Thermodynamics and transport near a quantum critical point

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Outline

- Introduction : (continuous) quantum phase transitions

- Thermodynamics near a QCP

- Conductivity near a QCP

T=0 quantum phase transitions – examples

- Transverse field Ising model $\hat{H} = -J \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - h \sum_i \hat{\sigma}_i^x$

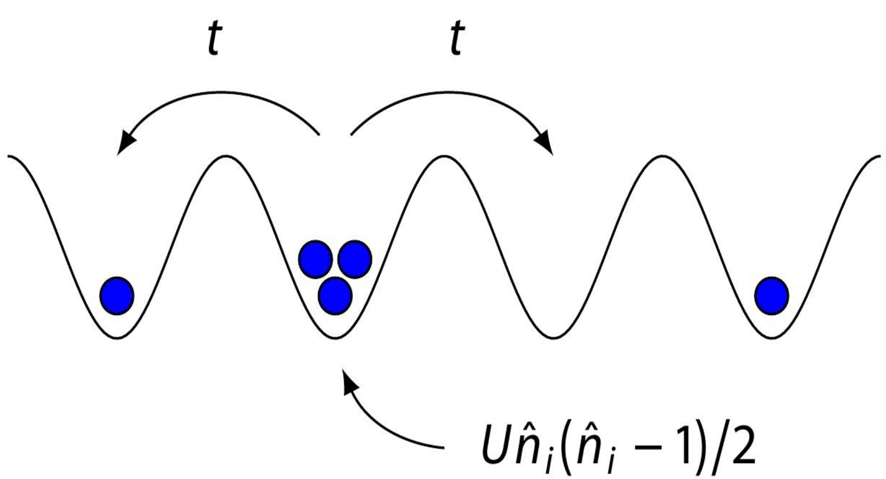
J/h

paramagnetic ground state
all spins aligned with h

$(J/h)_c$

ferromagnetic ground state
all spins parallel to z axis

- Interacting bosons (integer filling)



t/U

insulating phase
(localized bosons)

$(t/U)_c$

superfluid phase
(condensate)

2D quantum O(N) model

(bosons in optical lattices, quantum AFs, etc.)

$$S = \int_0^{\beta\hbar} d\tau \int d^2r \, \frac{1}{2}(\nabla\boldsymbol{\varphi})^2 + \frac{1}{2c^2}(\partial_\tau\boldsymbol{\varphi})^2 + \frac{r_0}{2}\boldsymbol{\varphi}^2 + \frac{u_0}{4!}(\boldsymbol{\varphi}^2)^2$$

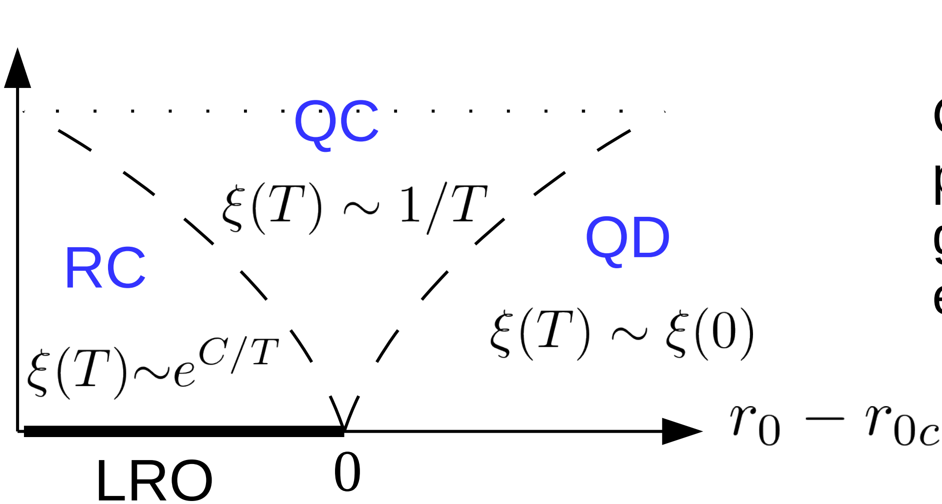
Lorentz-invariant action for a N-component real field with temperature-independent couplings

- T=0 : classical 3-dimensional O(N) model

  QPT for $r_0=r_{0c}$; 3D Wilson-Fisher fixed point

- T>0 : energy scales: T and T=0 gap Δ, crossover lines: $T \sim \Delta \sim |r_0 - r_{0c}|^\nu$

(2D, N>2)



Quantum Critical (QC) regime : physics determined by critical ground state and its thermal excitations

Method: nonperturbative functional RG

$$\partial_k \Gamma_k[\phi] = \frac{1}{2}\mathrm{Tr}\left\{\partial_k R_k\left(\Gamma_k^{(2)}[\phi] + R_k\right)^{-1}\right\}$$ [Wetterich'93]

- Derivative expansion

$$\Gamma_k[\phi] = \int_{x=(\mathbf{r},\tau)} \left\{ \frac{Z_k(\rho)}{2}(\nabla\phi)^2 + \frac{Y_k(\rho)}{4}(\nabla\rho)^2 + U_k(\rho) \right\}, \quad \rho = \frac{\phi^2}{2}$$

- Blaizot—Méndez-Galain—Weschbor approximation [Blaizot et al, 2006]

$$\partial_k \Gamma_k^{(2)}[\mathbf{p},\phi] = f\left(\Gamma_k^{(3)}, \Gamma_k^{(4)}\right) \simeq f\left(\frac{\partial \Gamma_k^{(2)}}{\partial\phi}, \frac{\partial^2 \Gamma_k^{(2)}}{\partial\phi\partial\phi}\right)$$

- LPA'' [Hasselmann'12; Ledowski, Hasselmann, Kopietz'04]

$$\Gamma_k[\phi] = \int_x \left\{ \frac{1}{2}\partial_\mu\phi \cdot Z_k(-\partial^2)\partial_\mu\phi + \frac{1}{4}\partial_\mu\rho\, Y_k(-\partial^2)\partial_\mu\rho + U_k(\rho) \right\}$$

What do we want do understand/calculate ?

T=0 and *T*>0 universal properties near the QCP

- thermodynamics : $$P(T) = P(0) + \frac{(k_B T)^3}{(\hbar c)^2} \mathcal{F}_N \left(\frac{\Delta}{k_B T} \right)$$

- time-dependent correlation functions (real time) $$\chi^R(\omega) \sim \Delta^{-x} \Phi_N \left(\frac{\hbar\omega}{k_B T}, \frac{\Delta}{k_B T} \right)$$

- conductivity $$\sigma(\omega, T) = \sigma_q \Sigma_N \left(\frac{\hbar\omega}{k_B T}, \frac{\Delta}{k_B T} \right), \quad \sigma_q = \frac{q^2}{h}$$

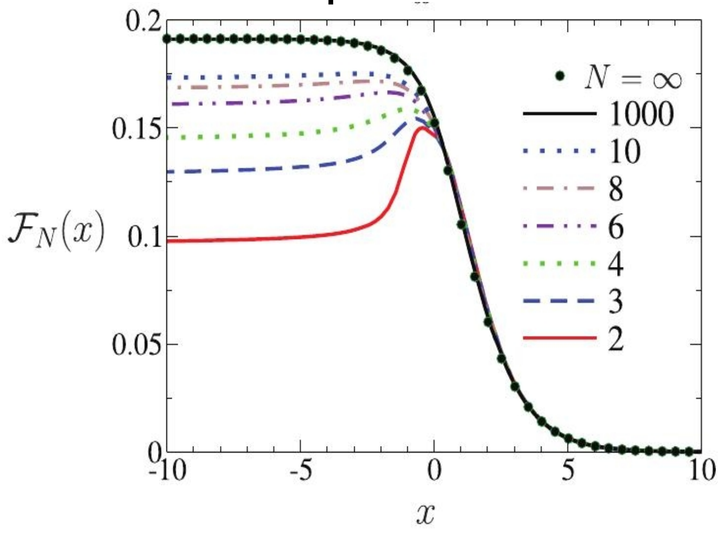
Benchmark test: thermodynamics

$$P(T) = P(0) + \frac{(k_B T)^3}{(\hbar c)^2} \mathcal{F}_N \left(\frac{\Delta}{k_B T} \right)$$

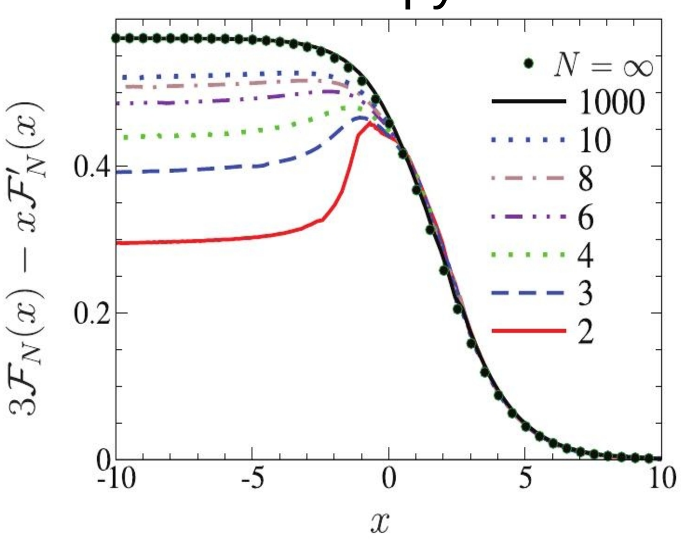
$$\epsilon(T) = \epsilon(0) - \frac{(k_B T)^3}{(\hbar c)^2} \vartheta_N \left(\frac{\Delta}{k_B T} \right)$$

Δ characteristic *T=0* energy scale

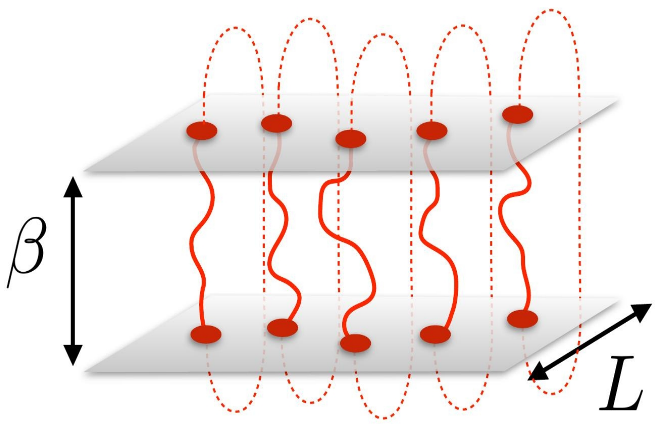
pressure

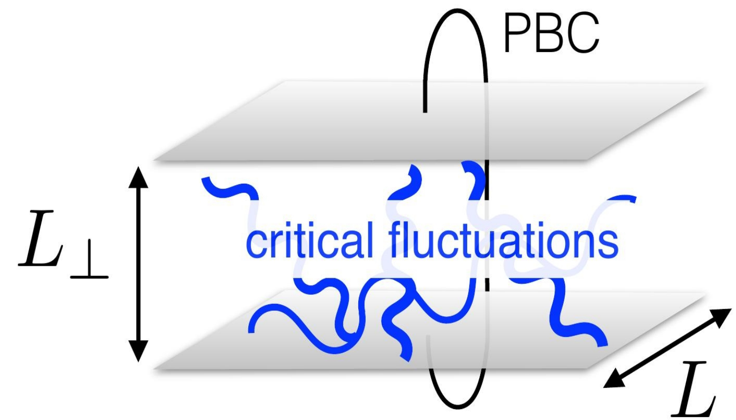


entropy



Rançon, Kodio, ND, Lecheminant, PRE'13



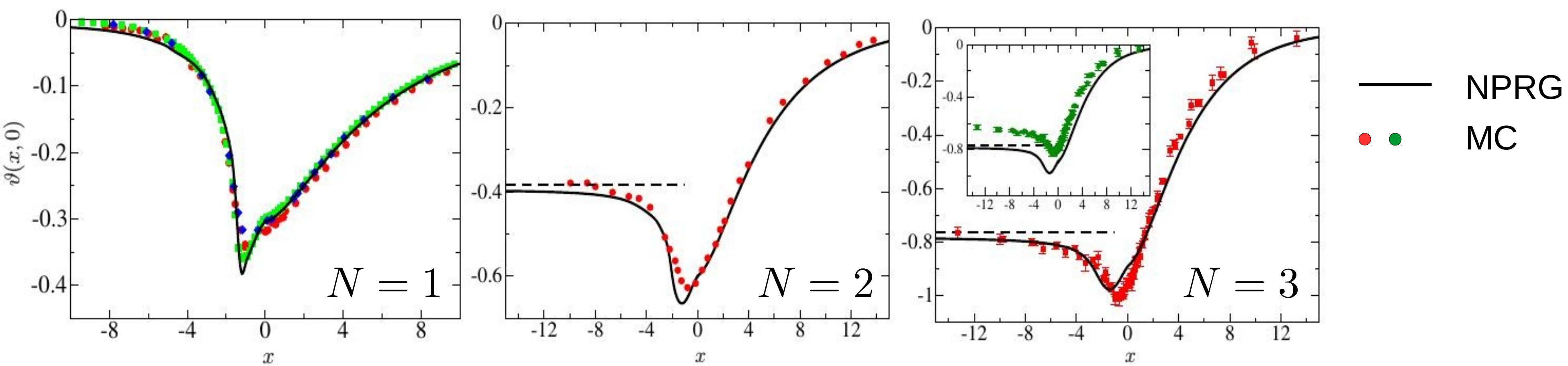


2D quantum system
at finite temperature
(equation of state)

quantum-classical mapping

$$L_\perp \sim \hbar\beta = \frac{\hbar}{k_B T}$$

3D classical system in
finite geometry with periodic
boundary conditions
(Casimir effect)



A. Rançon, L.-P. Henry, F. Rose, D. Lopes Cardozo, ND, P. Holdsworth, and T. Roscilde, PRB'16

Correlation functions

- Examples
  - o.p. susceptibility: $G_i(\mathbf{r},\tau) = \langle \varphi_i(\mathbf{r}\tau)\varphi_i(00)\rangle$
  - Scalar (Higgs) susceptibility: $\chi_s(\mathbf{r},\tau) = \langle \varphi^2(\mathbf{r}\tau)\varphi^2(00)\rangle$
  - Conductivity : $\chi^{ab}_{\mu\nu} = \langle j^a_\mu(\mathbf{r}\tau) j^b_\nu(00)\rangle$

- Difficulties
  - Strongly interacting theory (QCP)
  - Frequency/momentum dependence
  - 2- and 4-point functions
  - Analytical continuation $\chi^R(\omega) = \chi(i\omega_n \rightarrow i\omega + i0^+)$

Conductivity of the O(N) model

- O(N) symmetry → conservation of angular momentum $\partial_t L^a + \nabla \cdot \mathbf{j}^a = 0$
- we make the O(N) symmetry local by adding a gauge field

$$S = \int_x \frac{1}{2}[(\partial_\mu - A_\mu)\varphi]^2 + \frac{r_0}{2}\varphi^2 + \frac{u_0}{4!}(\varphi^2)^2$$

$$A_\mu = A_\mu^a T^a \in \mathrm{so}(N), \qquad T^a : \quad N(N-1)/2 \quad \text{generators of SO(N)}$$

- current density $\quad J_\mu^a = -\frac{\delta S}{\delta A_\mu^a} = j_\mu^a - A_\mu \varphi \cdot T^a \varphi, \qquad j_\mu^a = \partial_\mu \varphi \cdot T^a \varphi$

N=2 (bosons) $\quad j_\mu = -i(\psi^* \partial_\mu \psi - \mathrm{c.c.}), \quad \psi = \varphi_1 + i\varphi_2$

- linear response theory

$$K_{\mu\nu}^{ab}(x, x') = \langle j_\mu^a(x) j_\nu^b(x') \rangle - \delta_{\mu\nu}\delta(x - x')\langle T^a\varphi \cdot T^b \varphi \rangle = \frac{\delta^2 \ln Z[A]}{\delta A_\mu^a(x) \delta A_\nu^b(x')}$$

$$\sigma_{\mu\nu}^{ab}(\omega) = \frac{1}{i(\omega + i0^+)} K_{\mu\nu}^{ab}(p \to -i\omega + 0^+)$$ conductivity tensor

The conductivity tensor

- is diagonal: $\sigma^{ab}_{\mu\nu} = \delta_{\mu\nu}\delta_{ab}\sigma^{aa}$
- has two independent components:

$$\sigma^{aa}(\omega) = \begin{cases} \sigma_A(\omega) & \text{if} \quad T^a\boldsymbol{\phi} \neq 0 \\ \sigma_B(\omega) & \text{if} \quad T^a\boldsymbol{\phi} = 0 \end{cases}$$

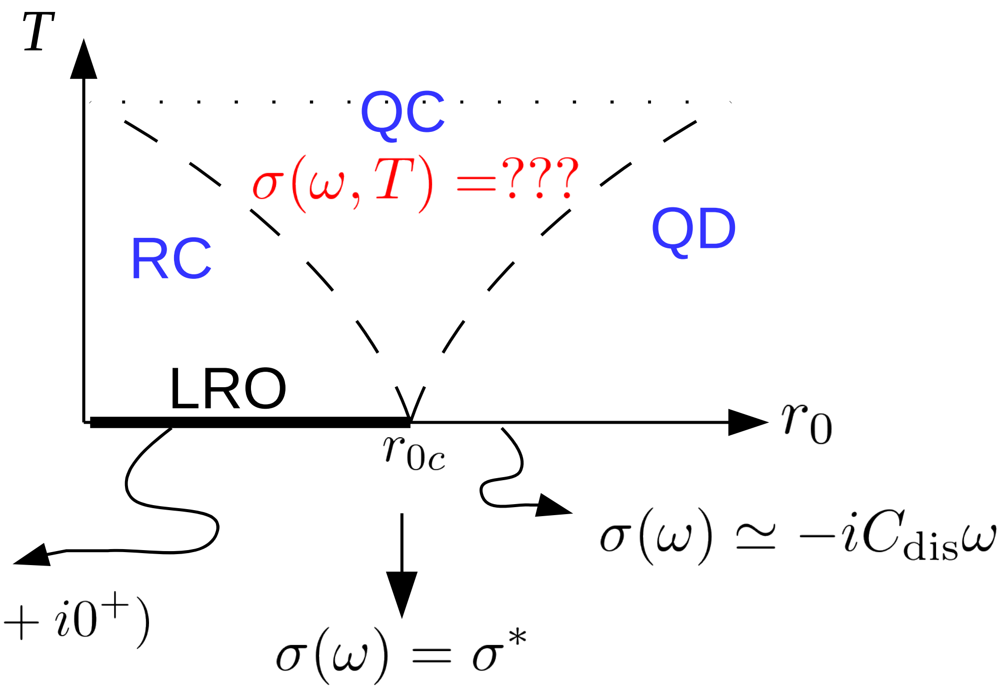
- in the disordered phase and at the QCP: $\sigma_A(\omega) = \sigma_B(\omega) = \sigma(\omega)$

For *N*=2, there is only one so(*N*) generator and the conductivity in the ordered phase reduces to σ_A

Universal properties

$$\sigma_{A,B}(\omega, T) = \sigma_q \Sigma_{A,B}\left(\frac{\hbar\omega}{k_B T}, \frac{\Delta}{k_B T}\right)$$

Low-frequency behavior:



$\sigma_A(\omega) \simeq i/L_{\rm ord}(\omega + i0^+)$

$\sigma_B(\omega) = ???$

(not much investigated as exists for *N*≥3)

σ^*/σ_q and $C_{\rm dis}/L_{\rm ord}\sigma_q^2$ are universal

[Fisher et al., PRL'89]

Long-term objective: determine the conductivity in the QC regime

(no quasi-particles → Boltzmann-like description not possible)

- Objective: determine the universal scaling form of the conductivity
  Technically: compute 4-point correlation function $\langle j_\mu^a j_\nu^b \rangle$

- Previous approaches
  - QMC (Sorensen, Chen, Prokof'ev, Pollet, Gazit, Podolsky, Auerbach)
  - CFT (Poland, Sachdev, Simmons-Duffin, Witzack-Krempa)
  - Holography (Myers, Sachdev, Witzack-Krempa)
  - NPRG – DE (F. Rose & ND, PRB'2017)

NPRG – LPA´´

- Gauge-invariant effective action

$$\Gamma_k[\boldsymbol{\phi}, A] = \int_x \Big\{ \frac{1}{2}\partial_\mu \boldsymbol{\phi} \cdot Z_k(-D^2)\partial_\mu \boldsymbol{\phi} + \frac{1}{4}\partial_\mu \rho\, Y_k(-D^2)\partial_\mu \rho + U_k(\rho) + \frac{1}{4}F^a_{\mu\nu} X_{1,k}(-D^2) F^a_{\mu\nu} + \frac{1}{4} F^a_{\mu\nu} T^a \boldsymbol{\phi} \cdot X_{2,k}(-D^2) F^b_{\mu\nu} T^b \boldsymbol{\phi} \Big\}$$

$$\text{where } D_\mu = \partial_\mu - A_\mu, \quad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu - [A_\mu, A_\nu]$$

- Gauge-invariant regulator

$$\Delta S_k = \tfrac{1}{2} \int_{x,x'} \boldsymbol{\varphi}(x) \cdot R_k\big(-D^2\big) \boldsymbol{\varphi}(x')$$

[Morris'00, Codello, Percacci et al.'16, Bartosh'13]

- Conductivity

$$K^{ab}_{\mu\nu} = -\Gamma^{(0,2)ab}_{\mu\nu} + \Gamma^{(1,1)a}_{\mu} \big(\Gamma^{(2,0)}\big)^{-1} \Gamma^{(1,1)b}_{\nu} \text{ with } \Gamma^{(n,m)} = \frac{\delta^{m+n}\Gamma}{\delta\boldsymbol{\phi}^n \delta A^m}$$

(Preliminary) results

- Universal conductivity at QCP (*N*=2) $\sigma^*/\sigma_q \simeq 0.32$

  QMC: 0.355-0.361

  bootstrap: 0.3554(6) [Kos et al., JHEP'15]

- Universal ratio

N	2	3	4	1000	∞ (exact)
$C/NL\sigma_q^2 \quad (\sigma_q = q^2/h)$	0.105	0.0742	0.0598	0.0416	0.04167

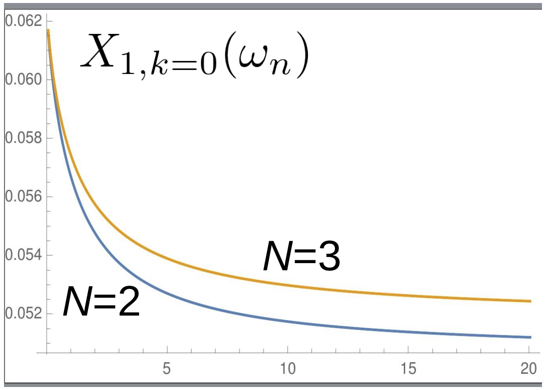
N=2: good agreement (~5%) with MC [Gazit et al.'14]

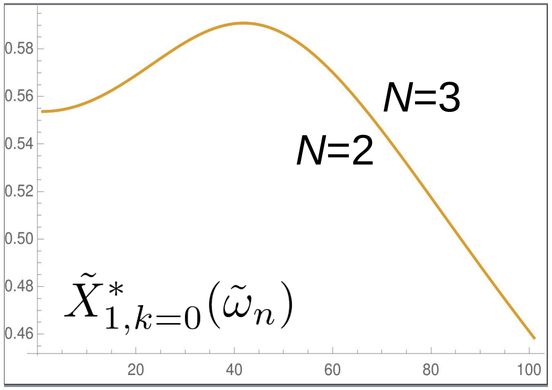
- Ordered phase

$$\sigma_A(\omega) = i/L_{\rm ord}(\omega + i0^+), \quad \sigma_B(\omega) = \frac{\pi}{8}\sigma_q \text{ is superuniversal}$$

$\sigma_B(\omega)$ *N* independent

$$\sigma_B(\omega)|_{N\to\infty} = \frac{\pi}{8}\sigma_q$$





- Frequency-dependence of the conductivity: $\sigma(\omega) = \sigma(i\omega_n \to \omega + i0^+)$
  - *T*=0: Padé approximant (work in progress)
  - *T*>0: analytical continuation from numerical data difficult when $\omega < T$
    - Strodthoff et al.: simplified RG schemes where sums over Matsubara frequencies (and analytical continuation) can be performed analytically
    - Pawlowski-Strodthoff, PRD'15

Conclusion

- Non-perturbative functional RG is a powerful tool to study QCP's.
- Finite-temperature thermodynamic near a QCP is fully understood
  - Universal scaling function compares well with MC simulations of classical 3D systems in finite geometry.
  - Pressure, entropy, specific heat are non-monotonous across the QCP; hence a clear thermodynamic signature of quantum criticality.
- Promising results for dynamic correlation functions (e.g. conductivity) but finite-temperature calculation still very challenging.
  - LPA'' appears as the best approximation scheme to compute $\sigma(\omega)$.
  - Low-frequency T=0 conductivity well understood. $\sigma_B(\omega)$ is found to be superuniversal.
  - How to perform analytic continuation at finite temperature?