

Dynamics and transport in the vicinity of a quantum phase transition

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Introduction and outline

Some physical systems display a zero-temperature **quantum phase transition** when an external parameter is tuned

→ interesting playground for condensed matter theory: exotic scaling laws, models without quasiparticles...

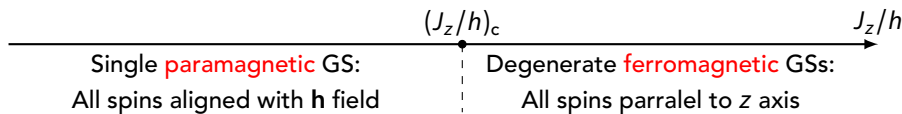
Our goal: study the **universal** properties of the quantum $O(N)$ model in the vicinity of its quantum critical point.

Outline:

- Introduction: QPTs and the quantum $O(N)$ model.
- Motivation for a (nonperturbative) functional renormalization group approach.
- Thermodynamics of the model.
- The “**Higgs**” amplitude mode.
- Universal scaling function of the **conductivity**.

Quantum phase transitions — examples

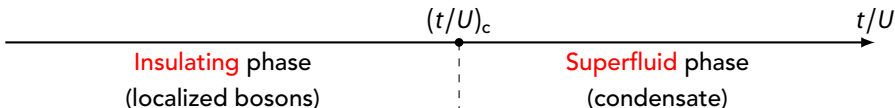
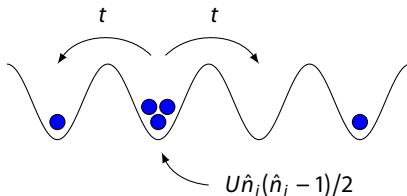
Transverse field Ising model: $\hat{H} = -J_z \sum_{\langle ij \rangle} \hat{s}_i^z \hat{s}_j^z - h \sum_i \hat{s}_i^x$



Interacting lattice bosons (integer filling):

t : hopping

U : on-site interaction energy



Describing QPTs

We restrict ourselves to **second order QPTs** for which at the transition:

- the gap Δ closes;
- the correlation length ξ diverges.

We are interested in the low-energy, long distance physics \rightarrow (effective) field theories.

The **path integral formalism** allows to rewrite the partition function.

Second quantization

$\hat{H}, \hat{\psi}(\mathbf{r})^\dagger, \hat{\psi}(\mathbf{r})$ operators

$$Z = \text{Tr} e^{-\beta \hat{H}}$$

Path integral formulation

$\psi(\mathbf{r}, \tau)$ complex fields

$$Z = \int D[\psi^*, \psi] e^{-S[\psi^*, \psi]}$$

Statistical field theory and QPT

$$\hat{H}[\hat{\psi}^\dagger, \hat{\psi}] \rightarrow S[\psi^*, \psi] = \int_0^\beta d\tau \left\{ H[\psi^*, \psi] + \int d^d \mathbf{r} \psi^* \partial_\tau \psi \right\}.$$

Periodic BCs: $\psi(\mathbf{r}, \tau + \beta) = \psi(\mathbf{r}, \tau)$.

- Transforms the d -dimensional quantum problem into a $d + 1$ **classical** field theory...
- ... at the cost of a new imaginary **time** dimension $\tau \in [0, \beta]$.
- A QPT manifests as a phase transition in the classical field theory.

→ QPTs show all features of classical critical phenomenons: universality classes, scaling,...

E.g. for a $2d$ theory pressure and conductivity scale like

$$P(T) = P(T = 0) + T^{2+z} F\left(\frac{T}{\Delta}\right), \quad \sigma(\omega) = \frac{q^2}{h} \Sigma\left(\frac{\omega}{\Delta}, \frac{T}{\Delta}\right)$$

with $F(x), \Sigma(x, y)$ **universal scaling functions**.

Quantum $O(N)$ model

Lorentz-invariant action, where $\boldsymbol{\varphi}$ is a real N -component field ($\sim \varphi^4$ model)

$$S[\boldsymbol{\varphi}] = \int_0^\beta d\tau \int d^d \mathbf{r} \left\{ \frac{1}{2} (\nabla \boldsymbol{\varphi})^2 + \frac{1}{2c^2} (\partial_\tau \boldsymbol{\varphi})^2 + r_0 \boldsymbol{\varphi}^2 + u_0 (\boldsymbol{\varphi}^2)^2 \right\}$$

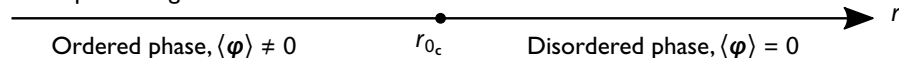
- The couplings are **temperature-independent**
- **Effective action** that describes several condensed matter phase transitions:
Bose–Hubbard model ($N = 2$), Quantum antiferromagnets ($N = 3$).

At zero T the model is strictly equivalent to the $d + 1$ classical $O(N)$ model.

Below a critical value of r_0 , $\langle \boldsymbol{\varphi} \rangle \neq 0$

→ the $O(N)$ symmetry is **spontaneously broken**.

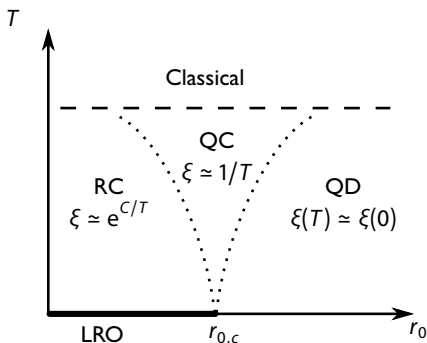
$T = 0$ phase diagram:



Qualitative $T > 0$ phase diagram

At finite T the QPT is destroyed (critical energy scales $\ll T$).

However there are **crossovers** between different regimes:



Typical ($N \geq 3$) $2d$ phase diagram.

- Energy scales: T and zero- T gap Δ .
- Crossover lines $T \sim \Delta \sim |\delta r_0|^\nu$.
- For $N = 1$ or 2 existence of a $T > 0$ “ordered” phase.

In the quantum critical fan, physical quantities are described by “exotic” scaling laws. E.g., in $2d$

$$P(T) = P(0) + T^{2+z} F_0,$$

$$\sigma(\omega) = \frac{q^2}{h} \Sigma \left(\frac{\hbar\omega}{k_B T} \right).$$

Why do we need to go beyond mean-field?

Like for classical phase transitions, the dimension plays an important role.

- For $d + 1 \geq 4$, the theory is controlled by a **Gaussian fixed point** and the MF is qualitatively correct.
- For $d = 2$ it is harder to answer. **Strongly interacting** Wilson–Fischer fixed point: MF is wrong.

Perturbation theories (weak/strong coupling, large- N) ill-suited to study the critical regime.

→ need for a **nonperturbative** framework: **FRG**

Complementary existing approaches:

- Analytical: holographic models, conformal field theories.
- Numerical: Monte Carlo, exact diagonalization.

The functional renormalization group: philosophy

FRG: implemented on effective action (Gibbs free energy) $\Gamma[\varphi]$. $(\equiv \Gamma[\langle\varphi\rangle])$.

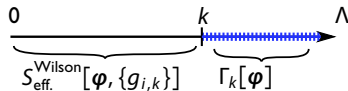
Γ : Legendre transform of free energy $\ln Z$.

$$Z[\mathbf{J}] = \int D[\varphi] \exp\left(-S[\varphi] + \int_x \mathbf{J} \cdot \varphi\right), \quad \Gamma[\varphi] = -\ln Z[\mathbf{J}] + \int_x \mathbf{J} \cdot \varphi.$$

Vertices $\Gamma^{(n)} \equiv \delta^n \Gamma / \delta \varphi^n$ contain the physical information:

- $\Gamma_{\varphi(x)=\text{const.}} = U$: potential \rightarrow thermodynamics (physical φ extremizes Γ).
- $\Gamma^{(2)} = [G]^{-1}$: inverse propagator.

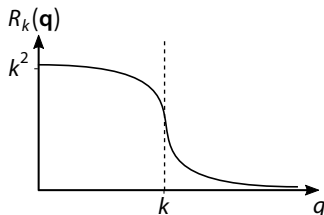
Similar in concept to Wilsonian RG: degrees of freedom are progressively integrated out.



The functional renormalization group: in practice

This is implemented by adding to the action a “mass-like” term:

$$S \rightarrow S_k = S + \Delta S_k,$$
$$\Delta S_k[\boldsymbol{\varphi}] = \frac{1}{2} \int_{\mathbf{q}} \boldsymbol{\varphi}(\mathbf{q}) \cdot R_k(\mathbf{q}) \boldsymbol{\varphi}(\mathbf{q}).$$



R_k gives a very large mass to modes at momenta $\lesssim k$.

New k -dependent effective action $\Gamma \rightarrow \Gamma_k$.

- $k = \Lambda$: all fluctuations are frozen and MF is exact, $\Gamma_\Lambda = S$.
- $k = 0$: all fluctuations are taken into account, $\Gamma_{k=0} = \Gamma$.

Exact flow equation

$$k \partial_k \Gamma_k[\boldsymbol{\varphi}] = \frac{1}{2} \text{Tr} \left\{ \partial_k R_k \left(\Gamma_k^{(2)}[\boldsymbol{\varphi}] + R_k \right)^{-1} \right\}$$

Functional renormalization group: approximation procedures

Simplest idea: the **derivative expansion** (DE).

$$\text{Ansatz: } \Gamma_k[\boldsymbol{\varphi}] = \int_{\mathbf{x}} \frac{Z_k(\boldsymbol{\varphi}^2)}{2} (\partial_\mu \boldsymbol{\varphi})^2 + U_k(\boldsymbol{\varphi}^2) + \frac{Y_k(\boldsymbol{\varphi}^2)}{4} (\boldsymbol{\varphi} \cdot \partial_\mu \boldsymbol{\varphi})^2.$$

- Nonperturbative (no small parameter) and 1-loop exact.
- Coupled PDEs for U_k, Z_k and Y_k : numerically solvable.
- Valid in principle at small momenta only.

Other example: the **Blaizot–Mendéz-Galain–Wschebor** procedure (BMW) where high-order vertices $\Gamma^{(3)}, \Gamma^{(4)}, \dots$ are approximated \rightarrow closed equation for $\Gamma^{(2)}(\mathbf{p})$.

Yields good results at finite momenta! **[Blaizot et al., PRE '06]** **[Benitez et al., PRE '09]**

Critical exponents for the $(2 + 1)d$
Ising model:

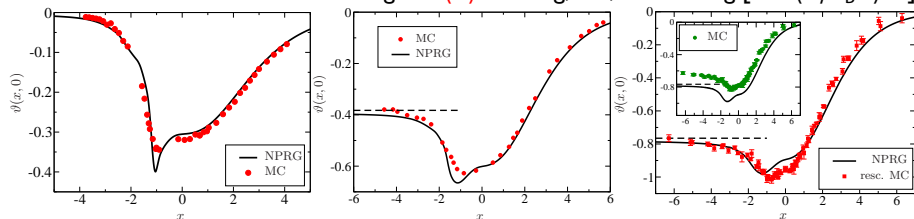
	FRG DE	FRG BMW	Bootstrap
η	.0443	.039	.036298(2)
ν	.6307	.632	.629971(4)

Thermodynamics

Application of the DE: we compute the universal scaling functions of the pressure and internal energy density.

$$P(T) = P(T=0) + \frac{(k_B T)^3}{(\hbar c)^2} F(\Delta/(k_B T)), \quad \epsilon(T) = \epsilon(T=0) - \frac{(k_B T)^3}{(\hbar c)^2} \theta(\Delta/k_B T).$$

Left to right: $\theta(x)$ for Ising, XY, Heisenberg [$x = (\Delta/k_B T)^{1/\nu}$].



[Rançon, F. R. et al., PRB '16].

Full lines: FRG; dots: Monte-Carlo simulations for 3D classical spin systems with PBC.

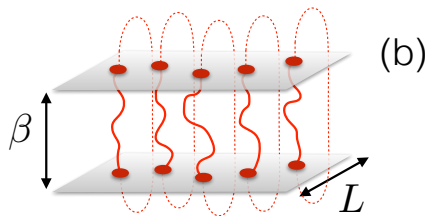
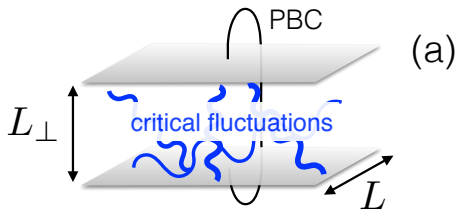
Full potential $O(\partial^2)$ DE, improvement over previous work by Rançon et al.

Classical — quantum mapping

A classical theory confined along a L_{\perp} direction and a quantum $T > 0$ theory are **equivalent!**

$$H_{\text{cl.}} = \int d^{D-1} \mathbf{x}_{\parallel} \int_0^{L_{\perp}} dx_{\perp} H,$$

$$H_{\text{q.}} = \int d^d \mathbf{r} \int_0^{\hbar\beta} d\tau H.$$



The scaling function θ describes the scaling of the critical Casimir force of a 3D classical model near criticality with periodic boundary conditions.

$$\text{Casimir force } f(L_{\perp}, \xi) \sim L_{\perp}^{-D} \theta(L_{\perp}/\xi).$$

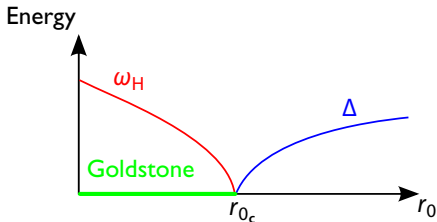
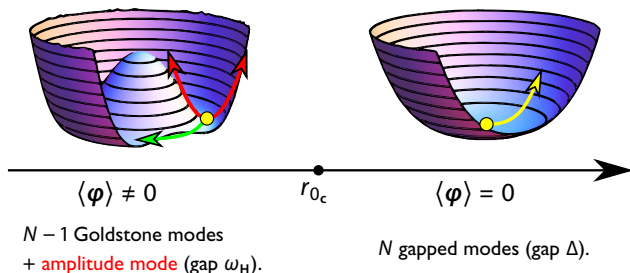
(Critical Casimir forces: **[Fisher and de Gennes, C.R.Acad. Sci. '78]**)

ξ : correlation length.

Dynamics: mean-field excitations

$$U(\varphi) = r_0 \varphi^2 + u_0 (\varphi^2)^2$$

Mean-field zero T phase diagram:



Mean-field:

$$\Delta = A |r_0 - r_{0c}|^{1/2}$$

$$\omega_H = A\sqrt{2} |r_0 - r_{0c}|^{1/2}$$

Beyond the Gaussian approximation

Question: what happens to the “Higgs” amplitude mode beyond MF?

- Is it a well defined mode? What is the quasiexcitation lifetime?
- What happens near the critical point?

“In general, this Higgs particle can decay into multiple lower-energy spin waves. It has been argued that such decay processes dominate for $d < 3$, and the Higgs particle is therefore not a stable excitation.”

[Sachdev, *Quantum Phase Transitions*, 2nd. ed]

Emission of Goldstone bosons \rightarrow IR divergence of the longitudinal susceptibility.

[Patasinskij et al., JETP' 73], [Zwenger, PRL '04], [Dupuis, PRE '11], ...

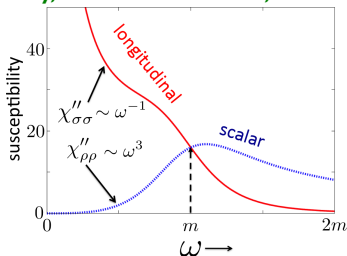
Scalar response function

Answer: consider a different response function. [Podolsky, Auerbach and Arovas, PRB '11]

Right probe: the **scalar susceptibility**.

$$\chi_s(\mathbf{r}, \tau) = \langle \varphi^2(\mathbf{r}, \tau) \varphi^2(0, 0) \rangle,$$

$$\chi_s''(\omega) = \text{Im}[\chi_s(\mathbf{q} = 0, i\omega_n \rightarrow \omega + i0^+)].$$



To compute the 4-point correlation function: introduce an additional source,

$$S \rightarrow S[\mathbf{J}, h] = S + \int d^{d+1}x \mathbf{J} \cdot \boldsymbol{\varphi} + \int d^{d+1}x h \varphi^2.$$

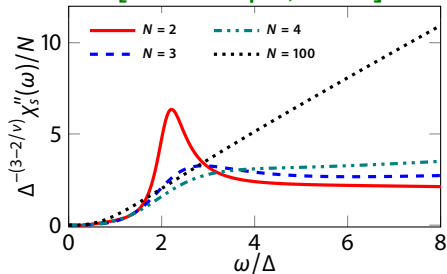
Effective action $\Gamma[\boldsymbol{\varphi}, h]$: Legendre transform wrt \mathbf{J} but not h . Then

$$\chi_s(\omega) = -\Gamma^{(0,2)}(\omega) + \left(\Gamma^{(2,0)}(\omega)\right)^{-1} \left(\Gamma^{(1,1)}(\omega)\right)^2, \quad \Gamma^{(n,m)} = \frac{\delta^{(n+m)}\Gamma}{\delta^{(n)}\varphi \delta^{(m)}h}.$$

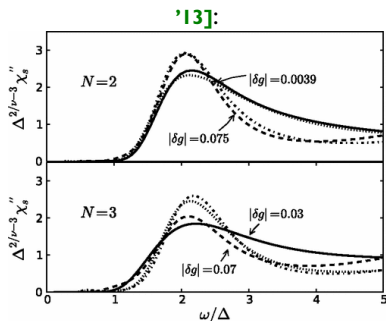
Approximation method: BMW to obtain **full frequency dependence**.

Results and comparison

FPRG BMW [Rose and Dupuis, PRB '15]:



MC [Gazit, Podolski, Auerbach PRL



Experimental observation: [Endres et al., Nature '12].

Higgs mass m_H/Δ	$N = 3$	$N = 2$	$N = 3$	$N = 2$
MF	$\sqrt{2}$	$\sqrt{2}$	2.7	2.2
QMC (Chen et al.)		3.3(8)	Lattice QMC (Löhöfer et al.)	2.6(4)
QMC (Gazit et al.)	2.2(3)	2.1(3)	Exact diag. (Nishiyama)	2.7
ϵ expansion (Katan et al.)	1.64	1.67		2.1(2)

Conductivity of the $O(N)$ model

$O(N)$ symmetry \rightarrow conservation of angular momentum L , current $\partial_t L + \nabla \cdot \mathbf{J} = 0$.

We make the $O(N)$ symmetry local by adding a **gauge field**, $\partial_\mu \rightarrow D_\mu = \partial_\mu - A_\mu$.

$$A_\mu = A_\mu^a T^a \in \mathfrak{so}(N) \quad T^a: N(N-1)/2 \text{ generators, } T_{ij}^a = -T_{ji}^a$$

Current densities $J_\mu^a = -\frac{\delta S}{\delta A_\mu^a} = j_\mu^a - A_\mu^a \boldsymbol{\varphi} \cdot T^a \boldsymbol{\varphi}, \quad j_\mu^a = \boldsymbol{\varphi} \cdot T^a \partial_\mu \boldsymbol{\varphi}$

$N = 2$ (bosons): $\mathbf{j} \sim i(\psi^* \nabla \psi - \psi \nabla \psi^*), \quad \psi = \varphi_1 + i\varphi_2.$

Linear response theory

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

$$\sigma_{\mu\nu}^{ab}(i\omega_n) = -\frac{1}{\omega_n} K_{\mu\nu}^{ab}(p_x = 0, p_y = 0, p_z = i\omega_n) \quad \text{conductivity tensor}$$

Conductivity: generalities

The conductivity tensor $\sigma_{\mu\nu}^{ab}$:

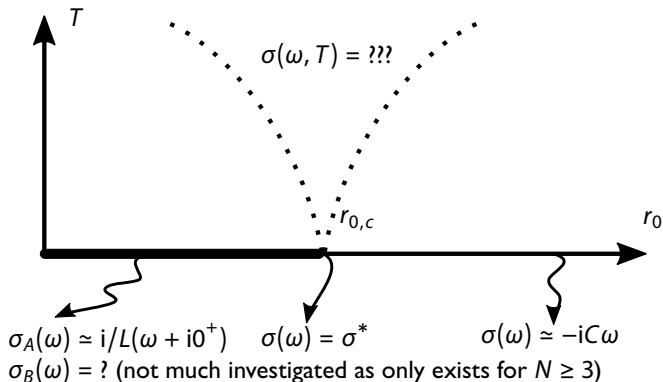
- is diagonal, $\sigma_{\mu\nu}^{ab} = \delta_{\mu\nu} \delta_{ab} \sigma^{aa}$;
- has two independent components, $\sigma^{aa}(\omega) = \begin{cases} \sigma_A(\omega) & \text{if } T^a \boldsymbol{\varphi} \neq 0, \\ \sigma_B(\omega) & \text{if } T^a \boldsymbol{\varphi} = 0; \end{cases}$
- in the disordered phase and at the QCP $\sigma_A = \sigma_B = \sigma$.

For $N = 2$, there is only one $\text{so}(N)$ generator and the conductivity in the ordered phase reduces to σ_A .

Universal properties

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

Low frequency behavior:



$\sigma^*/\sigma_q, C/L\sigma_q^2$ are universal! ($\sigma_q = q^2/h$)

[Fischer et al., PRL '89]

Goals

Objective: determine the universal scaling form of the conductivity.

Technically: compute **4 point correlation functions** $\langle j_{\mu}^a j_{\nu}^b \rangle$.

Approaches:

- QMC (**Sørensen, Chen, Prokof'ev, Pollet, Gazit, Podolsky, Auerbach**);
- Holography (**Myers, Sachdev, Witzack-Krempa**);
- CFT (**Poland, Sachdev, Simmons-Duffin, Witzack-Krempa**);
- FRG (us!).

Effective action formalism

Idea: use the same trick than for the Higgs.

The partition function depends on two sources, the gauge field and \mathbf{J} that couples linearly to φ :

$$Z[\mathbf{J}, \mathbf{A}] = \int D[\varphi] \exp(-S[\varphi, \mathbf{A}] + \int_{\mathbf{x}} \mathbf{J} \cdot \varphi).$$

The **effective action** is the Legendre transform of $\ln Z$ wrt \mathbf{J} but not \mathbf{A} :

$$\Gamma[\varphi, \mathbf{A}] = -\ln Z[\mathbf{J}, \mathbf{A}] + \int_{\mathbf{x}} \mathbf{J} \cdot \varphi.$$

$$K_{\mu\nu}^{ab} = \frac{\delta^{(2)} \ln Z}{\delta A_{\mu}^a \delta A_{\nu}^b} = -\Gamma_{a\mu, b\nu}^{(0,2)} + \Gamma_{i, a\mu}^{(1,1)} \left(\Gamma_{ij}^{(2,0)} \right)^{-1} \Gamma_{j, b\nu}^{(1,1)}$$

with

$$\Gamma^{(n,m)} = \frac{\delta^{(n+m)} \Gamma}{\delta^{(n)} \varphi \delta^{(m)} A}.$$

ERG formulation

Problem of the FRG: the regulator (\sim mass) breaks down gauge invariance:

$$\Delta S_k = \frac{1}{2} \int_{\mathbf{q}} \boldsymbol{\varphi}(\mathbf{q}) \cdot R_k(\mathbf{q}^2) \boldsymbol{\varphi}(-\mathbf{q}).$$

How to recover gauge invariance?

Answer: make the **regulator gauge dependent!**

[Morris, N. Phys. B '00] [Codello, Percacci et al., EPJC '16] [Bartosh, PRB '13]

$$\Delta S_k = \frac{1}{2} \int_{\mathbf{x}} \boldsymbol{\varphi}(\mathbf{x}) \cdot R_k(-\partial_\mu^2) \boldsymbol{\varphi}(\mathbf{x}) \rightarrow \Delta S_k[\mathbf{A}] = \frac{1}{2} \int_{\mathbf{x}} \boldsymbol{\varphi}(\mathbf{x}) \cdot R_k(-D_\mu^2) \boldsymbol{\varphi}(\mathbf{x})$$

Modified flow equations due to the presence of \mathbf{A} .

Which approximation procedure do we use?

First idea: BMW to obtain full momentum dependence (as done for the study of the Higgs mode).

Problem: it fails!

- Impossible to close the flow equations rigorously.
- Setting momenta to zero in flow equations breaks down gauge invariance.

Derivative expansion scheme

We try a **derivative expansion** scheme and project the flow equation onto a gauge-invariant Ansatz. $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu - [A_\mu, A_\nu]$ allows us to build two $O(A_\mu^2)$ gauge-invariant terms:

$$\Gamma_k[\boldsymbol{\varphi}, \mathbf{A}] = \int_{\mathbf{x}} \frac{1}{2} Z_k(\rho) (D_\mu \boldsymbol{\varphi})^2 + \frac{1}{4} Y_k(\rho) (\partial_\mu \rho)^2 + U_k(\rho) \quad (\text{standard } O(\partial_\mu^2) \text{ DE}) \\ + \frac{1}{4} X_{1,k}(\rho) \text{Tr}(F_{\mu\nu}^2) + \frac{1}{4} X_{2,k}(\rho) (F_{\mu\nu} \boldsymbol{\varphi})^2.$$

$\rho = \boldsymbol{\varphi}^2/2$, $\rho_{0,k}$: minimum of the potential.

Expression of the conductivity within the DE

$$\sigma_A(\omega) = 2\rho_0 Z(\rho_0) / (\omega + i0^+) + \omega [X_1(\rho_0) + 2\rho_0 X_2(\rho_0)],$$

$$\sigma_B(\omega) = \omega X_1(\rho_0).$$

Results

This simple DE scheme allows us to recover the low momenta physics! We retrieve the universal ratio C/L . Exact value for $N = \infty$, **good agreement with MC (~ 5%)** for $N = 2$.

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

The picture is more complicated in the critical regime.

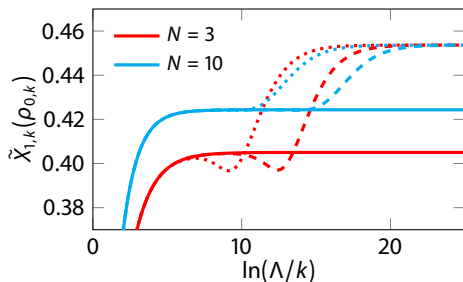
- DE can sometimes be extrapolated to finite ω but not always.
- $\Gamma^{(0,2)}(\omega) \sim 1/\omega$: divergence in the flow:

$$\sigma(\omega) \sim \tilde{X}_{1,\text{crit}}^* \frac{\omega}{k} \quad \text{with} \quad \tilde{X}_{1,\text{crit}}^* = \lim_{k \rightarrow 0} k\chi_1(\rho_{0,k}) \quad (\text{fixed point value}).$$

- Setting $\omega \sim k$ yields an estimate of the conductivity, $\sigma^* \sim \tilde{X}_{1,\text{crit}}^*$.

Similarly, in the ordered phase, $\sigma_B(\omega) \sim \tilde{\chi}_{1,\text{ord}}^* \omega/k$.

$\tilde{\chi}_{1,\text{ord}}^*$ is an universal number — verified for $N = \infty$, conjecture for $N < \infty$.



Full: QCP

Dashed: ordered

More surprising: $\tilde{\chi}_{1,\text{ord}}^*$ numerically does not depend on N !

$$\sigma_B(\omega) = \frac{\pi}{8} \sigma_q \text{ for all } N: \text{“superuniversality”!}$$

[Rose and Dupuis, PRB '17]

Beyond DE...?

Next project: use a momentum-dependent scheme to compute $\sigma(\omega)$ at finite ω .

From this: deduce $\sigma_B, \sigma^*, \dots$

Idea: DE-like *Ansatz* with momentum dependence.

Preliminary results:

- $\sigma^* \simeq 0.34\sigma_q$, bootstrap result: $\sigma^* = 0.3554(6)\sigma_q$ [Kos et al., JHEP '15], QMC predicts value from 0.355 to 0.361.
- The conjecture that $\sigma_B(\omega \rightarrow 0) = \frac{\pi}{8}\sigma_q$ for all N holds.

Review and conclusion

- Although harder than thermodynamics FRG can be successfully used to describe dynamics in the vicinity of QPTs and compare well with complementary approaches (holography, CFTs, numerics).
- Study of the excitation spectrum of the $O(N)$ model: Higgs [Rose et. al, PRB '15] (and bound states [Rose et. al, PRB '16]).
- Transport: a simple derivative expansion allows to obtain results that compare well with MC. Results allow to make a conjecture on the universal behavior of σ_B [Rose and Dupuis, PRB '17].
- This will soon be confirmed with a momentum-dependent scheme we are developing!
- Hardest part (and long term goal): $T > 0$, a little because of computational time and a lot because of analytic continuation! Proposals to overcome this difficulty (Strodthoff, Pawłowski).