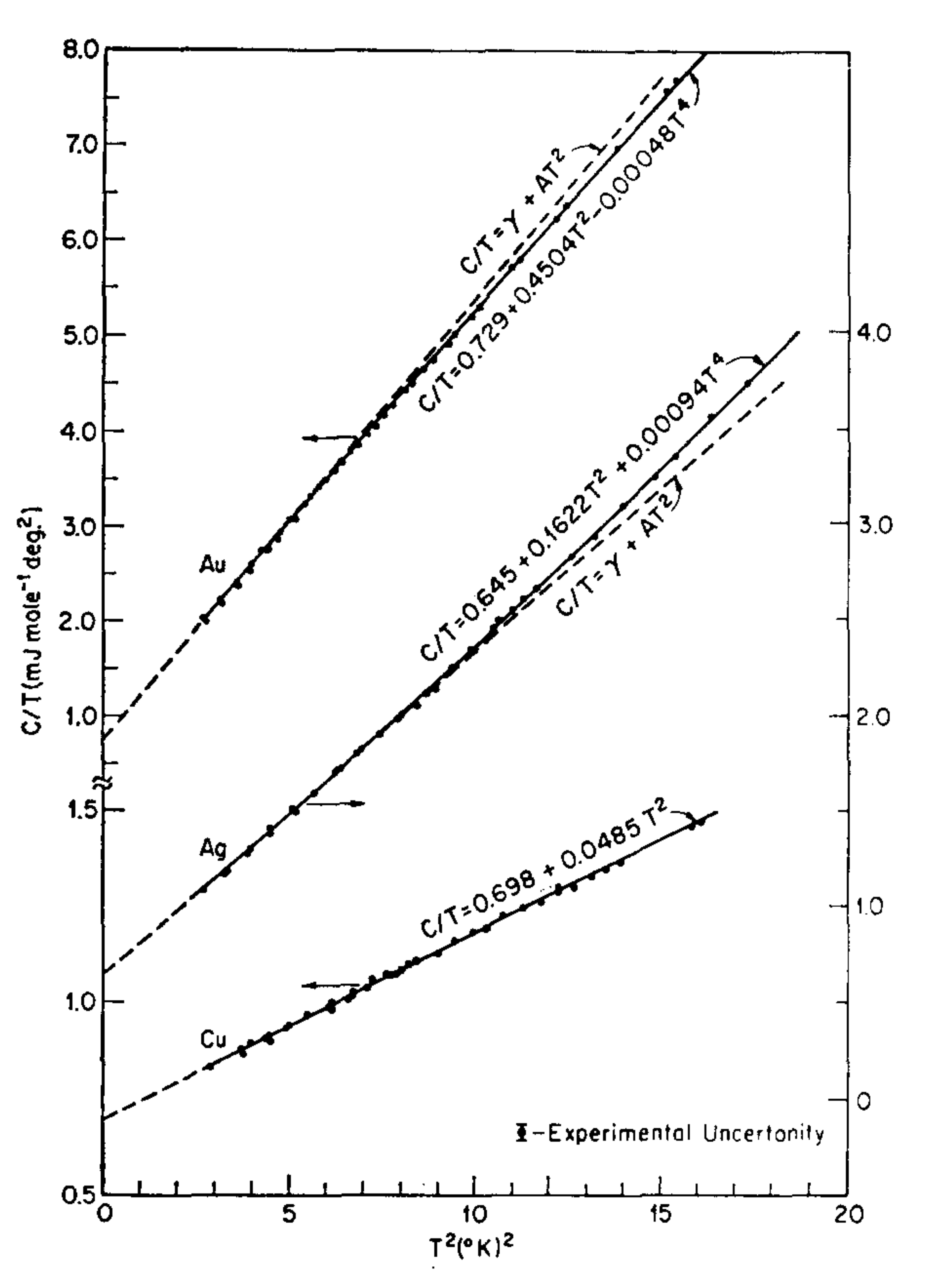


FIG. 1. The plots of C/T versus T^2 for gold, silver, and copper.

L. L. Isaacs, J. Chem. Phys. **43**, 307 (1965)

Metals = Au, Ag, Cu

$$C/T = \boxed{\gamma} + \boxed{A\,T^2}$$

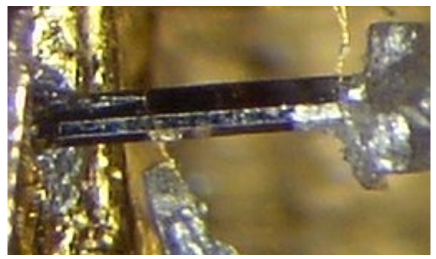
electrons   phonons

Deviations :

- even $T \ll \theta_D$: anharmonicity
- $T \to 0$: magnetic impureties

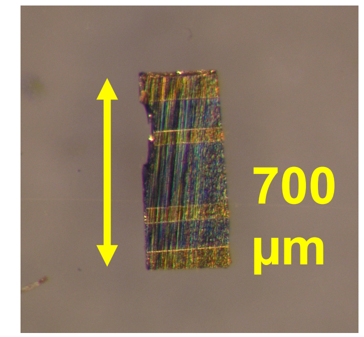
SPECIFIC HEAT
of a
SUPERCONDUCTOR

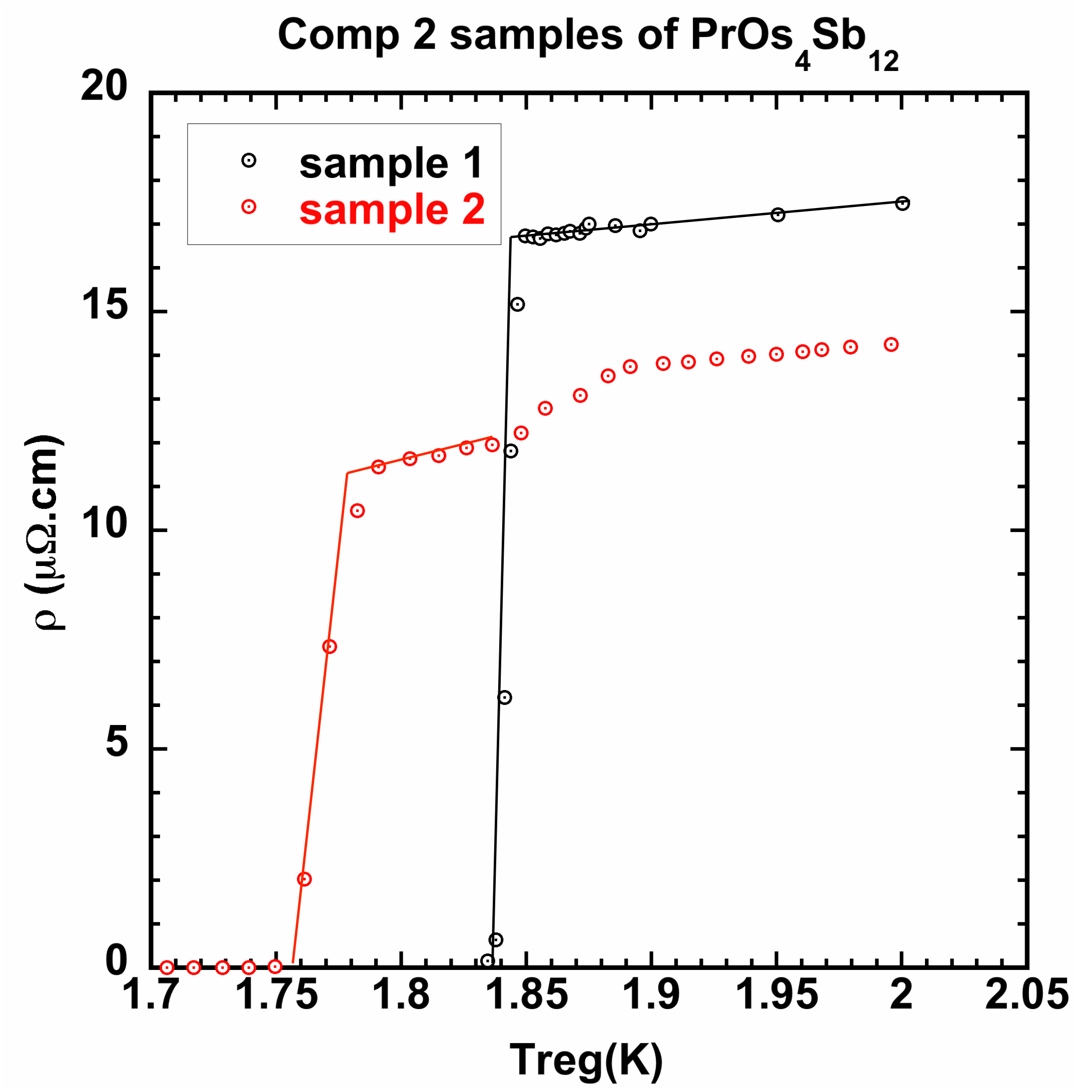
Cp = Bulk Probe !!

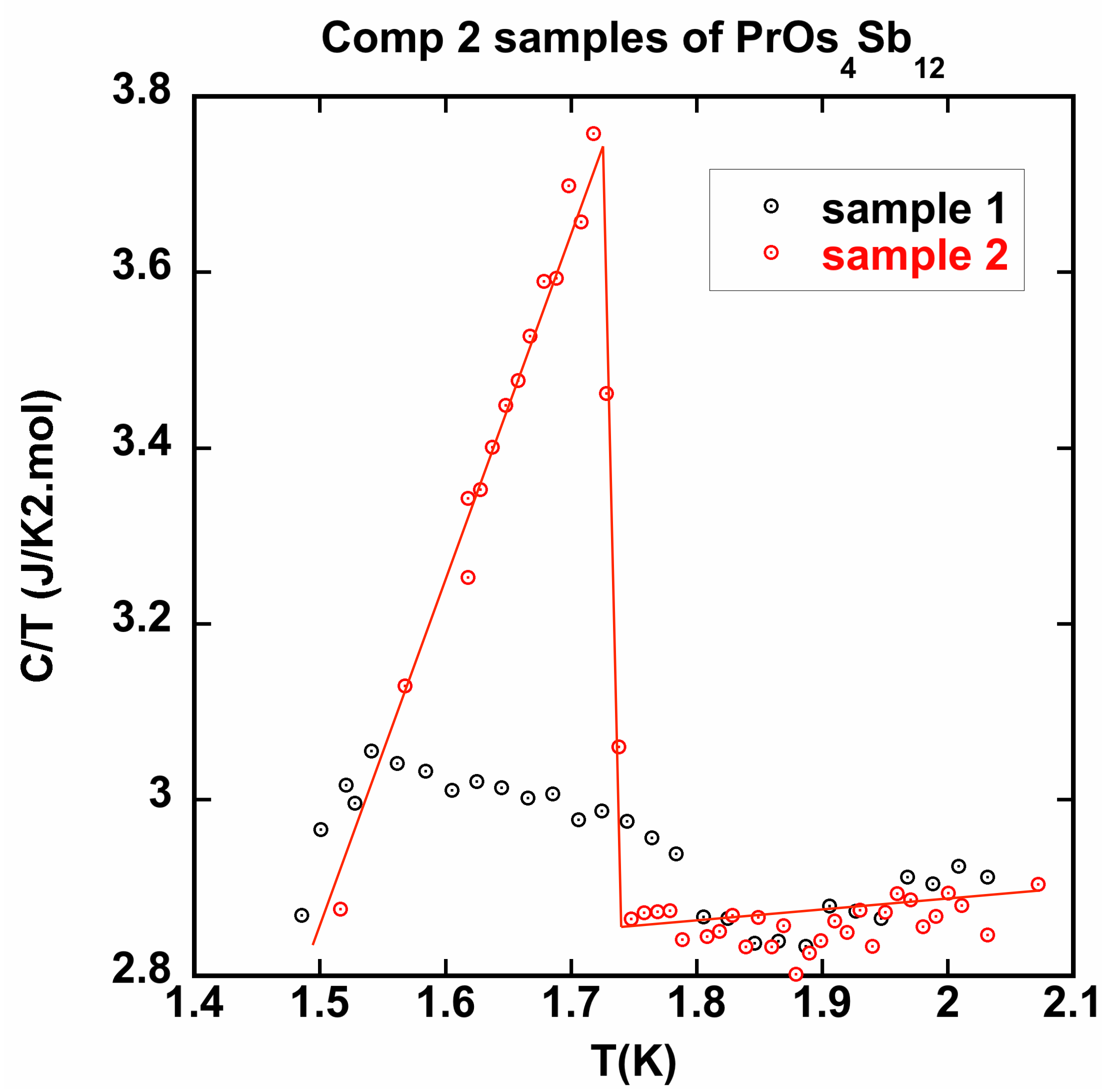


sample 1

sample 2



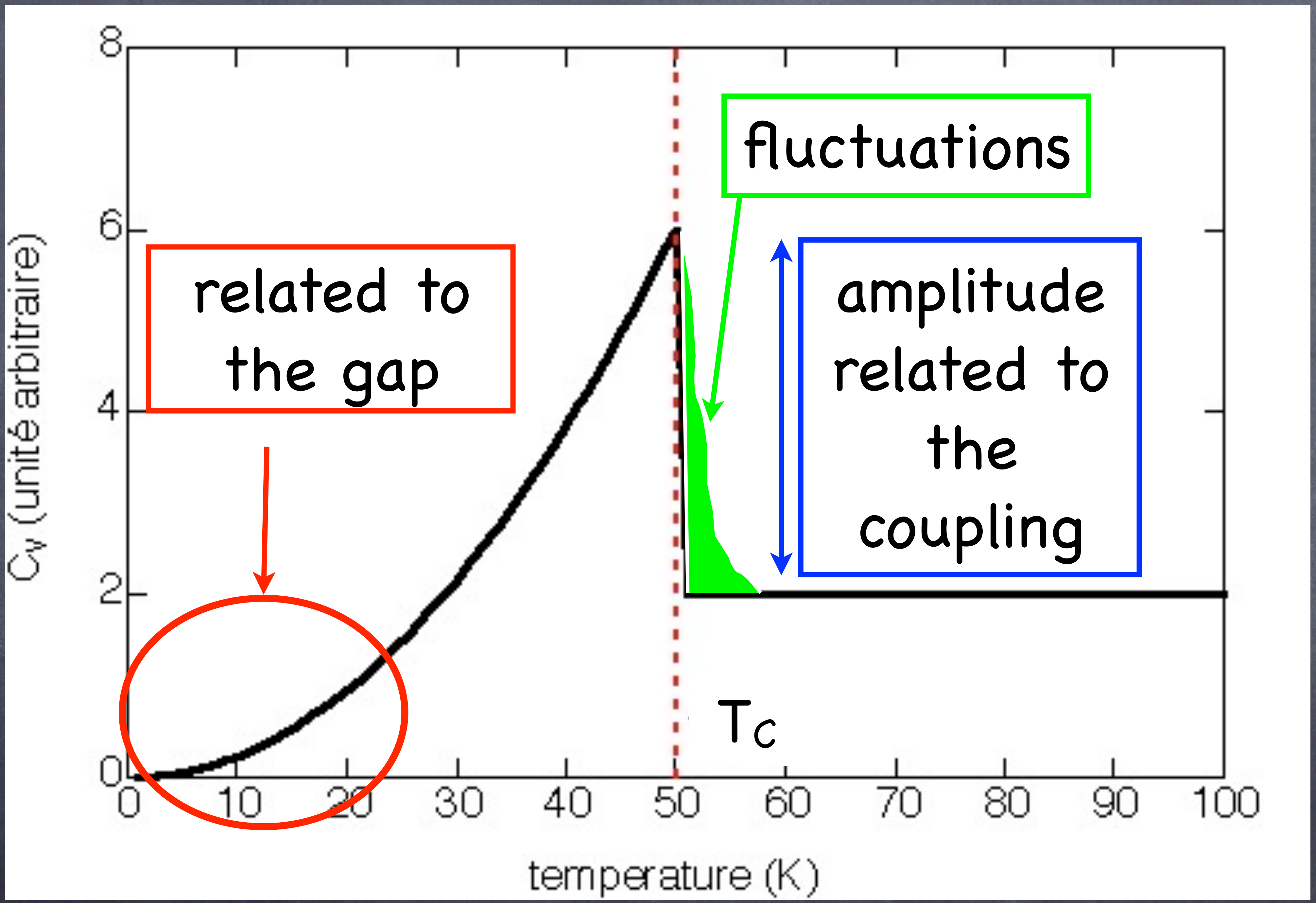




experimental goal

- Compute $\Delta C/ \Upsilon T_c$: substraction of BKG !!!!!!!!

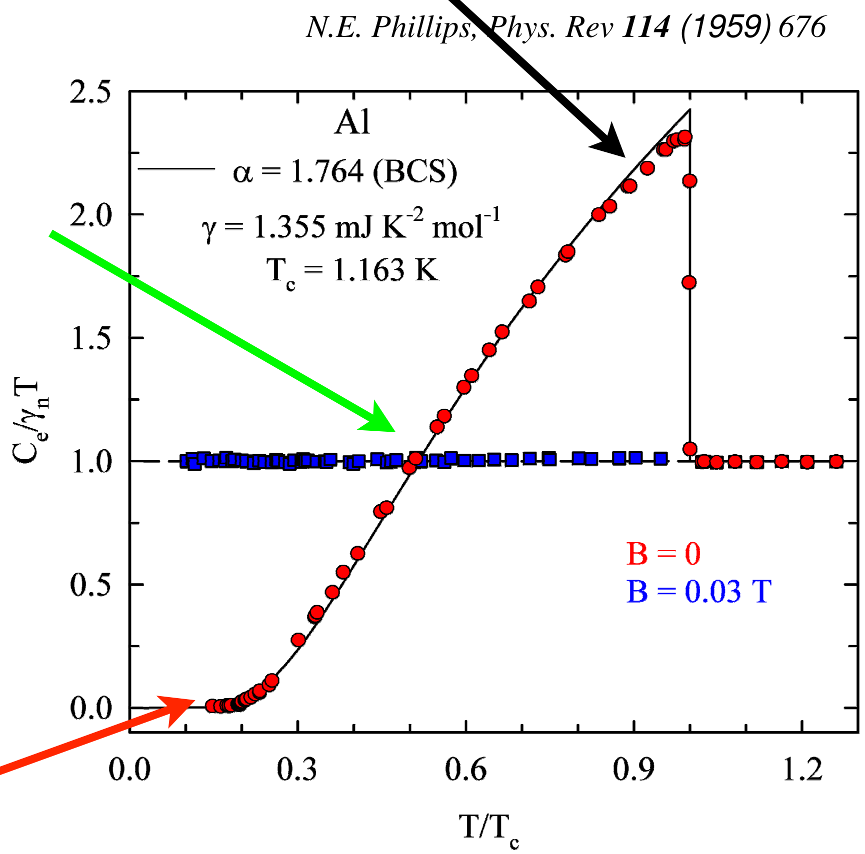
Superconductivity



BCS

normalized slope $d\Delta C/dT$ = 2.6 $\Delta C/T_c$ ind of γ

$T^* \approx 0.5\ T_c$



$\Delta C/\gamma T_c = 1.43$

$\Delta C/\gamma T_c = 8.5\ \exp(-1.44\ T_c/T)$ $\quad 2.5 < T_c/T < 6$

$\Delta C/\gamma T_c = 2.37\ (T_c/T)^{-3/2}\ \exp(-1.76\ T_c/T)$ $\quad 10 < T_c$

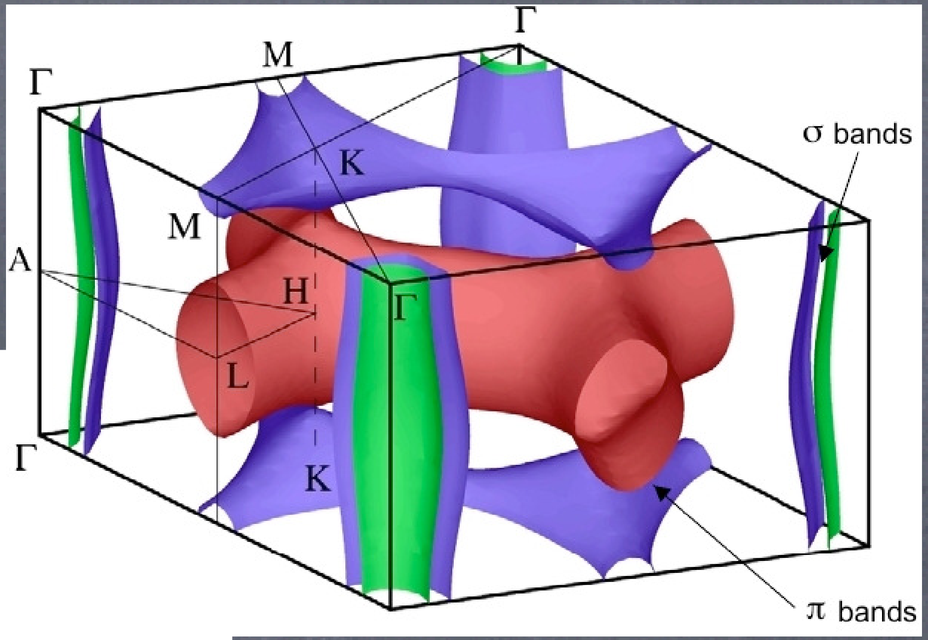
electron-phonon coupling (Eliashberg)

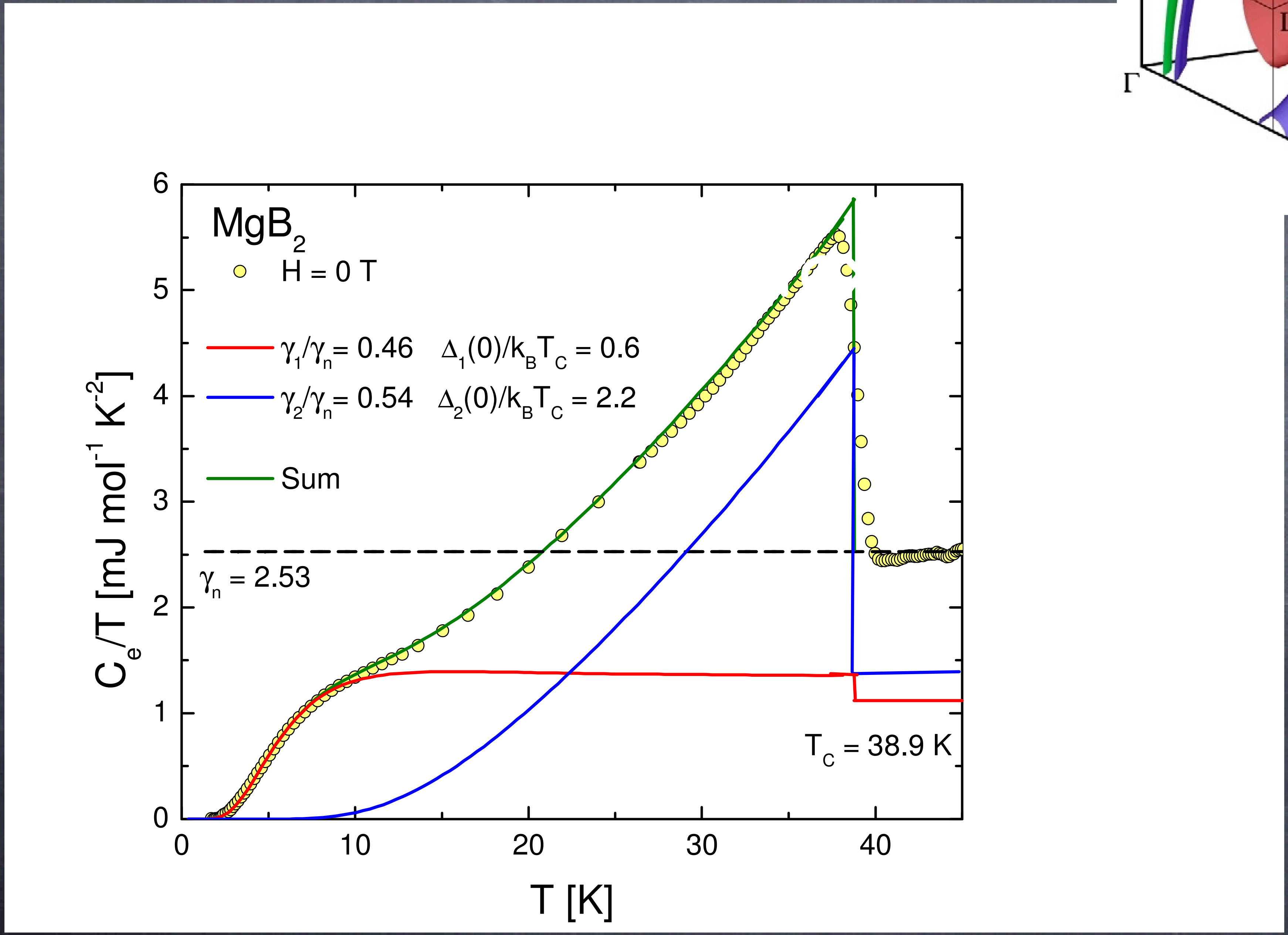
J.P.Carbotte, Rev. of Mod. Phys. 62 (1990) 1027

- e-ph renormalization $m^*=(1+\lambda)m_e$
- $\lambda = \int 2\alpha^2F(\omega)d\omega/\omega$, $\alpha^2F(\omega)$ spectral density contains N_e, N_{ph},V_{int}
- $\omega_{ln}=\exp(2/\lambda \times\int\alpha^2F(\omega)\ln(\omega)d\omega/\omega)$
  «mean» log energy of electron-phonon coupling
- $Tc/\omega_{ln} << 1$: weak-coupling limit
  and $\lambda(\omega)= \lambda$ for $\omega< \omega_c$ and =0 otherwise $\Big\}$ = BCS

multi-gap superconductivity

MgB_2





Gap nodes

- in a fully gapped superconductor :
  $C/T = f(T)\ e^{-\Delta/T}$ and prop to H/H_{c2}

- in a d-wave superconductor :
  line of nodes
  C/T prop to T and prop to $(H/H_{c2})^{1/2}$

symetry of the gap ex: Fe(Se,Te)

oscillations of Cp when rotating the magnetic field in presence of nodes