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INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
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**SMR. 758 - 16**

SPRING COLLEGE IN CONDENSED MATTER
ON QUANTUM PHASES
(3 May - 10 June 1994)

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**MAGNETIC PHASE TRANSITIONS AT LOW TEMPERATURES**

**PART I**

**MPTI Magnetic Fluctuation Spectra and the Quasiparticle Scattering Rate**

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These are preliminary lecture notes, intended only for distribution to participants.

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# *Magnetic Phase Transitions at Low Temperatures*

## *MPTI Magnetic Fluctuation Spectra and the Quasiparticle Scattering Rate*

- Spin Aligned to Fermi Liquid Transition
- Magnetic Fluctuation Model
- Fluctuation Spectrum and the Relaxation Rate $\Gamma_q$
- The Quasiparticle Scattering Rate

Appendices:

Notation and Key Relations

Review of Linear Response, Power Spectrum and the Fluctuation Dissipation Theorem

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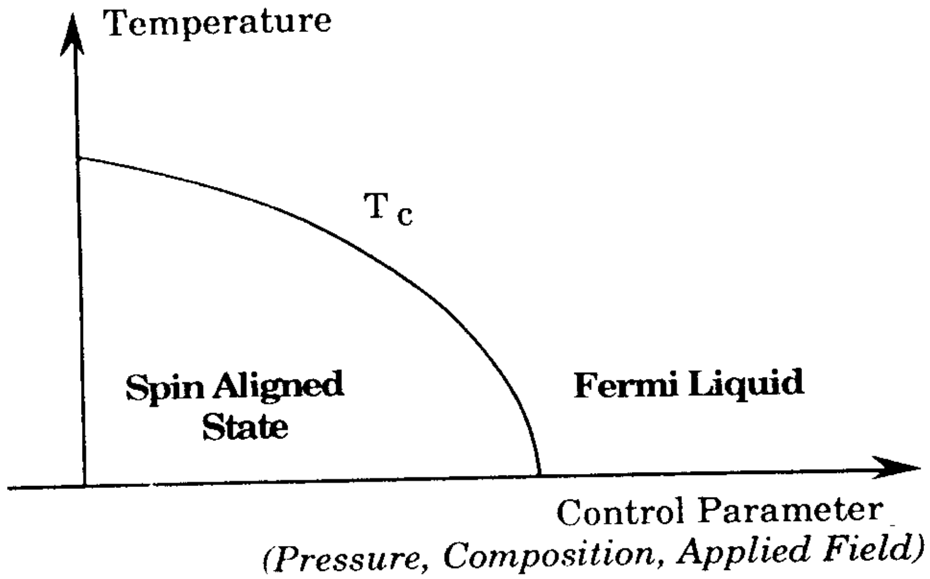
May 1994

## 1. *Ferromagnetic to Fermi Liquid Transitions at Low Temperatures*

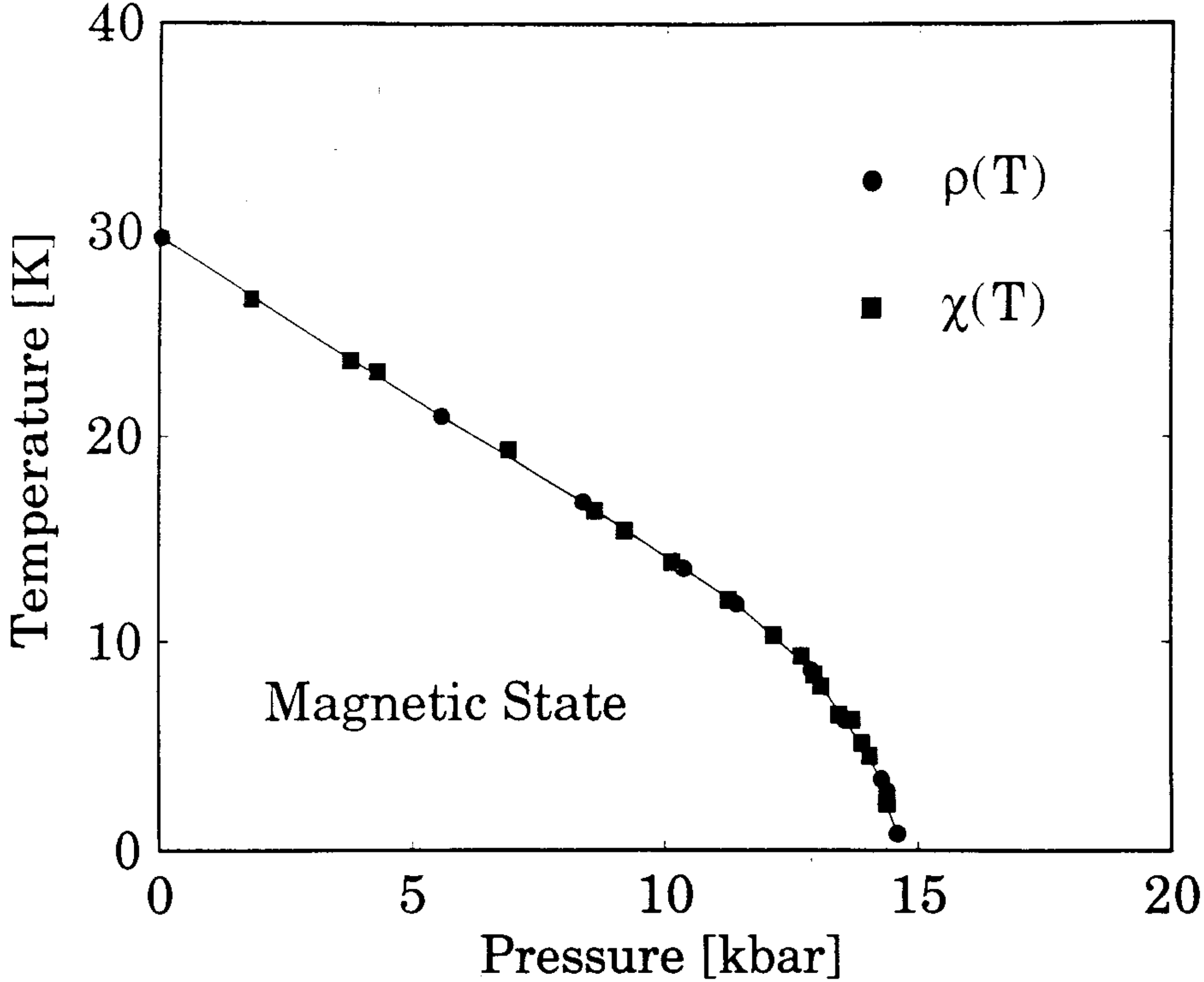



- Fluctuation frequency $\Gamma_q \geq kT_c/\hbar$ near the critical pressure or composition.
- 3d ferromagnetic metals near critical lattice spacing or composition

  heavy fermion compounds and low dimensional conductors
- Quantum Critical Phenomena (breakdown of conventional view of elementary excitations).
- Quantum Order (fermion condensations, novel magnetism and superconductivity).
- Millis, Sachdev
- Doniach, Hertz, Moriya

Pfleiderer, McMullan, Khmelnitskii
Cavendish Laboratory

# *Phase Diagram of MnSi*



## 2. *Magnetic Fluctuation Model for Nearly Ferromagnetic Metals*

- Low frequency (one pole) model for $\chi_{q\omega}$

$$\chi_{q\omega}^{-1} = \chi_q^{-1} - \frac{i\omega}{\gamma_q} = \chi_q^{-1}\left(1 - i\omega / \Gamma_q\right) \tag{2.1}$$

- The relaxation spectrum $\Gamma_q$

$$\Gamma_q = \gamma_q \chi_q^{-1} . \tag{2.2}$$

At low q

$$\gamma_q = \gamma q^n , \tag{2.3}$$

$$\chi_q^{-1} = \chi^{-1} + cq^2 . \tag{2.4}$$

- n = 1 : conserved variable decays via ballistic transport by quasiparticles (e.g. the magnetisation in a pure incipient ferromagnetic metal). In Fermi liquid theory at low q

$$\Gamma_q = \frac{2}{\pi} \upsilon_F^* q \frac{\chi^*}{\chi_q} , \quad \frac{\chi^*}{\chi} = 1 + F_o^a \tag{2.5}$$

- n = 2 : conserved variable decays via diffusive quasiparticle transport (e.g. the magnetisation in a disordered incipient ferromagnet with weak spin-orbit).

- n = 0 : non-conserved variable decays via local processes (e.g. the staggered magnetisation in an incipient antiferromagnet).

- Variance $\upsilon_q$ of $m_q(t)$ from $\chi''_{q\omega}$ via Nyquist's Theorem

$$\upsilon_q = \frac{2\hbar}{\pi} \int_0^\infty d\omega \, n_\omega \, \chi''_{q\omega} \, . \tag{2.6}$$

- Key results of model

$$\chi^{-1} = a + (2+N)\sum_q b\upsilon_q \, , \tag{2.7}$$

$$B = \chi^{-1} M + bM^3 \, , \tag{2.8}$$

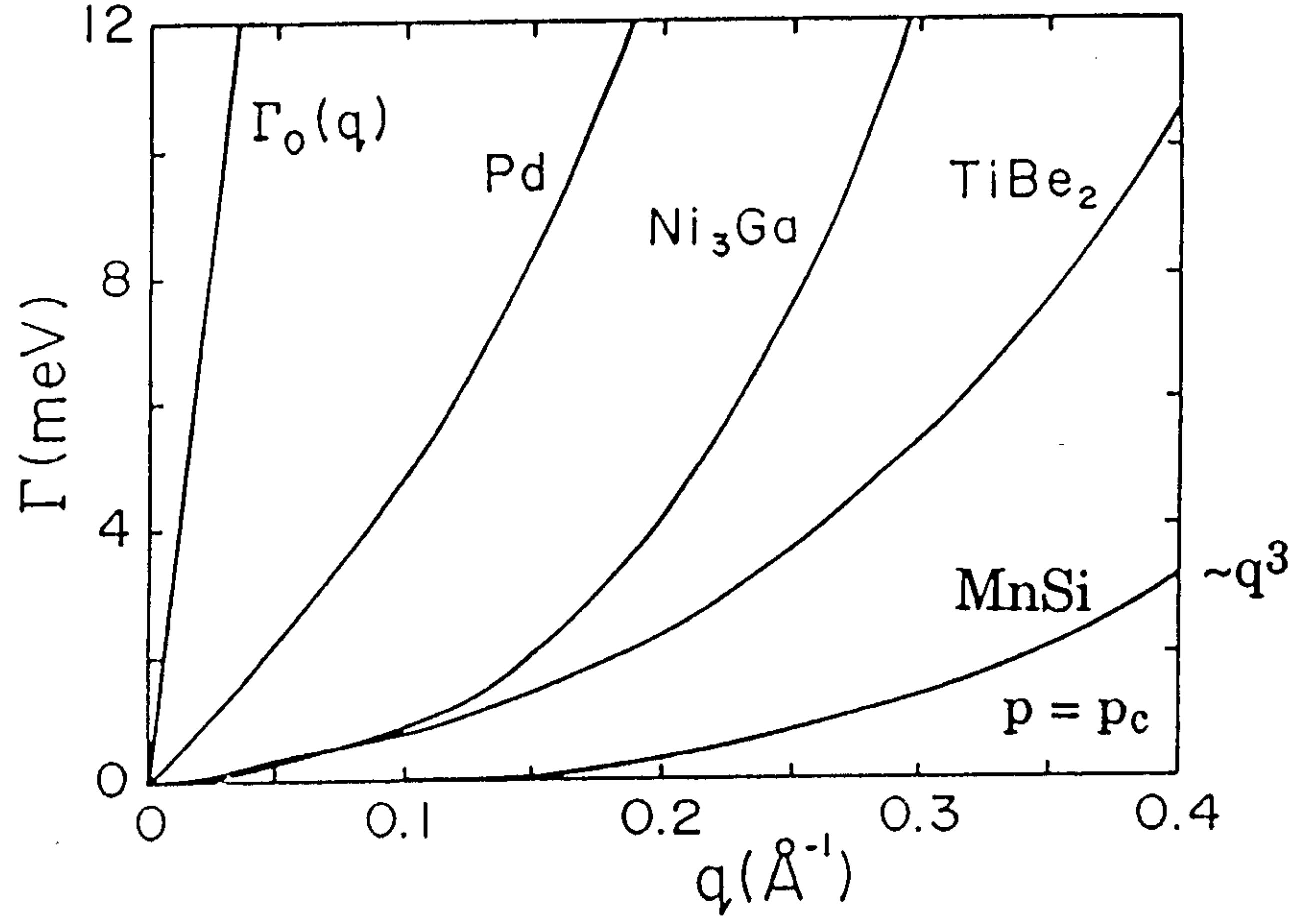
$$\Delta C = \frac{N}{2}\sum_q \chi_q^{-1} \frac{\partial \upsilon_q}{\partial T} \, , \tag{2.9}$$

$$\rho = \alpha T \sum_q q \left( \frac{\partial \upsilon_q}{\partial T} \right)_\chi \, . \tag{2.10}$$

| $d = 3$ | FL ($\Gamma_q \sim q$) | MFL ($\Gamma_q \sim q^{z=3}$) |
|---|---|---|
| $\Delta\chi^{-1}$ | $T^2$ | $T^{4/3}$ |
| $\Delta C$ | $T$ | $T \, ln \, (T^*/T)$ |
| $\rho$ | $T^2$ | $T^{5/3}$ |

- Temperature independent parameters a, b, c, $\gamma$.

## 3. *Spin Fluctuation Rate in Nearly Ferromagnetic Transition Metals*




Exp: Bernhoeft and Lonzarich; Ishikawa et al. (MnSi)
Calc: McMullan and Lonzarich; Winter et al.

$$\Gamma_q = \gamma q(\chi^{-1} + cq^2) \rightarrow q^{z=3} \quad \text{for} \quad T \rightarrow T_c.$$

z = Dynamical Exponent; $d_{eff} = d + z \rightarrow 6$.

# 4. *Neutron Scattering*

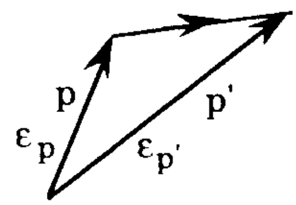
- Measurement of fluctuation spectra and introduction to electron scattering

- Assume potential v(ρ) seen by neutron is a classical stochastic process (high T approximation)

$$v(\rho) = \frac{1}{\sqrt{\rho_o}} \sum_k v_k e^{ik\cdot\rho}, \quad \begin{array}{l} \rho = (r,t) \;, \quad k = (q,\omega) \;, \\ \rho_o = \upsilon_o t_o \to \infty \;. \end{array} \tag{4.1}$$

- Rate of scattering from $p \to p'$ in Born approximation

$q = p - p'$
$\hbar\omega = \varepsilon_p - \varepsilon_{p'}$




Golden Rule:
$Ue^{ik\cdot\rho}$ yields transition rate
$\frac{|U|^2}{\hbar^2} t_o$ for $p \to p'$

$$\tau^{-1}_{p\to p'} = \frac{C^v_k}{\hbar^2 \upsilon_o} \tag{4.2}$$

- **Differential Cross section**

Incident flux × $d^2\sigma$ = # scattered from p to range $p'^2 d\Omega dp'$ per time = # in $\upsilon_o \times \tau^{-1}_{p\to p'} \times$ # states in $p'^2 d\Omega dp'$

$$\frac{d^2\sigma}{\upsilon_o d\Omega\, d\omega} = \frac{m_N^2}{8\pi^3\hbar^4} \frac{p'}{p} C^v_k \tag{4.3}$$

- **Nuclear Scattering** (single isotope):

$$v(\rho) = a\sum \delta(r - r_i(t)) = a\, n(\rho)$$

$$C_k^v = a^2 C_k^n \tag{4.4}$$

Thus, cross-section yields the nuclear density power spectrum.

- **Magnetic Scattering** (unpolarised system):

$$v(\rho) = -\mu_N \cdot B(\rho)$$

$$C_k^v = \left(\frac{1}{3}\right)\mu_N{}^2\, C_k^B \tag{4.5}$$

Field fluctuations in terms of spin magnetisation and transverse currents

$$\nabla \times B = \frac{4\pi}{c}\left(j_{spin} + j_{orbital}\right), \qquad j_{spin} = c\nabla \times m\ ,$$

$$iq \times B_q = \frac{4\pi}{c}\left(icq \times m_q + j_{\perp q}\right), \tag{4.6}$$

$$C_k^B = (4\pi)^2\left[C_k^m + C_k^{j\perp}/c^2q^2\right].$$

Thus, the cross-section has contributions from spin and transverse current power spectra.

- **Quantum Limit**: v(ρ) is an operator which does not commute with itself at different times, and hence

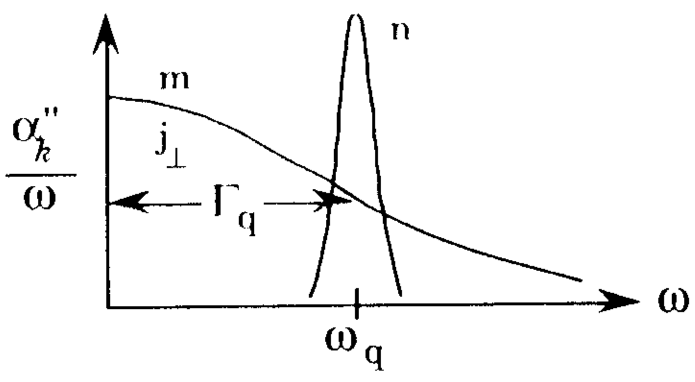
$$C_k = 2\hbar(1+n_\omega)\alpha''_k \tag{4.7}$$

replaces the classical form for the power spectrum. $C_k$ includes both zero point and thermal fluctuations (spontaneous and stimulated processes). Also factor of 1/3 in (5) is replaced by unity. Derivations are based on application of Born Approximation to the system as a whole or via an operator form of the one particle Schrodinger equation which yields an equation of motion for the single particle Green function. This operator description takes account not only of the non-commutation of v(t) and v(t + τ) but also the indistinguishability and statistics of the scattered particles which will be important in the electron scattering problem.

- **Comments**

i) Charge density fluctuations are normally suppressed at low q,ω but quadrupolar fluctuations may be important.

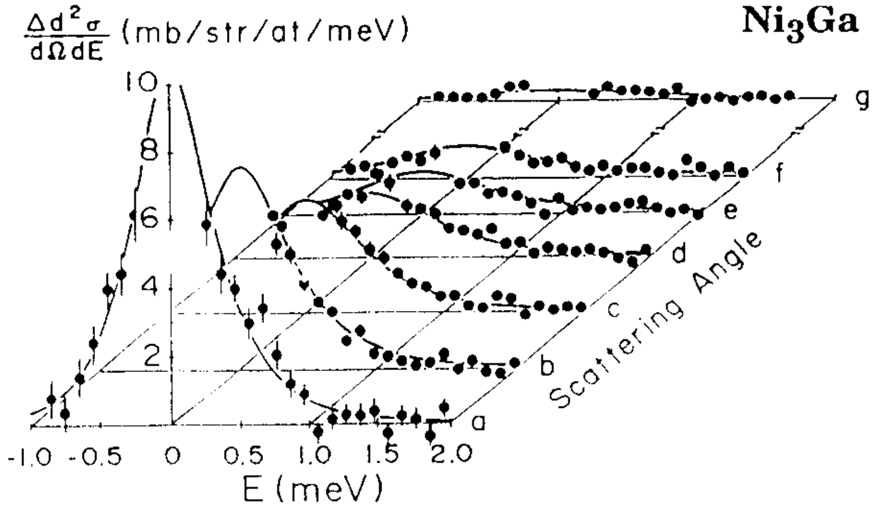
ii) Simplest models in the normal metallic state



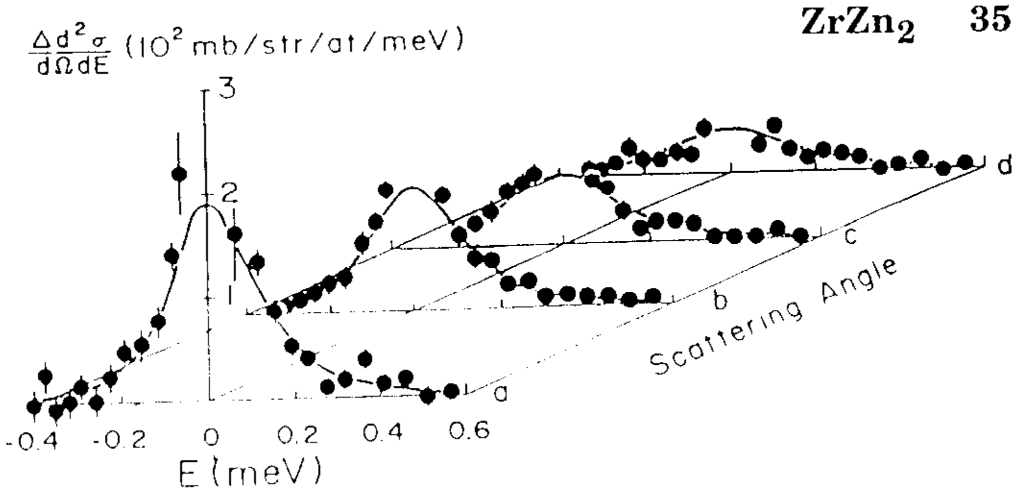

iii) Softening of $\Gamma_q$ may be expected (a) for $C^m_k$ in nearly magnetic metals around the ordering wavevector, (b) for $C^{j\perp}_k$ in incipient superconductors, and (c) in $C^m_k$ and the quadrupolar spectrum in heavy fermion systems.

# *Spin Fluctuation Spectra in d-Metals*

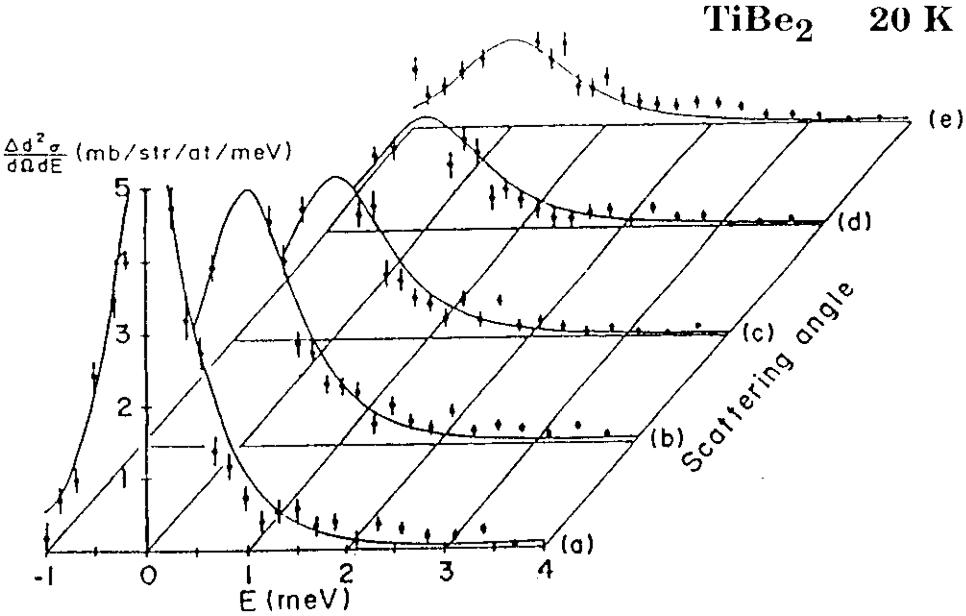
**$Ni_3Ga$ 22 K**



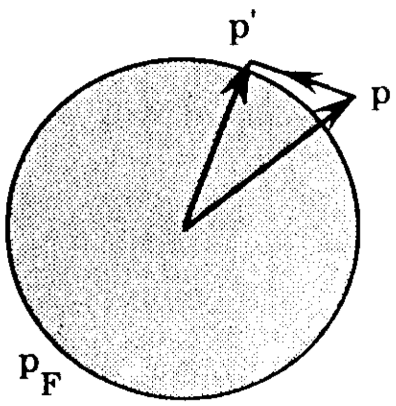

**$ZrZn_2$ 35 K**




**$TiBe_2$ 20 K**



## 5. *Electron Scattering*

- 


In Born approximation at T = 0

$$\tau_p^{-1} = \frac{1}{\hbar^2} \hat{\sum_{p'}} C_k^v \, , \qquad p' > p_F \, , \quad (5.1)$$

$$\left( \hat{\Sigma} \equiv \frac{1}{\rho_o} \Sigma = \int \frac{d^4 k}{(2\pi)^4} \right) .$$

- Phenomenological models of effective potentials

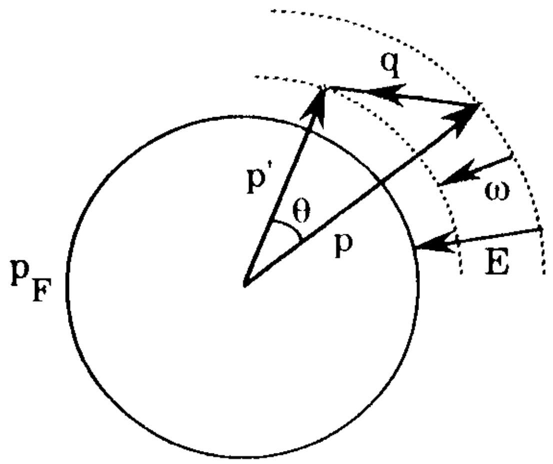
$$v(\rho) \cong \begin{cases} \eta^* n(\rho) & \text{nuclear} \\ -\mu \cdot \lambda m(\rho) & \text{magnetic} \end{cases} \qquad (5.2)$$

- Similar to neutron potential but with much greater strength. Born approximation *may* apply because of screening, use of final statistics of n(ρ) or m(ρ) and Pauli principle constraint on scattering for p very close to $p_F$ at T = 0.

- Simplest models for $\alpha''_k$ (associated with either n or m) and hence for $C_k^v$

$$\alpha''_k = \pi \, \alpha_q \omega \begin{cases} \frac{1}{2}\left[\delta(\omega - \omega_q) + \delta(\omega + \omega_q)\right] & \text{2 real poles at } \pm\omega_q, \quad (5.3a) \\ \frac{\Gamma_q / \pi}{\omega^2 + \Gamma_q^2} & \text{imaginary pole at } i\Gamma_q . \quad (5.3b) \end{cases}$$

- Express sum over p' as integral over q and $\omega$ for an isotropic system in 3 dimensions. First integrate over $\theta$, hence q, for fixed radius p' and then over the magnitude p' from p to $p_F$.




- $q^2 = p'^2 + p^2 - 2pp' \cos\theta$

  $d\cos\theta = -\frac{q\,dq}{pp'}$ .

- $2\frac{4\pi}{8\pi^3} p'^2 dp' = g(\varepsilon')d\varepsilon'$ . (5.4)

  $g(\varepsilon)$ = DOS of starting system for both spins per unit volume.

then if $p \approx p' \approx p_F$, $g(\varepsilon) \approx g(\varepsilon_F) = g_F$ for scattering near the Fermi surface.

$$\frac{1}{\hbar^2}\hat{\sum_{p'}} = \frac{g_F}{4\hbar p_F^2}\int_0^{E/\hbar}\int_0^{2p_F} q\,dq\,d\omega \qquad (5.5)$$

## 6. *Scattering from Acoustic Phonons*

- Consider $J = \int q\,dq\,d\omega\,\alpha''_k$ .

- Assume 2 pole form of $\alpha''_k$ with $\omega_q = \gamma q^n$ and $\alpha_q \rightarrow \alpha$ at low q.

- Integral over $\omega$ gives zero unless $\hbar\omega_q \leq E$ or $q < (E/\hbar\gamma)^{1/n}$ .

- Then integral over $q\omega_q$ finally yields

$$J = \frac{\pi\alpha\gamma}{2(n+2)}\left(\frac{E}{\hbar\gamma}\right)^{\frac{n+2}{n}} ,$$

$$\text{and} \qquad \tau_E^{-1} = \frac{\eta^2 g_F}{2p_F^2} J . \tag{6.1}$$

- For acoustic phonons at low q, n = 1 so that

$$\tau_E^{-1} \propto E^3 \tag{6.2}$$

## 7. *Scattering from Spin Fluctuations at Small q*

- Assume 1 pole form of $\alpha''_k \rightarrow \chi''_k$ with $\Gamma_q = \gamma q^n(\chi^{-1} + cq^2)$ $\rightarrow \zeta q^z$ at low q. $z = n$ if $\chi^{-1} \neq 0$, and $z = n + 2$ if $\chi^{-1} = 0$.

- $$J = \int q dq\, d\omega \frac{\omega\gamma q^n}{\omega^2 + (\zeta q^z)^2} \tag{7.1}$$

- If $\omega^2$ in denominator can be neglected in lowest order, then $\tau_E^{-1}$ has the form expected for a *Fermi Liquid*

$$\tau_E^{-1} \propto E^2. \tag{7.2}$$

This holds if the q integral does not diverge at low q, i.e. if there are more factors of q in numerator than in the denominator $(n + 2 > 2z)$, a condition satisfied for $\chi^{-1} \neq 0$, $n < 2$.

- For $n + 2 \leq 2z$, i.e. for $\chi^{-1} = 0$, the E dependence of J is determined by the low q (infrared) regime. Integrating over $\omega$

$$J = \frac{\gamma}{2}\int dq\, q^{n+1} ln\left(1 + \frac{E^2}{(\hbar\zeta q^z)^2}\right)$$

$$= \frac{\gamma}{2}\left(\frac{E}{\hbar\zeta}\right)^{\frac{n+2}{z}} \int dx\, x^{n+1} ln\left(1 + \frac{1}{x^{2z}}\right). \qquad (7.3)$$

The upper bound of the integral can be set to $\infty$ if $n + 2 \leq 2z$. For $z = n + 2$, $\tau_E^{-1}$ has the form of a *Marginal Fermi Liquid.*

$$\tau_E^{-1} \propto E \qquad (7.4)$$

## 8. *Large Angle Scattering Relaxation Rate and Thermal Averages*

- $\tau_E^{-1}$ is the total rate for all scattering processes. Define $\bar{\tau}_E^{-1}$ biased relative to $\tau_E^{-1}$ for large angle scattering by factor $(1 - \cos\theta) \simeq q^2 / 2p_F^2$

- For phonons $\bar{\tau}_E^{-1} \propto E^5$ # (8.1)

- For spin fluctuations

$$\bar{\tau}_E^{-1} \propto \begin{cases} E^2 & \text{if} \quad 4 + n > 2z \\ E^{\frac{4+n}{z}} & \text{if} \quad 4 + n \leq 2z \end{cases} \tag{8.2}$$

Thus, $\bar{\tau}_E^{-1} \propto E^{5/3}$ for a pure ferromagnetic metal in three dimensions at the critical point $\alpha^{-1} = 0$, $(n = 1, z = 3)$.

- Thermal average over $(-\partial f/\partial E)$ yields a temperature dependence with the same exponent as that of the energy dependence in leading order.

$$\left\langle \bar{\tau}_E^{-1} \right\rangle = \int \left( -\frac{\partial f}{\partial E} \right) \bar{\tau}_E^{-1} \, dE \propto T^{\alpha} \quad \text{if} \quad \bar{\tau}_E^{-1} \propto E^{\alpha} \, . \tag{8.3}$$

#Damping of phonon spectrum by coupling to electrons or impurities can lead to $E^2$ rather than $E^5$.

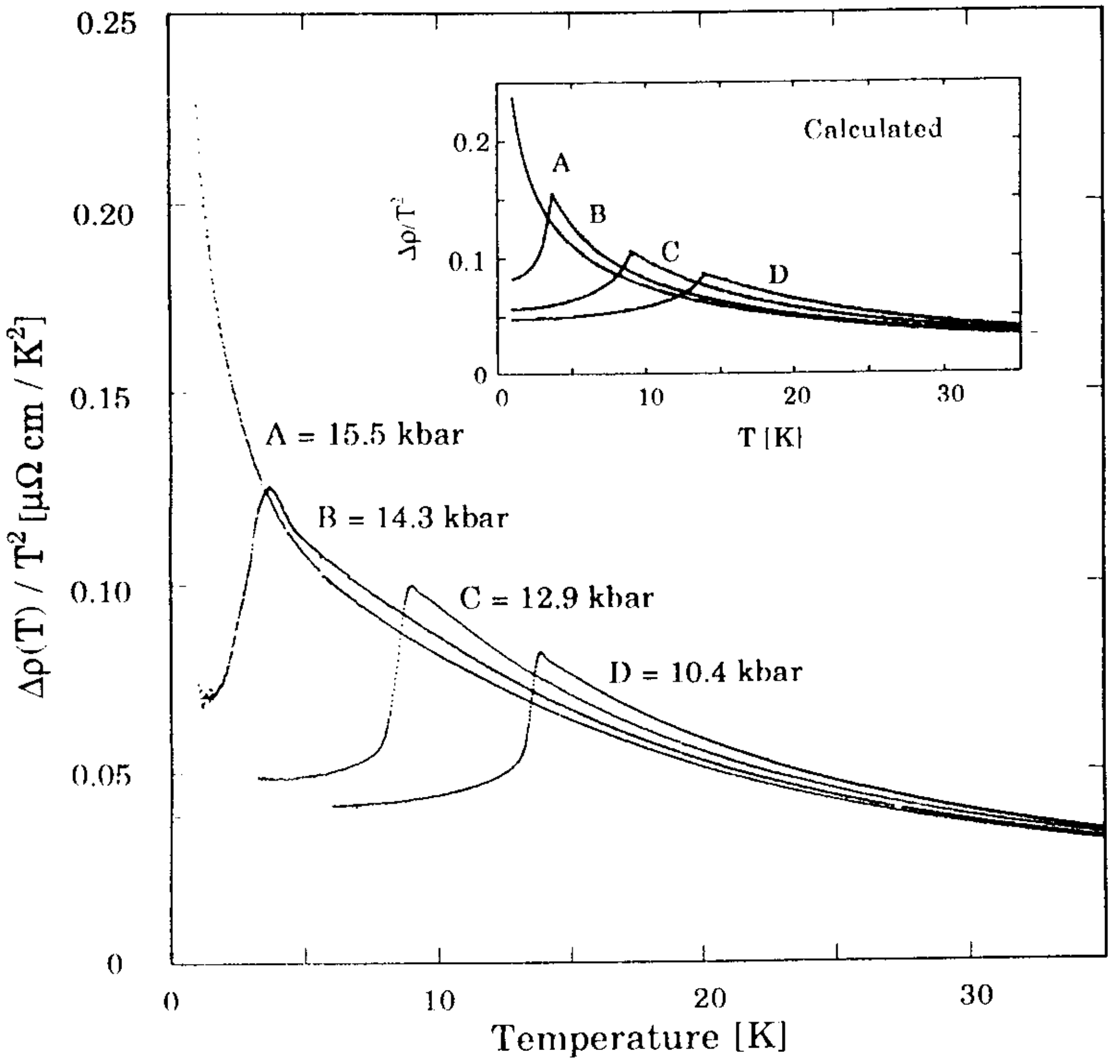
## 9. *The resistivity*

- Assume current is lost via transitions from states of low to high effective mass, or via Umklapp processes which transfer momentum to the lattice

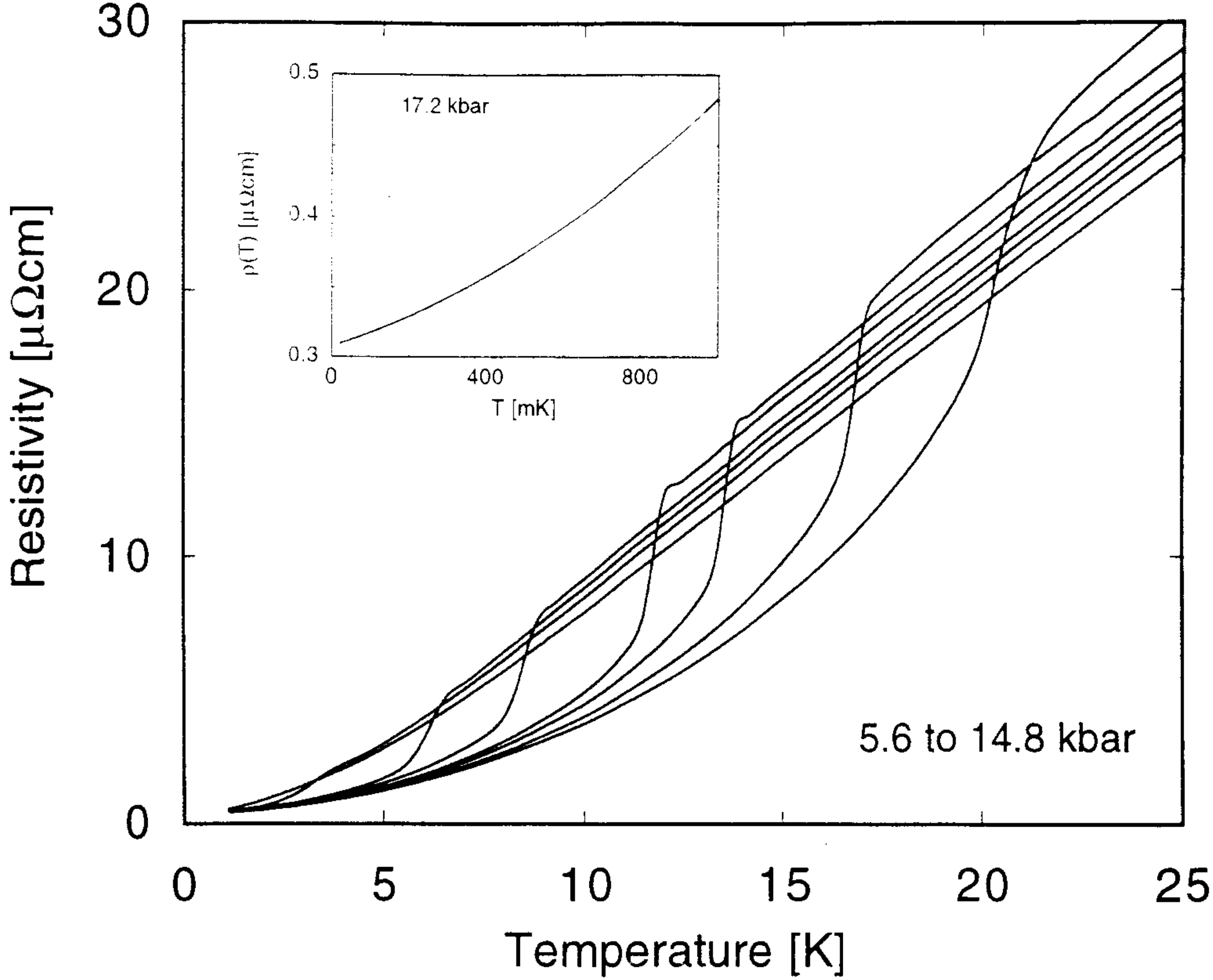
- From an analysis based on the Boltzmann equation, with scattering of carrier from spin fluctuations in the Born approximation, we find that ρ has same T dependence in leading order as $<\bar{\tau}_E^{-1}>$ and can be expressed in the form

$$
\begin{aligned}
\rho &\propto T \sum_k q \left( \frac{\partial C_k^m}{\partial T} \right)_\chi \\
&= \alpha T \sum_q q \left( \frac{\partial \upsilon_q}{\partial T} \right)_\chi \quad . \qquad (9.1)
\end{aligned}
$$

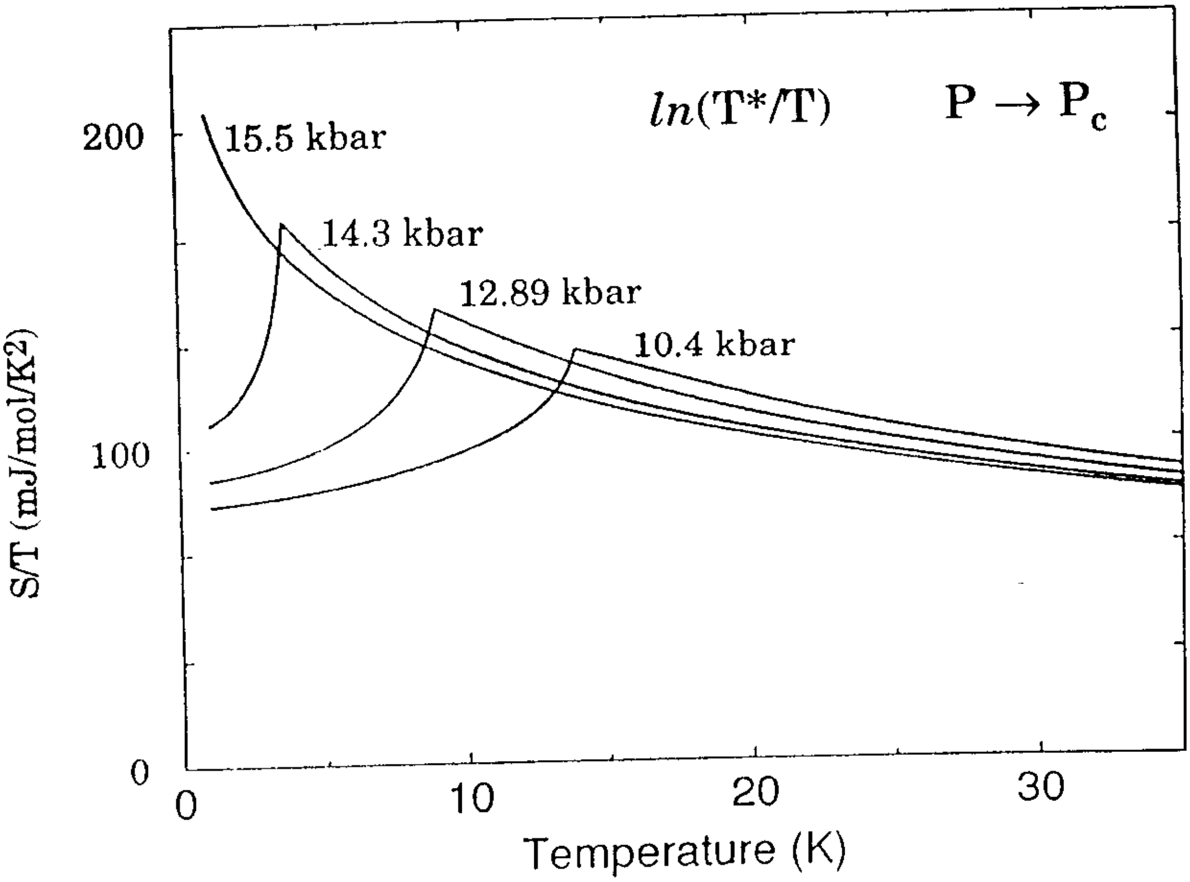
# *MnSi: Temperature Dependence of $\Delta\rho(T)/T^2$*

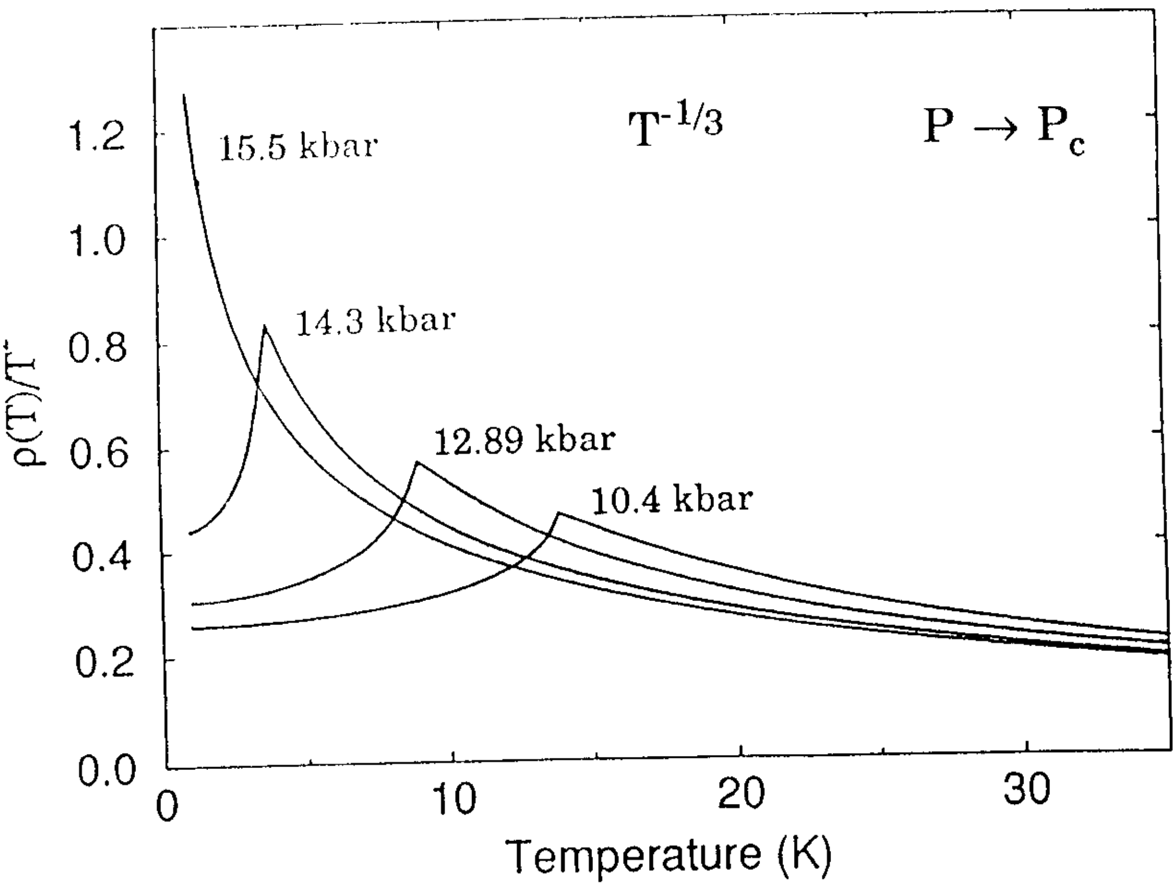


## ***Pressure and Temperature Dependence of the Resistivity***



# Calculated Temperature and Pressure Variations of the Entropy and Resistivity



## A1. Notation and Key Relations

- Space and time: $\rho = (r,t)$, $k = (q,\omega)$
  in large volume $\upsilon_o$ and long time $t_o$, $\rho_o = \upsilon_o t_o$

- Space and imaginary time: $u(r,\tau)$, $k = (q,\nu)$
  in $\upsilon_o$ and $\tau_o = \hbar\beta$, $u_o = \upsilon_o\tau_o$, $\beta = 1/k_B T$

- Fourier representation of fluctuating variables x and conjugate force f (assume translational invariance and $\bar{x} = 0$ if $f \to 0$):

$$x(\rho) = \frac{1}{\sqrt{\rho_o}} \sum_k x_k e^{ik\cdot\rho}, \quad x_k = \frac{1}{\sqrt{\rho_o}} \int d^4\rho\, x(\rho) e^{-ik\cdot\rho},$$

$$k \cdot \rho = q \cdot r - \omega t, \quad \frac{1}{\rho_o}\sum_k = \int \frac{d^4 k}{(2\pi)^4} \qquad (\text{or } \hat{\sum} = \int d^4\hat{k}) \ .$$

- **Response Function** and its Fourier representation :

Perturbation $= -\int d^3 r x f$, $\quad \overline{x(\rho)} = \int \alpha(\rho - \rho')\, f(\rho')\, d^4\rho'$,

$$\overline{x_k} = \alpha_k f_k \quad \text{if} \quad \alpha_k = \int d^4\rho\ \alpha(\rho)\ e^{-ik\cdot\rho}.$$

(nb: $\alpha_k$ is defined without $1/\sqrt{\rho_o}$ factor in $x_k$.)

- **Kramers Kronig**: $\alpha'_{q\omega} = P \int_{-\infty}^{\infty} \frac{d\Omega}{\pi} \frac{\alpha''_{q\Omega}}{\Omega - \omega}$, $\qquad \alpha = \alpha' + i\alpha''$.

$(\alpha' = \text{Re}\ \alpha, \quad \alpha'' = \text{Im}\ \alpha)$ .

- **Power Spectrum**:

$$C_k = C_k^L = \int \frac{d^4\rho'}{\rho_o} \int d^4\rho \, \overline{x(\rho'+\rho)x(\rho')} \, e^{-ik\cdot\rho} = \overline{x_k x_{-k}} \, .$$

$$C_k^R = \text{FT of } \overline{x(\rho')x(\rho'+\rho)} = \overline{x_{-k}x_k}, \quad C_k^S = \tfrac{1}{2}(C_k^L + C_k^R)$$

Bar denotes quantum-statistical average; result depends on order of products in quantum mechanics.

- **Fluctuation-Dissipation Theorem**:

$$C_k = 2\hbar(1+n_\omega)\alpha_k'' \, , \quad n_\omega = (e^{\beta\hbar\omega} - 1)^{-1}, \quad 1+n_\omega = -n_{-\omega}$$

$$= 2\hbar\alpha_{q,|\omega|}'' \begin{cases} 1+n_\omega & \omega > 0 \\ n_{|\omega|} & \omega < 0 \end{cases} .$$

Also $C_k^R = 2\hbar n_\omega \alpha_k''$ and $C_k^S = 2\hbar(\frac{1}{2} + n_\omega)\alpha_k''$.

## A2. *Response Function and Fluctuation Dissipation (Nyquist's) Theorem*

- Perturbation = -xf, $f = \frac{f_o}{2}(e^{i\omega t} + e^{-i\omega t})$.

- Transition rate =

$$\nu_{n'n} = \frac{2\pi}{\hbar^2}|x_{n'n}|^2\left(\frac{f_o}{2}\right)^2[\delta(\omega - \omega_{n'n}) + \delta(\omega + \omega_{n'n})] .$$

- Power absorption

$$= \sum P_n \nu_{n'n} \hbar\omega_{n'n}$$
$$= -\overline{x_f \dot{f}} = \alpha''_\omega f_o^2 \omega / 2$$

- Thus $\alpha''_\omega = \frac{\pi}{\hbar}\sum P_n |x_{n'n}|^2 \left[\delta(\omega - \omega_{n'n}) - \delta(\omega + \omega_{n'n})\right]$

$$= \frac{\pi}{\hbar}(1 - e^{-\beta\hbar\omega})\sum P_n |x_{n'n}|^2 \delta(\omega - \omega_{n'n}) .$$

Real part from the Kramers-Kronig relation.

- The correlation function: $C(\tau) = C^L(\tau) = \overline{x(\tau)x(0)}$

$$= \sum P_n \langle n|x(\tau)x(0)|n\rangle = \sum P_n |x_{n'n}|^2 e^{-i\omega_{n'n}\tau} .$$

- Power Spectrum: $C_\omega = C^L_\omega = 2\pi \sum P_n |x_{n'n}|^2 \delta(\omega - \omega_{n'n})$ .

- The Fluctuation Dissipation Theorem:

$$C_\omega = 2\hbar(1 + n_\omega)\alpha''_\omega, \quad n_\omega = (e^{\beta\hbar\omega} - 1)^{-1} .$$

- $C^R(\tau) = \overline{x(0)x(\tau)}$ ,

$$C^R_\omega = 2\pi \sum P_n |x_{n'n}|^2 \delta(\omega + \omega_{n'n}) = e^{-\beta\hbar\omega} C^L_\omega = 2\hbar n_\omega \alpha''_\omega ,$$

$$C^S_\omega = 2\hbar\left(\frac{1}{2} + n_\omega\right)\alpha''_\omega .$$