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2. Non-equilibrium critical relaxation, coupling to conserved modes

critical initial slip and aging: non-equilibrium relaxation

"quench" system from disordered state ($T \rightarrow \infty$)

to - $T > T_c$: finite relaxation time t_c

→ system "forgets" initial state for $t > t_c$

- $T < T_c$: totally different ground state

(broken ergodicity) → slow coarsening dynamics,
typical scale: domain wall size $L(t)$

- $T = T_c$: $\xi \rightarrow \infty$, $t_c \sim \xi^z \rightarrow \infty$

"never" fully equilibrates,

dynamics non-stationary

"initial-slip" scaling:

$$\langle S(\tau=0, t) \rangle = S_0 t^{\theta'} \tilde{S}(S_0 t^{\theta' + \frac{\beta}{2\nu}}) \sim \begin{cases} S_0 t^{\theta'} & t \rightarrow 0 \text{ grows} \\ t^{-\frac{\beta}{2\nu}} & t \rightarrow \infty \text{ decays} \end{cases}$$

dynamic response function in "aging" scaling limit $t' \ll t$:

$$\chi(\tau, \vec{q}, \frac{t'}{t} \rightarrow 0) = |\vec{q}|^{-2+z+\eta} \left(\frac{t}{t'}\right)^{\theta} \hat{\chi}(|\vec{q}|\xi, |\vec{q}|^2 t)$$

$$\chi(\tau, \vec{x}, t, t'=0) = t^{-\lambda_R/2} \tilde{\chi}\left(\frac{|\vec{x}|}{\xi}, |\vec{x}| t^{-1/2}\right) \sim t^{-\lambda_R/2}$$

as $|\vec{x}| \rightarrow 0, t \rightarrow \infty$

autoresponse exponent: $\lambda_R = d + z - 2 + \eta - z\theta$

dynamic correlation function:

↓ equilibrium FDT

$$C(\tau, \vec{q}, \frac{t'}{t} \rightarrow 0) = |\vec{q}|^{-2+z+\eta} \left(\frac{t}{t'}\right)^{\theta-1} \hat{C}(|\vec{q}|\xi, |\vec{q}|^2 t)$$

$$C(\tau, \vec{x}, t, t'=0) = t^{-\lambda_c/2} \tilde{C}\left(\frac{|\vec{x}|}{\xi}, |\vec{x}| t^{-1/2}\right) \sim t^{-\lambda_c/2}$$

autocorrelation exponent: $\lambda_c = d - 2 + \eta - z(\theta - 1) = \lambda_R$
(in equilibrium)

model B: $\theta' = \theta = 0$ (conserved order parameter!), $\lambda_R = d + 2$

model A: $\theta' = \theta - 1 + \frac{z-\eta}{z}$, $\lambda_R = d - z\theta'$, $\theta' = \frac{\eta+2}{z} \in +O(\epsilon^2)$
(independent exponent)

non-equilibrium perturbations for relaxational critical dynamics:

violate Einstein relation, noise strength $D k_B T \rightarrow \tilde{D}$

$\rightarrow$ effective noise temperature $k_B T' = \frac{\tilde{D}}{D}$

rescale $\vec{r} \rightarrow \vec{r}' = \sqrt{\frac{D k_B T}{\tilde{D}}} \vec{r}$, $S \rightarrow S' = \sqrt{\frac{D k_B T}{\tilde{D}}} S$

gives original model A/B Langerin equation with $u \rightarrow u' = \frac{\tilde{D}}{D k_B T} u$

critical properties: fixed point $u^* \rightarrow$ prefactor irrelevant for universal scaling behavior

$\rightarrow$ model A (B) also prominent non-equilibrium dynamic universality class

anisotropic detailed balance violation for model B:

$$D \vec{\nabla}^2 \rightarrow D_{\perp} \vec{\nabla}_{\perp}^2 + D_{\parallel} \vec{\nabla}_{\parallel}^2, \text{ noise: } \tilde{D}_{\perp} \vec{\nabla}_{\perp}^2 + \tilde{D}_{\parallel} \vec{\nabla}_{\parallel}^2, \text{ let } T'_{\perp} < T'_{\parallel}$$

$\rightarrow$ transverse spatial sector "softens" first, longitudinal non-critical

yields effective two-temperature or randomly driven model B:

$$\frac{\partial S^{\alpha}(\vec{x}, t)}{\partial t} = D \left(\vec{\nabla}_{\perp}^2 \left[\tau - \vec{\nabla}_{\perp}^2 + \frac{u'}{6} \vec{S}(\vec{x}, t)^2 \right] + c \vec{\nabla}_{\parallel}^2 \right) S^{\alpha}(\vec{x}, t) + \zeta^{\alpha}(\vec{x}, t)$$

$$\langle \zeta^{\alpha}(\vec{x}, t) \rangle = 0, \langle \zeta^{\alpha}(\vec{x}, t) \zeta^{\beta}(\vec{x}', t') \rangle = -2D k_B T' \vec{\nabla}_{\perp}^2 \delta(\vec{x} - \vec{x}') \delta(t - t') \delta^{\alpha\beta}$$

equivalent to effective equilibrium model B:

$$\frac{\partial S^{\alpha}(\vec{x}, t)}{\partial t} = D \vec{\nabla}_{\perp}^2 \frac{\delta H'[S^{\alpha}]}{\delta S^{\alpha}(\vec{x}, t)} + \zeta^{\alpha}(\vec{x}, t) \quad \text{with long-range (dipolar)}$$

$$\text{Hamiltonian } H'[S^{\alpha}] = \int \frac{d^d q}{(2\pi)^d} \frac{\vec{q}_{\perp}^2 (\tau + \vec{q}_{\perp}^2) + c \vec{q}_{\parallel}^2}{2 \vec{q}_{\perp}^2} |\vec{S}(\vec{q})|^2 + \frac{u'}{4!} \int d^d x [\vec{S}(\vec{x})^2]^2$$

$\rightarrow$ anisotropic scaling laws, e.g.: reduced critical dimension $d_c = 4 - d_{\parallel}$

$$X(\tau, \vec{q}_{\perp}, \vec{q}_{\parallel}, \omega) = |\vec{q}_{\perp}|^{-2+\eta} \hat{X} \left(\frac{\tau}{|\vec{q}_{\perp}|^{1/\nu}}, \frac{|\vec{q}_{\parallel}|}{|\vec{q}_{\perp}|^{1+\Delta}}, \frac{\omega}{|\vec{q}_{\perp}|^2} \right)$$

scaling relations: $z = 4 - \eta$, $\Delta = 1 - \frac{\eta}{2} = \frac{z}{2} - 1$; η, ν not equilibrium

longitudinal sector: $z_{\parallel} = \frac{z}{1+\Delta} = 2$, $\nu_{\parallel} = \nu(1+\Delta) = \frac{2\nu}{2} = \frac{\nu}{2} (4 - \eta)$

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(static) coupling to non-critical conserved (scalar) energy density g :

$$\Delta H[g, S^\alpha] = \frac{1}{2C} \int d^d x \left[g(\vec{x})^2 + g(\vec{x}) \vec{S}(\vec{x})^2 \right]$$

$$\rightarrow \langle g(\vec{x}) g(\vec{x}') \rangle = k_B T C \delta(\vec{x} - \vec{x}'), \quad (\Delta E)^2 = k_B T^2 C_V \rightarrow C = \frac{C_V T}{V}$$

complete square in Hamiltonian to integrate out $g(\vec{x})$:

$$\int dg \exp\left(-\frac{g^2 + g \vec{S}^2}{2C k_B T}\right) = \int dg \exp\left(-\frac{(g + \frac{g \vec{S}^2}{2})^2}{2C k_B T}\right) \cdot \exp\left(\frac{g^2 (\vec{S}^2)^2}{8C k_B T}\right)$$

$\rightarrow$ merely shifts non-linear coupling $u \rightarrow \tilde{u} = u - \frac{3g^2}{C}$

$$C_V \sim |T|^{-\alpha} : \quad \tilde{u} \rightarrow u \text{ as } |T| \rightarrow 0 \text{ for } \alpha > 0$$

non-conserved / conserved order parameter: model C / D relaxational kinetics

$$\frac{\partial S^\alpha}{\partial t} = -D(\vec{\nabla})^2 \frac{\delta H}{\delta S^\alpha} + \zeta^\alpha = -D(\vec{\nabla})^2 \left[\tau - \vec{\nabla}^2 + \frac{u}{6} \vec{S}^2 + \frac{g}{C} S \right] S^\alpha + \zeta^\alpha$$

$$\langle \zeta^\alpha \zeta^\beta \rangle = 2D k_B T (\vec{\nabla})^2 \delta(\vec{x} - \vec{x}') \delta(t - t') \delta^{\alpha\beta}$$

$$\frac{\partial g}{\partial t} = \lambda \vec{\nabla}^2 \frac{\delta H}{\delta g} + \eta = \frac{\lambda}{C} \vec{\nabla}^2 \left[g + \frac{g}{2} \vec{S}^2 \right] + \eta$$

$$\langle \eta \eta \rangle = -2\lambda k_B T \vec{\nabla}^2 \delta(\vec{x} - \vec{x}') \delta(t - t')$$

$g=0$: just heat diffusion $\omega(\tau, \vec{q}) = -i\kappa(\tau) \vec{q}^2$

with thermal conductivity $\kappa(\tau) = \frac{\lambda}{C(\tau)} \sim |\tau|^\alpha$

assume single diverging characteristic relaxation time scale $t_c(\tau)$:

"strong" dynamic scaling, $\omega_c(\tau, \vec{q}) \sim |\vec{q}|^z \hat{\omega}(|\vec{q}| \xi) \sim \vec{q}^2 |\tau|^\alpha$

requires

$$\sim (|\vec{q}| \xi)^{-\alpha/2} \rightarrow z = 2 + \frac{\alpha}{\nu}$$

holds indeed for scalar (Ising, $n=1$) model C:

$$z = 2 + \frac{\alpha}{\nu} = 2 + \frac{5}{3} + O(\epsilon^2)$$

model C ($a=0$) with $n \geq 2$: $\alpha < 0$

$\rightarrow$ order parameter S^α , energy density g decouple:

"weak" dynamic scaling: $z_S = 2 + c\eta$ (model A), $z_g = 2$

model D ($a=2$): $z_S = 4 - \eta$ (model B), $z_g = \begin{cases} 2 + \frac{\alpha}{\nu}, & n=1 \text{ (g slower)} \\ 2, & n \geq 2 \text{ (g much faster)} \end{cases}$

10 aside from irreversible relaxation terms, there can also be reversible dynamical couplings between order parameter components and/or other conserved modes
 microscopic dynamics: $\frac{\partial S^\alpha(t)}{\partial t} = \{H[S^\alpha], S^\alpha(t)\}$ Poisson brackets
 $\rightarrow \frac{i}{\hbar} [H[S^\alpha], S^\alpha(t)]$ commutator in quantum mechanics
 long-wavelength, large-time "hydrodynamic" limit:

slow modes $\{S^\alpha(\vec{x}, t)\}$ should represent complete basis for coarse-grained dynamics: $\{H[S^\alpha], S^\alpha(\vec{x})\} = \int d^d x' \sum_\beta \frac{\delta H[S^\alpha]}{\delta S^\beta(\vec{x}')} \{S^\beta(\vec{x}'), S^\alpha(\vec{x})\}$
 antisymmetric Poisson bracket: $Q^{\beta\alpha}(\vec{x}', \vec{x}) = -Q^{\alpha\beta}(\vec{x}, \vec{x}')$

$\rightarrow$ reversible mode couplings at $T=0$:

$$F_{\text{rev}}^\alpha[S^\alpha](\vec{x}) = - \int d^d x' \sum_\beta Q^{\alpha\beta}(\vec{x}, \vec{x}') \frac{\delta H[S^\alpha]}{\delta S^\beta(\vec{x}')}$$

Langevin equations: $\frac{\partial S^\alpha(\vec{x}, t)}{\partial t} = F_{\text{rev}}^\alpha[S^\alpha](\vec{x}, t) + F_{\text{rel}}^\alpha[S^\alpha](\vec{x}, t) + \zeta^\alpha(\vec{x}, t)$

with relaxation terms $F_{\text{rel}}^\alpha[S^\alpha](\vec{x}) = -D^\alpha (i\vec{\nabla})^{a_\alpha} \frac{\delta H[S^\alpha]}{\delta S^\alpha(\vec{x})}$, $a_\alpha = 0$ or 2

associated Fokker-Planck equation:

$$\frac{\partial P[S^\alpha](t)}{\partial t} + \int d^d x \sum_\alpha \frac{\delta}{\delta S^\alpha(\vec{x}, t)} = 0 \quad \text{divergence in space of dynamical variables}$$

probability current: $J[S^\alpha] = (F_{\text{rev}}^\alpha[S^\alpha] + F_{\text{rel}}^\alpha[S^\alpha])P[S^\alpha] - \frac{\lambda}{2} \frac{\delta P[S^\alpha]}{\delta S^\alpha}$

with noise correlator $\langle \zeta^\alpha \zeta^\beta \rangle = \lambda \delta(\vec{x} - \vec{x}') \delta(t - t') \delta^{\alpha\beta}$

$\rightarrow$ two conditions to reach equilibrium $P_{\text{st}}[S^\alpha] \sim e^{-H[S^\alpha]/k_B T}$ as $t \rightarrow \infty$:

- from relaxation: $\lambda = 2 k_B T D^\alpha (i\vec{\nabla})^{a_\alpha}$ Einstein relation

- reversible terms: divergence-free in dynamical space

$$\int d^d x \sum_\alpha \frac{\delta}{\delta S^\alpha(\vec{x})} (F_{\text{rev}}^\alpha[S^\alpha](\vec{x}) e^{-H[S^\alpha]/k_B T}) = 0$$

requires amendment for $T > 0$:

$$F_{\text{rev}}^\alpha[S^\alpha](\vec{x}) = - \int d^d x' \sum_\beta \left[Q^{\alpha\beta}(\vec{x}, \vec{x}') \frac{\delta H[S^\alpha]}{\delta S^\beta(\vec{x}')} - k_B T \frac{\delta Q^{\alpha\beta}(\vec{x}, \vec{x}')}{\delta S^\beta(\vec{x}')} \right]$$

11 example: isotropic ferromagnet, Heisenberg model $H = -\frac{1}{2} \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j - \vec{h} \cdot \sum_i \vec{S}_i$

spin $\vec{S}_i$, satisfies $[S_i^\alpha, S_j^\beta] = i\hbar \sum_\gamma \epsilon^{\alpha\beta\gamma} S_i^\gamma \delta_{ij}$

total magnetization $\vec{M} = \sum_i \vec{S}_i$ conserved:

$$\begin{aligned} [H, M^\alpha] &= -\frac{1}{2} \sum_{i,j,k} \sum_\beta J_{ij} (S_i^\beta [S_j^\beta, S_k^\alpha] + [S_i^\beta, S_k^\alpha] S_j^\beta) \\ &= \frac{i\hbar}{2} \sum_{i,j} J_{ij} \sum_{\beta,\gamma} \underbrace{\epsilon^{\alpha\beta\gamma}}_{\text{antisymmetric } \beta \leftrightarrow \gamma} (S_i^\beta S_j^\gamma + S_i^\gamma S_j^\beta) = 0 \end{aligned}$$

mesoscopic description: $S_i^\alpha \rightarrow S^\alpha(\vec{x})$ local magnetization density

$\frac{i}{\hbar} [\dots, \dots] \rightarrow \{\dots\}$ Poisson brackets, $H \rightarrow$ Ginzburg-Landau Hamiltonian, $n=3$

$$Q^{\alpha\beta}(\vec{x}, \vec{x}') = -g \sum_\gamma \epsilon^{\alpha\beta\gamma} S^\gamma(\vec{x}) \delta(\vec{x} - \vec{x}') \quad \text{coupling } g: \text{ from continuum limit}$$

$$\frac{\delta Q^{\alpha\beta}(\vec{x}, \vec{x}')}{\delta S^\beta(\vec{x}')} = -g \sum_\gamma \epsilon^{\alpha\beta\gamma} \delta^{\beta\gamma} \delta(\vec{x} - \vec{x}') = 0$$

$$\rightarrow F_{\text{rev}}^\alpha[S^\alpha](\vec{x}) = g \sum_{\beta\gamma} \epsilon^{\alpha\beta\gamma} S^\gamma(\vec{x}) \frac{\delta H[S^\alpha]}{\delta S^\beta(\vec{x})}$$

yields "model J ":

$$\frac{\partial \vec{S}(\vec{x}, t)}{\partial t} = -g \vec{S}(\vec{x}, t) \times \frac{\delta H[\vec{S}]}{\delta \vec{S}(\vec{x}, t)} + D \nabla^2 \frac{\delta H[\vec{S}]}{\delta \vec{S}(\vec{x}, t)} + \vec{S}(\vec{x}, t)$$

explicit: Spin precession in local field diffusive relaxation

$$\begin{aligned} \frac{\partial S^\alpha(\vec{x}, t)}{\partial t} &= g \sum_{\beta\gamma} \epsilon^{\alpha\beta\gamma} S^\beta(\vec{x}, t) [\vec{\nabla}^2 S^\gamma(\vec{x}, t) + h^\gamma(\vec{x}, t)] \\ &\quad + D \nabla^2 \left(\left[\tau - \vec{\nabla}^2 + \frac{u}{6} \vec{S}(\vec{x}, t)^2 \right] S^\alpha(\vec{x}, t) - h^\alpha(\vec{x}, t) \right) + S^\alpha(\vec{x}, t) \end{aligned}$$

$$\langle S^\alpha(\vec{x}, t) \rangle = 0, \quad \langle S^\alpha(\vec{x}, t) S^\beta(\vec{x}', t') \rangle = -2Dk_B T \vec{\nabla}_x^2 \delta(\vec{x} - \vec{x}') \delta(t - t') \delta^{\alpha\beta}$$

• paramagnetic phase ($T > 0$): linear model $J \hat{=} \text{linear model } B$

excitations: diffusive paramagnons, $\omega(\vec{q}) = -iD\vec{q}^2(\tau + \vec{q}^2)$

• critical scaling: $\left. \begin{aligned} g \vec{\nabla}^2 S^\alpha &\sim t^{-1} \sim |\vec{x}|^{-2} \\ &\sim |\vec{x}|^{-2+\eta} = \frac{d-2+\eta}{2} \end{aligned} \right\} \text{ compare: } z = \frac{d+2-\eta}{2}$

$d > 4$: $\eta = 0$, $z = \frac{d+2}{2}$ faster than mean-field model B $z=4$ for $d \leq 6$
 $\rightarrow$ dynamical upper critical dimension $d_c' = 6$

• ferromagnetic phase ($T < 0$): let $\langle S^3 \rangle = \phi = \sqrt{\frac{6|T|}{u}} > 0$

introduce fluctuating fields: $\pi^{1/2} = S^{1/2}$, $\sigma = S^3 - \phi$

→ linearized Langevin equations:

$$\frac{\partial \sigma(\vec{x}, t)}{\partial t} = D \vec{\nabla}^2 [2|T| - \vec{\nabla}^2] \sigma(\vec{x}, t) - h^3(\vec{x}, t) + \zeta^3(\vec{x}, t)$$

like model B for $T < T_c$, "Higgs" mode

$$\chi_o^L(\vec{q}, \omega) = \frac{1}{-\frac{i\omega}{Dq^2} + 2|T| + q^2}, \quad C_o^L(\vec{q}, \omega) = \frac{2Dk_B T q^2}{\omega^2 + [Dq^2(2|T| + q^2)]^2}$$

"massive", damped, (sub)diffusive

with non-linear fluctuations actually: $\chi_o^L(\vec{q}) \sim \frac{1}{|\vec{q}|^{4-d}}$ for $d < d_c = 4$
transverse "massless" Goldstone modes:

$$\frac{\partial \pi^\alpha(\vec{x}, t)}{\partial t} = -g\phi \sum_\beta \epsilon^{\alpha\beta\gamma} [\vec{\nabla}^2 \pi^\beta(\vec{x}, t) + h^\beta(\vec{x}, t)] - D \vec{\nabla}^2 [\vec{\nabla}^2 \pi^\alpha(\vec{x}, t) + h^\alpha(\vec{x}, t)] + \zeta^\alpha(\vec{x}, t)$$

diagonalize via circularly polarized spin wave modes: magnons

$$\pi^\pm(\vec{x}, t) = \frac{1}{\sqrt{2}} [\pi^1(\vec{x}, t) \pm i\pi^2(\vec{x}, t)], \quad \text{similarly } h^\pm, \zeta^\pm$$

$$\rightarrow \frac{\partial \pi^\pm(\vec{x}, t)}{\partial t} = (\pm ig\phi - D \vec{\nabla}^2) [\vec{\nabla}^2 \pi^\pm(\vec{x}, t) + h^\pm(\vec{x}, t)] + \zeta^\pm(\vec{x}, t)$$

$$\chi_o^\pm(\vec{q}, \omega) = \frac{\partial \langle \pi^\pm(\vec{q}, \omega) \rangle}{\partial h^\pm(\vec{q}, \omega)} \Big|_{\vec{h}=0} = \frac{\pm ig\phi + Dq^2}{-i(\omega \mp g\phi q^2) + Dq^4}$$

$$C_o^\pm(\vec{q}, \omega) = \frac{2k_B T D q^2}{(\omega \mp g\phi q^2)^2 + (Dq^4)^2}$$

→ propagating modes, quadratic dispersion $\omega_\pm(\vec{q}) = \pm g\phi q^2 - iDq^4$

dynamic scaling: $\text{Im} \omega_\pm(\vec{q}) \sim -|\vec{q}|^z$ as $T \rightarrow T_c$

with $\phi \sim |T|^\beta \sim |\zeta|^{-\beta/\gamma}$: $\text{Re} \omega_\pm(\vec{q}) \sim \phi |\vec{q}|^{2+\eta}$

same time scale if $z = 2 - \eta + \frac{\beta}{\gamma} = 2 - \eta + \frac{d-2+\eta}{2} = \frac{d+2-\eta}{2}$

even modes for itinerant ferromagnets (delocalized spins)

planar ferro-, isotropic antiferromagnet: order parameter non-conserved, $z = \frac{d}{2}$

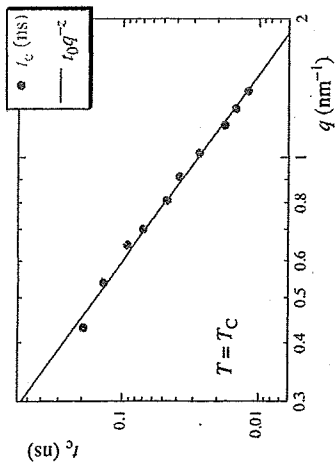


Fig. 3.7 Critical slowing-down of the characteristic relaxation time $t_c(q) = t_0 |q|^{-z}$ of the magnetic fluctuations in the three-dimensional Heisenberg ferromagnet CdCr_2S_4 . The solid line represents a power law fit with $z = 2.47 \pm 0.02$ and $t_0 = 0.02813 \text{ ns nm}^{-z}$. [Data and figure reproduced with permission from M. Alba, S. Pouget, P. Fouquet, B. Farago, and C. Pappas, Preprint arXiv:cond-mat/0703702 (2007).]

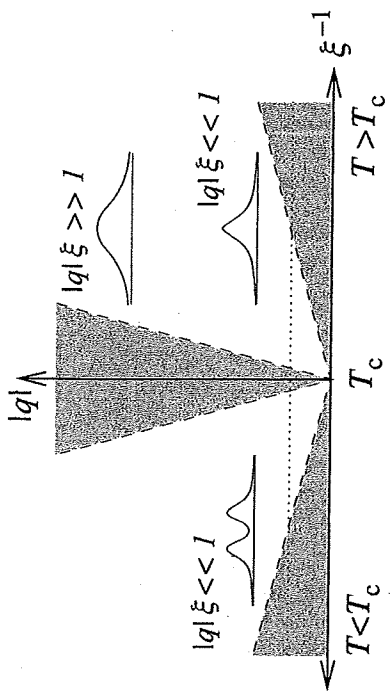


Fig. 3.8 Critical vs. hydrodynamic regions in the temperature-wavenumber plane. The (transverse) dynamic correlation function is sketched in both hydrodynamic regimes with $|q|\xi \ll 1$ (to the right for $T > T_c$, left for $T < T_c$); and in the critical region with $|q|\xi \gg 1$. The horizontal dotted line indicates a constant $|q|$ scan. [Figure adapted from Frey and Schwabl (1994).]

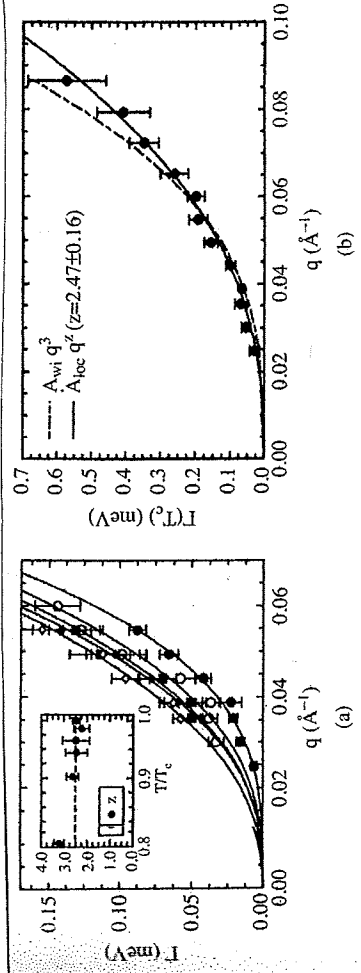


Fig. 6.8 Inelastic neutron scattering data showing dynamic scaling for the itinerant ferromagnet Ni_3Al . (a) Measured line widths for the spin wave peak at various temperatures; from top to bottom: $T/T_c = 0.98$ (open diamonds $\diamond$), 0.96 (filled diamonds), 0.94 (filled squares), 0.90 (open circles $\circ$), and 0.80 (filled circles $\bullet$); the data match power laws $\Gamma_x(q) \sim |q|^z$ with $z \approx 2.5$ (inset). (b) Quasielastic line width for the paramagnetic fluctuations at T_c ; the data fit yields $z = 2.47 \pm 0.16$ in good agreement with the prediction (6.76). [Data and figures reproduced with permission from: P. Semadeni, B. Rössli, P. Böni, P. Vorderwisch, and T. Chatterji, *Phys. Rev. B* 62, 1083–1088 (2000), DOI: 10.1103/PhysRevB.62.1083; copyright (2000) by the American Physical Society.]

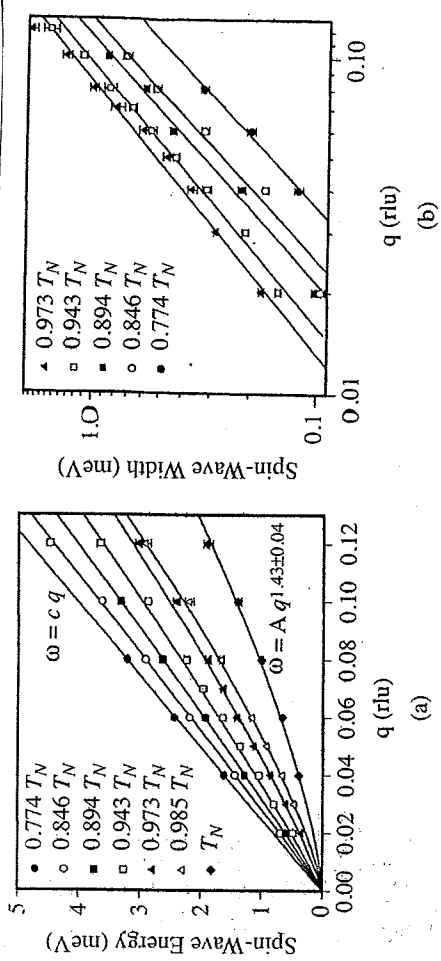


Fig. 6.14 (a) Spin wave dispersion in the Heisenberg antiferromagnet RbMnF_3 , obtained from neutron scattering data. (b) The Lorentzian halfwidth of the spin wave peaks as function of wavevector at different temperatures, yielding $\Gamma(q) \sim |q|^z$ with dynamic critical exponent $z = 1.41 \pm 0.05$. [Data and figures reproduced with permission from: R. Coldea, R. A. Cowley, T. G. Perring, D. F. McMorrow, and B. Rössli, *Phys. Rev. B* 57, 5281 (1998), DOI: 10.1103/PhysRevB.57.5281; copyright (1998) by the American Physical Society.]