Critical Dynamics

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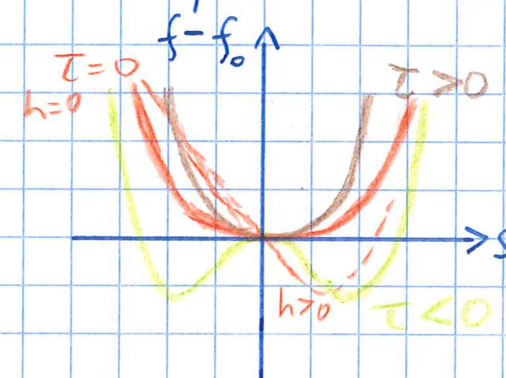
- originally refers to dynamic scaling for kinetics near critical points in thermal equilibrium
- also: generic scale invariance, prominent in dynamics far from equilibrium
- and: universal behavior at continuous non-equilibrium phase transitions

1. Near-equilibrium critical dynamics: relaxational kinetics

recall Landau's description of continuous (second-order) phase transition:



- (scalar) order parameter S
- expand free energy density $f(S)$

in powers of S: $\mathbb{Z}_2$ symmetry $S \leftrightarrow -S$

$$\rightarrow \quad f(S) = (f_0 +) \frac{\tau}{2} S^2 + \frac{u}{4!} S^4 + \ldots - h S$$

h: symmetry-breaking external field, conjugate to S

assume $u > 0$ $\rightarrow$ continuous phase transition at critical point

$$\tau = 0 \quad \rightarrow \quad \tau = \frac{T - T_c}{T_c} \; ; \; h = 0$$

dimensional analysis, power counting: $\langle S \rangle \sim \begin{cases} 0 & \tau > 0 \\ \sqrt{-\tau} & \tau < 0 \end{cases}$

$$\chi_\tau \sim \left.\frac{\partial \langle S \rangle}{\partial h}\right|_\tau \sim \frac{1}{|\tau|} \qquad \text{isothermal susceptibility, diverges at } T_c$$

$$\sim (\Delta S)^2 \qquad \rightarrow \text{ large fluctuations near } T_c$$

$$f \sim \begin{cases} f_0 & \tau > 0 \\ f_0 - \frac{a}{2}\tau^2 & \tau < 0 \end{cases} \quad \rightarrow \quad C_{h=0} \sim -\frac{\partial^2 f}{\partial \tau^2} \sim \begin{cases} 0 & T > T_c \\ a > 0 & T < T_c \end{cases}$$

specific heat, discontinuous at T_c

$T = T_c$: $\quad h \sim S^3 \quad$ critical isotherm

$\rightarrow$ mean-field critical exponents: $\alpha = 0$, $\beta = \frac{1}{2}$, $\gamma = 1$, $\delta = 3$

scaling form of free energy density: homogeneous function of τ, h

$$f_{\text{sing.}}(\tau,h) = |\tau|^{2-\alpha}\,\hat{f}_\pm\left(\frac{h}{|\tau|^{\beta\delta}}\right)$$, regular scaling functions $\hat{f}_\pm$ for $T \gtrless T_c$

$\rightarrow C_{h=0} \sim |\tau|^{-\alpha}$

equation of state: $\langle S(\tau,h\rangle = -\frac{\partial f_{\text{sing.}}}{\partial h} \sim |\tau|^{\beta}$, $\beta = 2-\alpha-\beta\delta$

at $\tau = 0$: $\sim h^{1/\delta}$ critical isotherm

susceptibility: $\chi_\tau \sim |\tau|^{-\gamma}$, $\gamma = \beta(\delta-1)$

scaling relations connect critical exponents, only two are independent

$\rightarrow$ thermodynamic scale invariance

incorporate spatial fluctuations: order parameter (vector) field $S^\alpha(\vec{x})$, $\alpha = 1,\dots,n$

assume $O(n)$ rotational symmetry: Ginzburg-Landau effective Hamiltonian

$$H[\vec{S}] = \int d^dx \left[\frac{\tau}{2}\,\vec{S}(\vec{x})^2 + (c)\frac{1}{2}\left[\vec{\nabla}\vec{S}(\vec{x})\right]^2 + \frac{u}{4!}\left(\vec{S}(\vec{x})^2\right)^2 - \vec{h}(\vec{x})\cdot\vec{S}(\vec{x})\right]$$

gradient term penalizes spatial inhomogeneities if $c > 0$ $(c \rightarrow 1)$

$\tau < 0$: spontaneously broken symmetry

$n = 1$: Ising model; $n = 2$: XY model or complex order parameter (superfluid)

$n = 3$: Heisenberg model; $n \rightarrow \infty$: spherical model

$n \rightarrow 0$: polymers, self-avoiding random walks

canonical equilibrium distribution: $P_{st}[S^\alpha] = \frac{1}{Z(T,h)}\, e^{-H[S^\alpha]/k_BT}$

expectation value of observable A: $\langle A \rangle = \int \mathcal{D}[S^\alpha]\, A[S^\alpha]\, P_{st}[S^\alpha]$

canonical partition function $(A=1)$: $Z(T,h) = \int \mathcal{D}[S^\alpha]\, e^{-H[S^\alpha]/k_BT}$

$\rightarrow$ functional integrals, over all possible configurations $\{S^\alpha(\vec{x})\}$

computation: discretize on lattice or Fourier transform

$$S(\vec{x}) = \frac{1}{V}\sum_{\vec{q}} S(\vec{q})\, e^{i\vec{q}\cdot\vec{x}} \rightarrow \mathcal{D}[S^\alpha] = \prod_\alpha \prod_{\vec{q},\, q_1>0} \frac{1}{V}\, d\,\mathrm{Re}\, S^\alpha(\vec{q})\, d\,\mathrm{Im}\, S^\alpha(\vec{q})$$

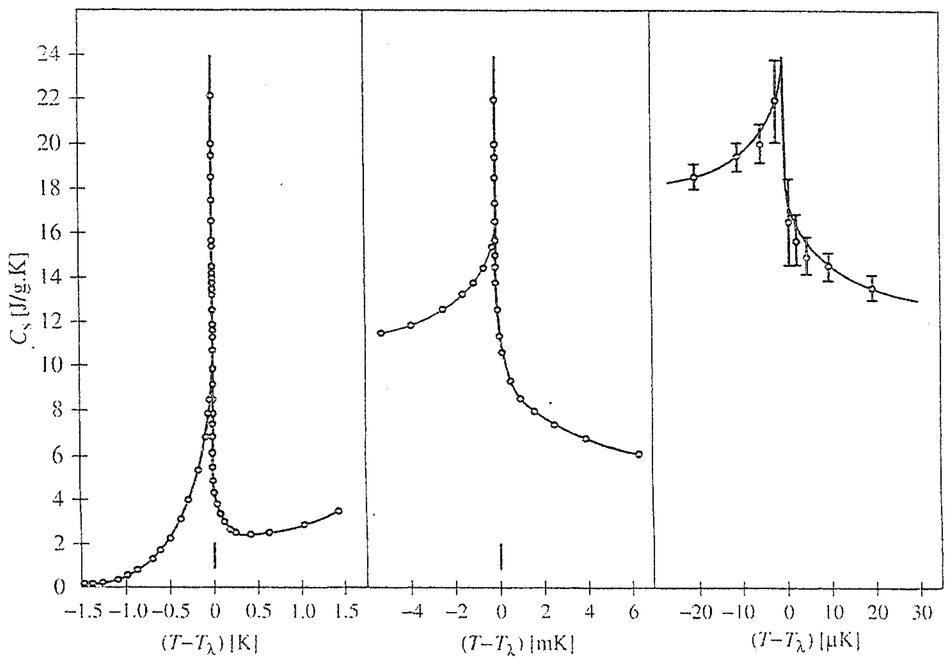


Fig. 1.6 Temperature dependence of the specific heat near the normal- to superfluid transition of helium 4, shown in successively reduced temperature scales. Close to the phase transition, the different graphs look remarkably alike. [Figure reproduced with permission from M. J. Buckingham and W. M. Fairbank, in: *Progress in Low Temperature Physics*, Vol. III, C. J. Gorter (ed.), 80–112, North-Holland (Amsterdam, 1961); copyright (1961) by Elsevier Ltd.]

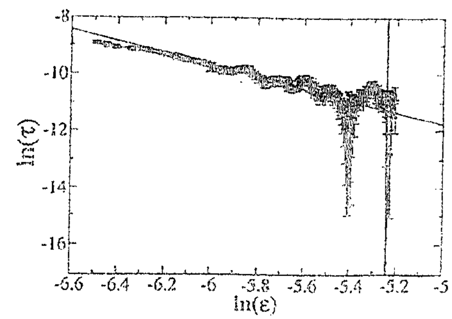


Fig. 3.1. Critical slowing-down of the relaxation time in the magnetization dynamics of a Fe bilayer grown on top of a W (110) substrate near its Curie temperature (T_c = 453.03 K). The experimental data for this two-dimensional Ising ferromagnet yield $z\nu$ = 2.09 ± 0.06. Data and figure reproduced with permission from: M.J. Dunlavy and D. Venus, Phys. Rev. B 71, 144406 (2005); DOI: 10.1103/PhysRevB.71.144406; copyright (2005) by the American Physical Society.

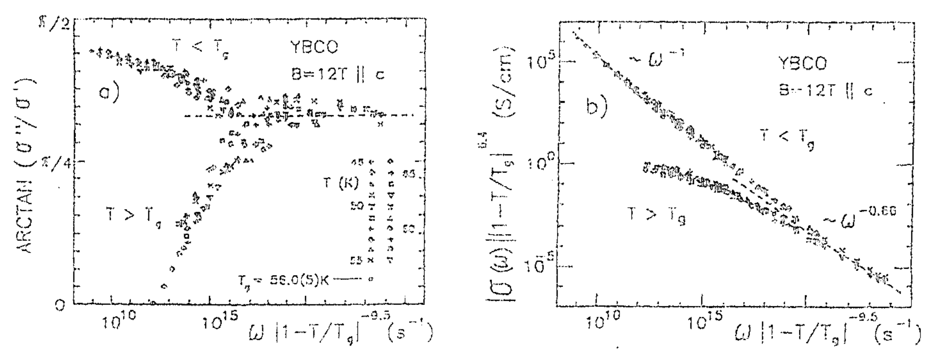


Fig. 3.2. (a) Phase and (b) scaled amplitude of the linear conductivity vs. rescaled frequency measured for the normal- to superconducting phase transition (occuring at $T_g \approx 56$ K) in an external magnetic field of B = 12 T in a twinned YBCO crystal. Data and figure reproduced with permission from: J. Kötzler, M. Kaufmann, G. Nakielski, R. Behr, and W. Assmus, Phys. Rev. Lett. 72, 2081 (1994); DOI: 10.1103/PhysRevLett.72.2081; copyright (1994) by the American Physical Society.

scaling ansatz for order parameter correlation function (d dimensions):

$$C(\tau,\vec{x}) = \langle S(\vec{x})S(0)\rangle - \langle S(\vec{x})\rangle\langle S(0)\rangle = \frac{1}{|\vec{x}|^{d-2+\eta}}\,\tilde{C}_\pm\left(\frac{|\vec{x}|}{\xi}\right)$$

with characteristic correlation length $\xi(\tau) \sim |\tau|^{-\nu}$

$\rightarrow$ large correlated clusters near T_c

$C(\tau, |\vec{x}|\to\infty) \to 0$ yields $\langle S\rangle^2 \sim |\tau|^{2\beta} \sim \xi^{-(d-2+\eta)} \rightarrow \beta = \frac{\nu}{2}(d-2+\eta)$

$f_{sing.} \sim |\tau|^{2-\alpha} \sim \xi^{-d} \rightarrow \alpha = 2 - d\nu$ hyperscaling relations ($d \leq d_c = 4$)

Fourier transform $C(\vec{q}) = \int d^dx\, e^{-i\vec{q}\cdot\vec{x}}\, C(\vec{x})$

$$\rightarrow C(\tau,\vec{q}) = k_B T\,\chi(\tau,\vec{q}) = \frac{1}{|\vec{q}|^{2-\eta}}\,\hat{C}_\pm(|\vec{q}|\xi)$$

thermodynamic susceptibility $\chi(\tau) = \chi(\tau,\vec{q}\to 0) \sim \xi^{2-\eta} \rightarrow \gamma = \nu(2-\eta)$

$\rightarrow$ diverging correlation length origin of thermodynamic singularities

systematic analysis of critical scaling laws: renormalization group

- compare effective coupling parameters at different length scales
- fixed points in ensuing RG flow describe scale-invariant regimes
- perform computations in safe UV region (small $\vec{x}$, large $\vec{q}$)

allows (non-)perturbative calculation of critical exponents

"small" expansion parameter: $\epsilon = d_c - d$

d_c: upper critical dimension; $d > d_c$: mean-field exponents $\eta = 0,\ \nu = \frac{1}{2}$

$O(n)$ Ginzburg-Landau model: $d_c = 4$

$$\frac{1}{\nu} = 2 - \frac{n+2}{n+8}\epsilon + O(\epsilon^2), \quad \eta = \frac{n+2}{2(n+8)^2}\epsilon^2 + O(\epsilon^3)$$

only depend on d, n: universal (short-range interactions)

spherical limit $n\to\infty$: $\nu = \frac{1}{2-\epsilon} = \frac{1}{d-2}$, $\eta = 0$, $d_{lc} = 2$ lower critical dimension dynamic scaling hypothesis:

- order parameter $\langle S(\tau,t)\rangle = |\tau|^\beta \, \hat{S}\left(\frac{t}{t_c(\tau)}\right)$

  characteristic relaxation time $t_c(\tau) \sim \xi(\tau)^z \sim |\tau|^{-z\nu}$

  diverges at T_c: critical slowing down, dynamic critical exponent z

  critical decay as $t \to \infty$ at T_c: $\langle S(0,t)\rangle \sim t^{-\frac{\beta}{z\nu}}$

  characteristic relaxation rate $\omega_c(\tau) \sim |\tau|^{z\nu}$

  generalize to dispersion relation $\omega_c(\tau,\vec{q}) = \underbrace{|\vec{q}|^z}_{\text{critical dispersion}} \hat{\omega}_\pm(|\vec{q}|\xi)$

- dynamic correlation function, static limit $t \to 0$:

  $$C(\tau,\vec{x},t) = \frac{1}{|\vec{x}|^{d-2+\eta}} \tilde{C}_\pm\left(\frac{|\vec{x}|}{\xi}, \frac{t}{t_c}\right) = \frac{1}{|\vec{x}|^{d-2+\eta}} \tilde{C}_\pm\left(\frac{|\vec{x}|}{\xi}, \frac{t}{\xi^z}\right)$$

  $$C(\tau,\vec{q},\omega) = \int d^dx \int dt \; e^{-i(\vec{q}\cdot\vec{x}-\omega t)} \, C(\tau,\vec{x},t) = \frac{1}{|\vec{q}|^{z+2-\eta}} \hat{C}_\pm(|\vec{q}|\xi, \omega\xi^z)$$

→ "time-temperature superposition", akin to anisotropic scaling governed by z

- dynamic response function, static limit $\omega \to 0$:

  $$\chi(\tau,\vec{q},\omega) = \frac{1}{|\vec{q}|^{2-\eta}} \hat{\chi}_\pm\left(|\vec{q}|\xi, \frac{\omega}{\omega_c}\right)$$

  thermal equilibrium, linear response: fluctuation-dissipation theorem (FDT)

  $$\chi(\vec{x},t) = -\frac{\Theta(t)}{k_BT} \frac{\partial C(\vec{x},t)}{\partial t} \qquad \text{(note causality)}$$

  $$C(\vec{q},\omega) = \frac{2k_BT}{\omega} \operatorname{Im} \chi(\vec{q},\omega) \qquad \text{(all consistent of course)}$$

continuum description of critical dynamics:

exploit time scale separation afforded by critical slowing down

→ effective coarse-grained Langevin-type description

- slow, relevant modes: order parameter, hydrodynamic modes (conserved fields)
- fast, irrelevant degrees of freedom: everything else → white "noise"

- simplest scenario: purely relaxational kinetics, non-conserved order parameter

$$\frac{\partial S^\alpha(\vec{x},t)}{\partial t} = -D \frac{\delta H[S^\alpha]}{\delta S^\alpha(\vec{x},t)} + \zeta^\alpha(\vec{x},t) \qquad \text{relaxation constant } D$$

$$= -D\left[\tau - \vec{\nabla}^2 + \frac{u}{6}\vec{S}(\vec{x},t)^2\right] S^\alpha(\vec{x},t) + D h^\alpha(\vec{x},t) + \zeta^\alpha(\vec{x},t)$$

stochastic forcing / noise: $\langle \zeta^\alpha(\vec{x},t)\rangle = 0$

Einstein relation: $\langle \zeta^\alpha(\vec{x},t)\zeta^\beta(\vec{x}',t')\rangle = 2Dk_BT\,\delta(\vec{x}-\vec{x}')\delta(t-t')\delta^{\alpha\beta}$

via associated Fokker-Planck equation: ensures relaxation to thermal equilibrium $P_{st}[S^\alpha]$

$\rightarrow$ time-dependent noisy Ginzburg-Landau equation, "model A"

- conserved fields satisfy continuity equation $\frac{\partial \rho(\vec{x},t)}{\partial t} + \vec{\nabla}\cdot\vec{j}(\vec{x},t) = 0$

Fourier transform: $-i\omega\,\rho(\vec{q},\omega) + i\vec{q}\cdot\vec{j}(\vec{q},\omega) = 0$, , $\frac{\partial \rho(\vec{q}=0,t)}{\partial t} = 0$

typically: $\vec{j}(\vec{x},t) = -D\vec{\nabla}\rho(\vec{x},t)$ $\rightarrow$ diffusive dispersion $\omega(\vec{q}) = -iD\vec{q}^2$

conserved order parameter: $\frac{\partial S^\alpha(\vec{x},t)}{\partial t} = -\vec{\nabla}\cdot\vec{J}^\alpha(\vec{x},t)$

current density $\vec{J}^\alpha(\vec{x},t) = -D\vec{\nabla}\frac{\delta H[S^\alpha]}{\delta S^\alpha(\vec{x},t)} + \vec{\eta}^\alpha(\vec{x},t)$

$$\rightarrow \frac{\partial S^\alpha(\vec{x},t)}{\partial t} = D\vec{\nabla}^2\frac{\delta H[S^\alpha]}{\delta S^\alpha(\vec{x},t)} + \zeta^\alpha(\vec{x},t), \quad \zeta^\alpha(\vec{x},t) = -\vec{\nabla}\cdot\vec{\eta}^\alpha(\vec{x},t)$$

$\langle \zeta^\alpha(\vec{x},t)\rangle = 0$, $\langle \zeta^\alpha(\vec{x},t)\zeta^\beta(\vec{x}',t')\rangle = -2Dk_BT\,\vec{\nabla}_x^2\,\delta(\vec{x}-\vec{x}')\delta(t-t')\delta^{\alpha\beta}$

$\rightarrow$ noisy Cahn-Hilliard equation, "model B"

combine models A/B: $D \rightarrow D(i\vec{\nabla})^a$, $a = 0, 2$ respectively

linearize for $T > T_c$ ($\tau > 0$): Gaussian approximation

Fourier transform: $\left[-i\omega + Dq^a(\tau + q^2)\right] S^\alpha(\vec{q},\omega) = Dq^a h^\alpha(\vec{q},\omega) + \zeta^\alpha(\vec{q},\omega)$

with $\langle \zeta^\alpha(\vec{q},\omega)\rangle = 0$, $\langle \zeta^\alpha(\vec{q},\omega)\zeta^\beta(\vec{q}',\omega')\rangle = 2Dk_BT\,q^a(2\pi)^{d+1}\delta(\vec{q}+\vec{q}')\delta(\omega+\omega')\delta^{\alpha\beta}$

→ dynamic response function for Gaussian relaxational models:

$$\chi_0(\tau,\vec{q},\omega)\,\delta^{\alpha\beta} = \frac{\partial\langle S^\alpha(\vec{q},\omega)\rangle_e}{\partial h^\beta(\vec{q},\omega)}\bigg|_{\vec{h}=0} = \frac{Dq^a}{-i\omega + Dq^a(\tau+q^2)}\,\delta^{\alpha\beta}$$

assumes scaling form: $\chi_0(\tau,\vec{q},\omega) = \frac{1}{q^2}\,\frac{1}{\frac{\tau}{q^2}+1-\frac{i\omega}{Dq^{2+a}}}$

note: $\xi(\tau) \sim \tau^{-1/2}$

$$\rightarrow \eta = 0,\; \nu = \frac{1}{2},\quad z = 2+a = \begin{cases} 2 & \text{model A} \\ 4 & \text{model B} \end{cases}$$

$$\chi_0(\tau,\vec{q},t) = Dq^a\, e^{-Dq^a(\tau+q^2)t}\,\Theta(t)$$

→ relaxation time $t_c(\tau,\vec{q}) = \frac{1}{Dq^a(\tau+q^2)}$

model A: $T>T_c$: $t_c = \frac{1}{D\tau}$, $T=T_c$: $t_c(T_c) = \frac{1}{Dq^2}$ diffusive

model B: $T>T_c$: $t_c = \frac{1}{D\tau q^2}$, $T=T_c$: $t_c(T_c) = \frac{1}{Dq^4}$ subdiffusive

dynamic correlation function ($\vec{h}=0$):

$$\langle S^\alpha(\vec{q},\omega)\,S^\beta(\vec{q}',\omega')\rangle_0 = C_0(\tau,\vec{q},\omega)\,(2\pi)^{d+1}\,\delta(\vec{q}+\vec{q}')\,\delta(\omega+\omega')\,\delta^{\alpha\beta}$$

$$C_0(\tau,\vec{q},\omega) = \frac{2Dk_BT\,q^a}{\omega^2+[Dq^a(\tau+q^2)]^2} = \frac{2k_BT}{Dq^{4+a}}\,\frac{1}{\left[\left(\frac{\tau}{q^2}+1\right)^2+\left(\frac{\omega}{Dq^{2+a}}\right)^2\right]}$$

$$C_0(\tau,\vec{q},t) = \underbrace{\frac{k_BT}{\tau+q^2}}_{\text{static Ornstein-Zernicke correlation function}}\, e^{-Dq^a(\tau+q^2)|t|}$$

if relaxation rate does not acquire renormalization: prefactor $q^2 \to q^{2-\eta}$

→ suggests $z = 2+a-\eta$, $\eta>0$: fluctuations slow down kinetics

correct in fact for model B: $z = 4-\eta$ scaling relation

not valid for model A: $z = 2+c\eta$, faster critical relaxation

perturbative dimensional expansion: $c = 6\ln\frac{4}{3} - 1 + \mathcal{O}(\epsilon)$