

# Renormalization of microscopic Hamiltonians

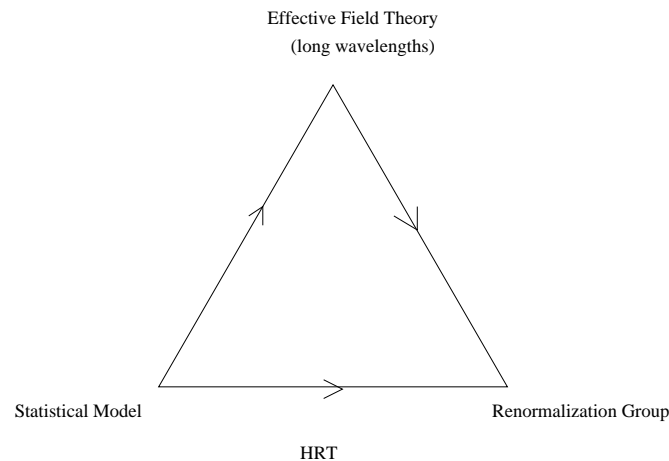
Renormalization Group without Field Theory

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# Renormalization Group $\Rightarrow$ Universality

Only dimensionality and symmetry matter



## Hierarchical Reference Theory

- Keeps track of higher order operators
- Provides information on non universal properties (critical temperature, crossovers etc.)

A.P. & L.Reatto: PRL, **53**, 2417 (1984); PRA **31**, 3309 (1985);  
Adv. Phys. **44**, 211, (1995).

# Outline

- Wilson's **momentum-shell** integration RG for microscopic models
- Sharp & Smooth cut-off formulations
- Approximate **non perturbative** closures
- Relation to the **Local Potential Approximation**
- **First order** transition and the convexity requirement
- Extension to **Quantum** Hamiltonians
- Open problems

# HRT vs. RG: A short story

(scalar order parameter)

$\Phi^4$  Field Theory

$$S = \int d\mathbf{r} \left[ \frac{1}{2} |\nabla \Phi|^2 + \frac{r}{2} \Phi^2 + \frac{u}{4!} \Phi^4 \right]$$

$$Z = \int \mathcal{D}\Phi(\mathbf{r}) e^{-S}$$

Perturbation theory in  $u$

Statistical Model

$$H = \frac{1}{2} \sum_{i \neq j} v(\mathbf{r}_i - \mathbf{r}_j)$$

$$Z = \int d\mathbf{r}_1 \cdots d\mathbf{r}_N e^{-\beta H}$$

Perturbation theory in  $\beta$

# Formal Perturbation Theory

- Split the potential into a **Hard Sphere part** and an **Attractive tail**

$$v(r) = v_{HS}(r) + w(r)$$

- Expand the free energy ( $\ln Z$ ) in powers of  $w(r)$
- Order the diagrams according to the number of loops



## Correspondence Field Theory $\Leftrightarrow$ Statistical Model

Propagator:  $\frac{1}{r + q^2} \Leftrightarrow [-\beta\tilde{w}(q)] \frac{[\rho S_{HS}(q)]^2}{1 + \beta\rho S_{HS}(q)\tilde{w}(q)}$

Vertex:  $u_n(\mathbf{r}_1, \dots, \mathbf{r}_n) \Leftrightarrow c_n(\mathbf{r}_1, \dots, \mathbf{r}_n) \equiv \frac{\delta^n \ln Z_{HS}[\rho(\mathbf{r})]}{\delta\rho(\mathbf{r}_1) \dots \delta\rho(\mathbf{r}_n)}$

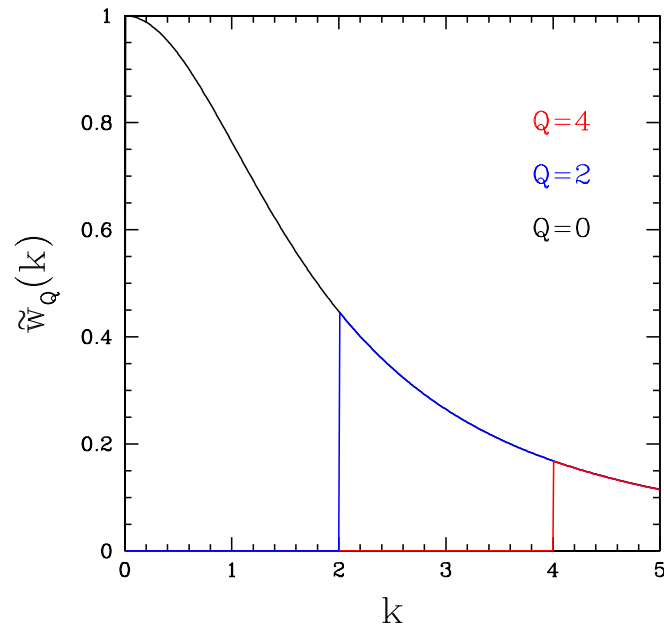
## Momentum Shell Integration RG

Cut-off on the propagator  $\Leftrightarrow$  Cut-off on the interaction  $\tilde{w}(q)$

# Sharp cut-off implementation

Sequence of intermediate  $Q$ -systems

$$\tilde{w}_Q(k) = \begin{cases} \tilde{w}(k) & \text{for } k > Q \\ 0 & \text{for } k < Q \end{cases}$$



$$Q : \infty \rightarrow 0$$

$$\lim_{Q \rightarrow \infty} \tilde{w}_Q(k) = 0$$

$$\lim_{Q \rightarrow 0} \tilde{w}_Q(k) = \tilde{w}(k)$$

The cut-off  $Q$  limits the range of density fluctuations included in the  $Q$ -system  
Liquid-vapor transition inhibited at every  $Q \neq 0$



## Evolution of the free energy with $Q$

$$\begin{aligned} \frac{dA_Q}{dQ} &= -\frac{d}{2} \Omega_d Q^{d-1} \ln \left[ 1 - F_Q(Q) \beta \tilde{w}(Q) \right] \\ &= -\frac{d}{2} \Omega_d Q^{d-1} \ln \left[ 1 + \frac{\beta \tilde{w}(Q)}{C_Q(Q)} \right] \end{aligned}$$

- $-kT A_Q$  = Free energy density of the  $Q$ -system  
+ Mean field contribution [  $\Gamma_k$  ]
  
- $C_Q(k)$  = Direct correlation function of the  $Q$ -system [  $\Gamma_k^{(2)}(q)$  ]  
+ Mean field contribution  $\implies C_Q(\mathbf{r}_1 - \mathbf{r}_2) = \frac{\delta^2 A_Q}{\delta \rho(\mathbf{r}_1) \delta \rho(\mathbf{r}_2)}$
  
- $\Omega_d$  = volume of the unit sphere in  $d$ -dimension

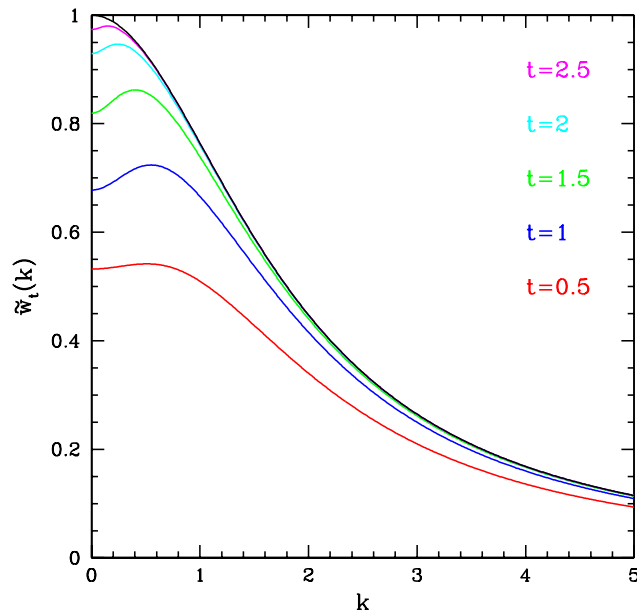
Exact hierarchy of differential equations for  $C_Q$  and  $c_n^Q$  ( $n = 3, \dots, \infty$ )

# Smooth cut-off implementation

Sequence of intermediate  $t$ -systems

$$w_t(r) = w(r) - e^{-(d+2-\eta)t} w(r/e^t)$$

$$\tilde{w}_t(k) = \tilde{w}(k) - e^{-(2-\eta)t} \tilde{w}(k e^t)$$



$$t : 0 \rightarrow \infty$$

$$Q \sim e^{-t}$$

$$\lim_{t \rightarrow 0} \tilde{w}_t(k) = 0$$

$$\lim_{t \rightarrow \infty} \tilde{w}_t(k) = \tilde{w}(k)$$

Phase transitions are suppressed at all finite  $t$ 's

A.P: J. Phys. C **26**, 5071 (1986)

A.P., D.Pini and L.Reatto: PRL **100**, 165704 (2008)

## Evolution of the free energy with $t$

$$\frac{d\mathcal{A}_t}{dt} = \frac{\beta}{2} \int \frac{d^d k}{(2\pi)^d} \frac{d\tilde{w}_t(k)}{dt} \left[ \mathcal{C}_t(k) + e^{-(2-\eta)t} \beta \tilde{w}(k e^t) \right]^{-1}$$

- $-kT \mathcal{A}_t =$  Free energy density of the  $t$ -system

+ Mean field contribution

$[\Gamma_k]$

- $\mathcal{C}_t(k) =$  Direct correlation function of the  $t$ -system

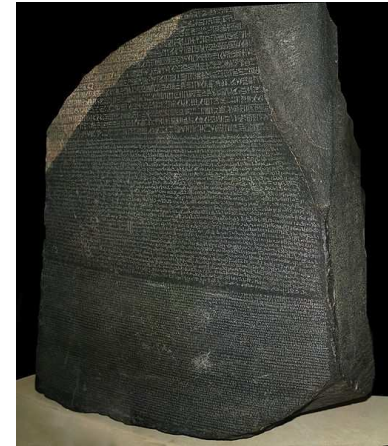
$[\Gamma_k^{(2)}(q)]$

+ Mean field contribution  $\implies \mathcal{C}_t(\mathbf{r}_1 - \mathbf{r}_2) = \frac{\delta^2 \mathcal{A}_t}{\delta \rho(\mathbf{r}_1) \delta \rho(\mathbf{r}_2)}$

Exact hierarchy of differential equations for  $\mathcal{C}_t$  and  $c_n^t$  ( $n = 3, \dots, \infty$ )

# The Dictionary

NPRG	Smooth cut-off HRT
$k$	$Q = e^{-t}$
$\phi$	$\rho$
$R_k(q)$	$-e^{-(2-\eta)t} \beta w(q e^t)$
$\Gamma_k[\phi]$	$-\mathcal{A}_t(\rho)$
$\Gamma_k^{(2)}(q)$	$-\mathcal{C}_t(q)$
$\Gamma_k^{(n)}(q_1 \cdots q_n)$	$-c_t^n(q_1 \cdots q_n)$



## Highlights of the exact HRT equations

- For  $Q \rightarrow 0$  and in the critical region the HRT equations simplify and, through a simple rescaling, reduce to the standard RG hierarchy of equations for a scalar field theory.
- The HRT smooth cut-off prescription depends on the interparticle potential  $w(r)$  and corresponds to the smooth cut-off RG with a suitable choice of smearing function
- The full HRT equations retain information on non-universal properties and short range correlations (i.e. the full UV behavior of the statistical model is preserved in the RG procedure)
- The HRT strategy can be trivially generalized to  $O(n)$  spin models on a lattice

## An approximate closure

$$C_t(k) = c_{HS}(k) - \lambda_t(\rho) \beta \tilde{w}(k)$$

$\lambda(\rho) = 1 \implies$  Mean Field

$\lambda_t(\rho)$  defined by the compressibility sum rule  $\implies C_t(k=0) = \frac{\partial^2 \mathcal{A}_t}{\partial \rho^2}$

**Local Potential Approximation** at long wavelengths

$$C_t(k) \xrightarrow{k \sim 0} \frac{\partial^2 \mathcal{A}_t}{\partial \rho^2} - b k^2$$

- Closed (approximate) **partial** differential equation for the thermodynamics of the  $t$ -system
- To be solved with initial condition  $\mathcal{A}_t = -\beta A_{MF}/V$  for  $t = 0$
- In the  $t \rightarrow \infty$  limit  $\mathcal{A}_t \rightarrow$  Physical free energy density of the fully interacting model

# Critical Properties

Formal structure of the HRT evolution equation at large  $t$

$$\frac{d\mathcal{A}_t}{dt} = e^{-dt} \Phi \left( e^{2t} \frac{\partial^2 \mathcal{A}_t}{\partial \rho^2} \right)$$

where  $\Phi(x)$  is a non-linear function  
depending on the choice of sharp/smooth cut-off

- **Rescaling:**  $z = (\rho - \rho_c) e^{\frac{d-2}{2}t}$

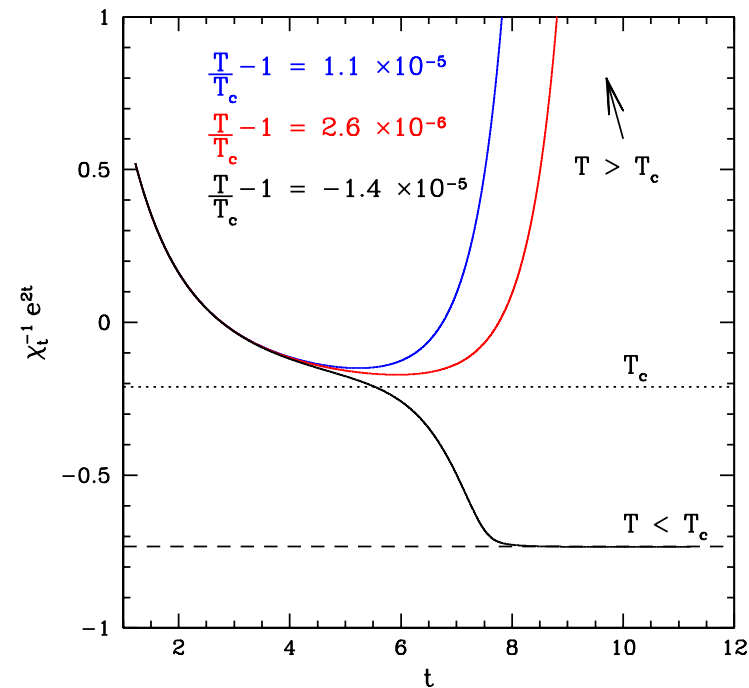
$$H_t(z) = e^{dt} [\mathcal{A}_t(\rho) - \mathcal{A}_t(\rho_c)]$$

- **Fixed point equation:** the standard RG structure in LPA is recovered

$$\frac{d-2}{2} z H'_*(z) - d H_*(z) = \Phi(H''_*(z)) - \Phi(H''_*(0))$$

## HRT flow of the inverse susceptibility

$$\chi_t^{-1} = - \left. \frac{\partial^2 \mathcal{A}_t(\rho)}{\partial \rho^2} \right|_{\rho_c}$$



- Approach to the fixed point value in the critical region
- Flow to the low temperature fixed point in the two-phase region



## Critical exponents and amplitudes

$$\chi^{-1} = - \left. \frac{\partial^2 \mathcal{A}_\infty(\rho)}{\partial \rho^2} \right|_{\rho_c} \sim \frac{1}{C_\pm} \left| \frac{T - T_c}{T_c} \right|^\gamma$$

$$|\rho_x - \rho_c| \propto (T_c - T)^\beta$$

$\epsilon$ -expansion

$d = 3$

$$\gamma = 1 + \frac{\epsilon}{6} + \dots$$

$$\beta = \frac{1}{2} - \frac{\epsilon}{6} + \dots$$

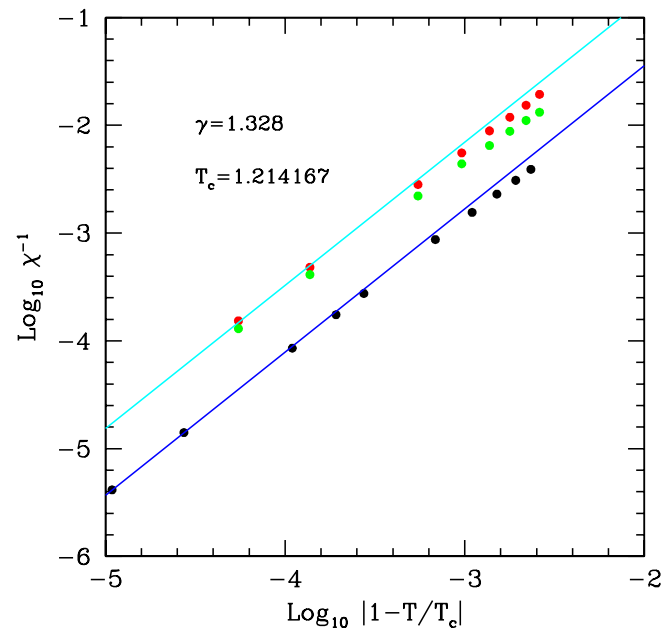
	HRT sharp	HRT smooth	Exact
$\gamma$	1.378	1.328	1.237
$\beta$	0.345	0.332	0.326
$\eta$	0	0	0.036
$U_2 = C_+/C_-$	—	4.16	4.76

PRL, **53**, 2417 (1984); PRL **100**, 165704 (2008)

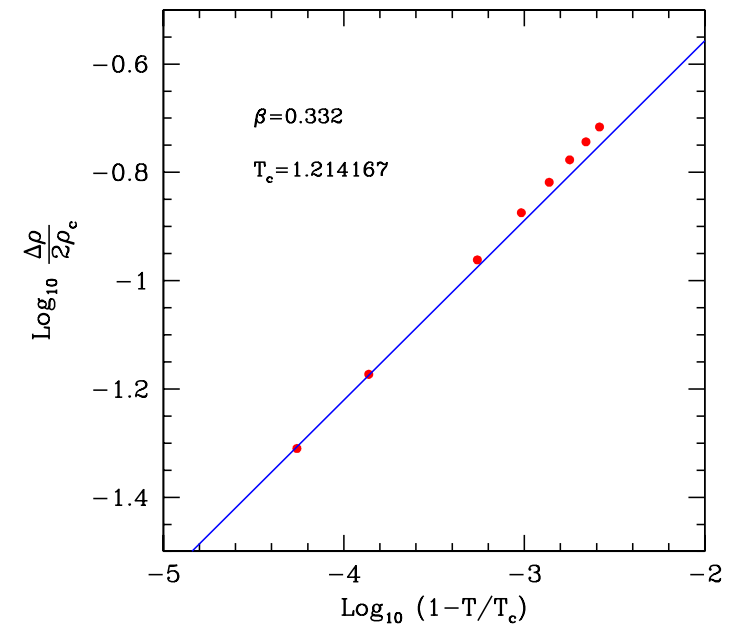
# Numerical integration of the full HRT equation

Smooth cut-off

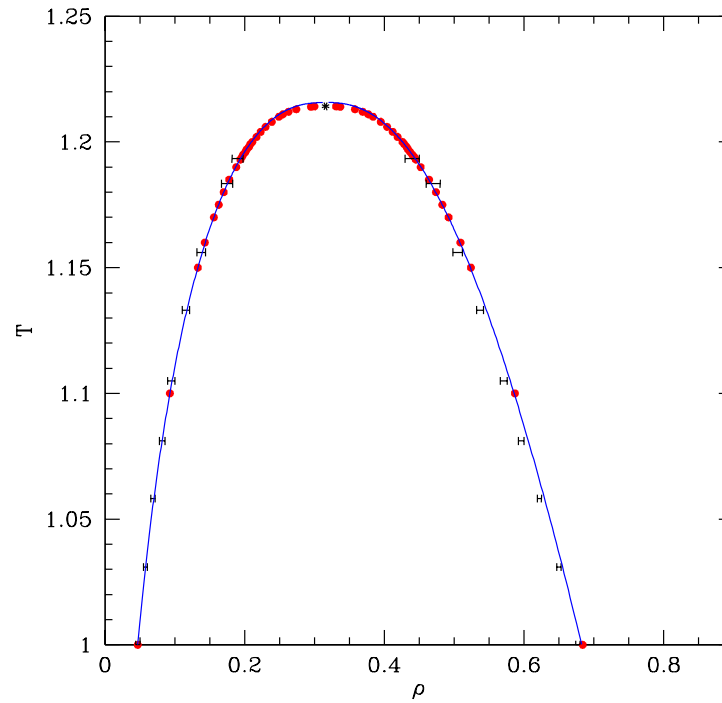
Inverse susceptibility



Coexistence curve

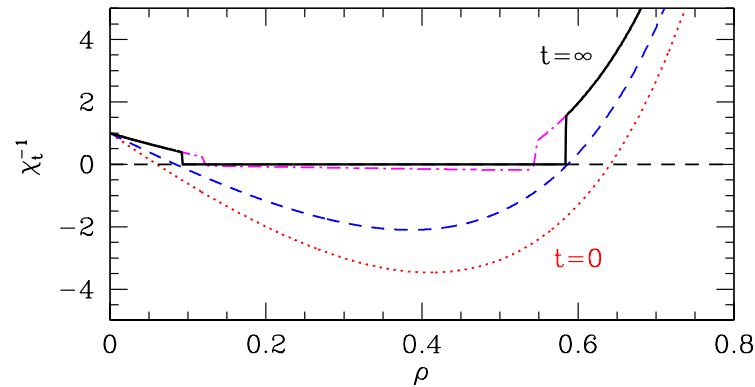


# Phase diagram of a fluid



	HRT-smooth	MC
$T_c$	1.2142	1.212(2)
$\rho_c$	0.3157	0.312(2)

# First order transition



- Fluctuations restore the convexity of the free energy
- For  $t \rightarrow \infty$ :

In one-phase regions the susceptibility is always **positive**

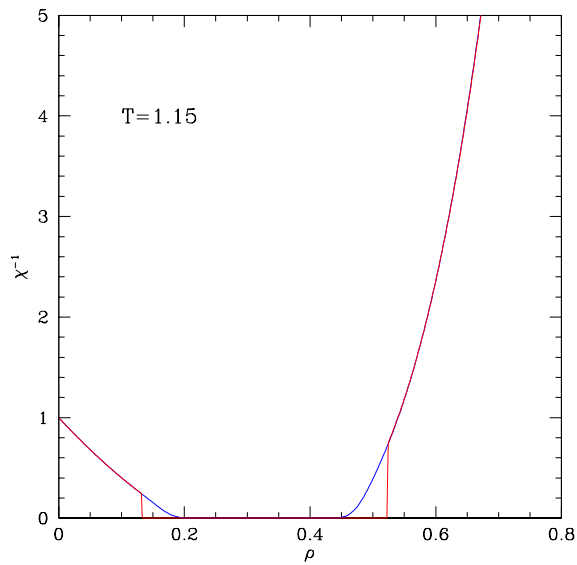
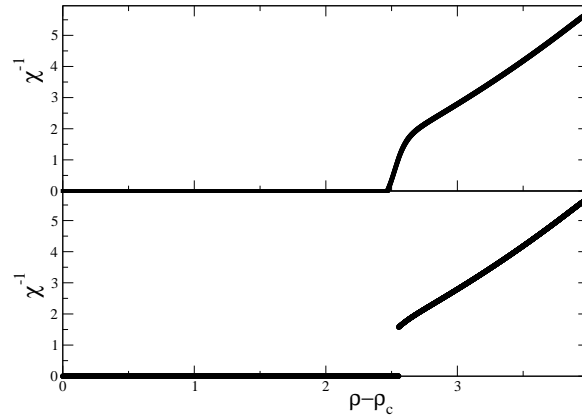
At coexistence the susceptibility identically **vanishes**

# First order transition

## Sharp vs Smooth cut-off

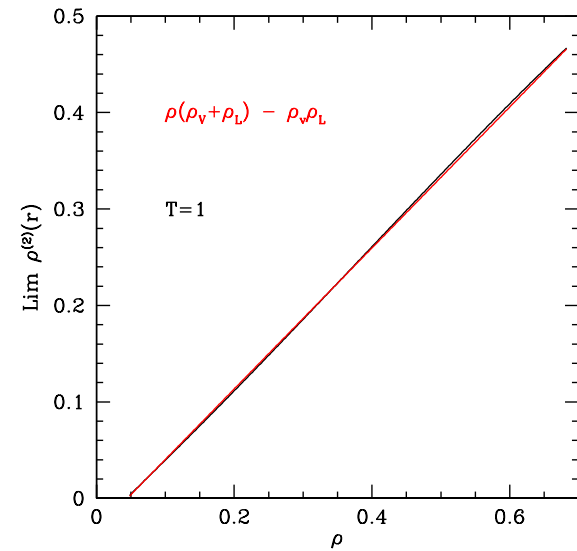
Sharp cut-off

Smooth cut-off



At coexistence

$$\lim_{r \rightarrow \infty} \rho^2 g(r) = \rho(\rho_v + \rho_l) - \rho_v \rho_l$$



# Quantum HRT

- General **interacting** quantum system of **bosons/fermions/spins**

$$\hat{H} = \hat{H}_R + \hat{V} = \hat{H}_R + \frac{1}{2} \int d\mathbf{x} d\mathbf{y} \hat{\rho}(\mathbf{x}) w(\mathbf{x} - \mathbf{y}) \hat{\rho}(\mathbf{y})$$

- Order parameter  $\langle \hat{\rho}(\mathbf{x}) \rangle \implies$  Perturbative expansion in  $w(\mathbf{x})$

$$\begin{aligned} \frac{\Xi}{\Xi_R} &= \frac{\text{Tr} e^{-\beta \hat{H}}}{\text{Tr} e^{-\beta \hat{H}_R}} \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n}{2^n n!} \int ds_1 ds'_1 \dots ds_n ds'_n \rho_R(s_1, \dots, s'_n) \phi(s_1, s'_1) \dots \phi(s_n, s'_n) \end{aligned}$$

$$\phi(s, s') = w(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau') \quad \tau \in (0, \beta) \quad s = (\mathbf{x}, \tau)$$

$$\rho_R(\mathbf{x}_1, \tau_1; \dots, \mathbf{x}_n, \tau_n) = \frac{1}{\Xi_R[J]} \frac{\delta^n \Xi_R[J]}{\delta J(\mathbf{x}_1, \tau_1) \dots \delta J(\mathbf{x}_n, \tau_n)} \Big|_{J=0}$$

## Formal analogy with a classical model in $d + 1$ dimension

- Sharp cut-off on the Fourier components of  $w(\mathbf{x})$
- Exact evolution equation for the Helmholtz free energy density

$$\frac{d\mathcal{A}_Q}{dQ} = -Q^{d-1} \frac{d}{2} \Omega_d \sum_{\omega_n} \ln[1 - F_Q(Q, \omega_n) \tilde{w}(Q)]$$

- Connected two point function in imaginary time:

$$F(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_2) = \frac{\delta^2 \ln \Xi[J]}{\delta J(\mathbf{x}_1, \tau_1) \delta J(\mathbf{x}_2, \tau_2)} \Big|_{J=0}$$

- Matsubara frequencies at finite temperature:  $\omega_n = \frac{2\pi}{\beta} n$

# The antiferromagnetic Heisenberg model

$$\hat{H} = J \sum_{\langle \mathbf{R}, \mathbf{R}' \rangle} \hat{\mathbf{S}}_{\mathbf{R}} \cdot \hat{\mathbf{S}}_{\mathbf{R}'} - h \sum_{\mathbf{R}} e^{i\vec{\pi} \cdot \mathbf{R}} \hat{S}_{\mathbf{R}}^z$$

- Order parameter: **staggered** magnetization  $\langle \hat{S}_{\mathbf{R}}^z \rangle = m e^{i\vec{\pi} \cdot \mathbf{R}}$

## Parametrization of the two point functions

$$(\alpha_{\perp Q}, \alpha_{\parallel Q})$$

$$F_Q^{xx}(\mathbf{k}, \omega) = \frac{\alpha_{\perp Q} - \tilde{w}(\mathbf{k})}{m^{-2}\omega^2 + \alpha_{\perp Q}^2 - \tilde{w}(\mathbf{k})^2}$$

$$F_Q^{xy}(\mathbf{k}, \omega) = \frac{m^{-1}\omega}{m^{-2}\omega^2 + \alpha_{\perp Q}^2 - \tilde{w}(\mathbf{k})^2}$$

$$F_Q^{zz}(\mathbf{k}, \omega) = \frac{\delta_{\omega,0}}{\alpha_{\parallel Q} + \tilde{w}(\mathbf{k})}$$



## Physical response functions

### Single mode approximation

$$\text{Im } S^{xx}(\mathbf{k}, \omega) = \frac{\pi\omega}{1 - \exp(-\beta\omega)} \frac{\delta(\omega - \epsilon_k) + \delta(\omega + \epsilon_k)}{\alpha_{\perp} + \tilde{w}(\mathbf{k})}$$

$$\text{Im } S^{zz}(\mathbf{k}, \omega) = \frac{2\pi}{\beta} \frac{\delta(\omega)}{\alpha_{\parallel} + \tilde{w}(\mathbf{k})}$$

- Spin wave dispersion:  $\epsilon_k = m \sqrt{\alpha_{\perp}^2 - \tilde{w}(\mathbf{k})^2}$

## LPA-like closure

$$\chi_{\perp}^s = \left(\frac{h}{m}\right)^{-1} = -\beta m \left(\frac{\partial \mathcal{A}}{\partial m}\right)^{-1} = F^{xx}(\vec{\pi}, 0) = (\alpha_{\perp} - 2Jd)^{-1}$$
$$\chi_{\parallel}^s = \left(\frac{\partial h}{\partial m}\right)^{-1} = -\beta \left(\frac{\partial^2 \mathcal{A}}{\partial m^2}\right)^{-1} = F^{zz}(\vec{\pi}, 0) = (\alpha_{\parallel} - 2Jd)^{-1}$$

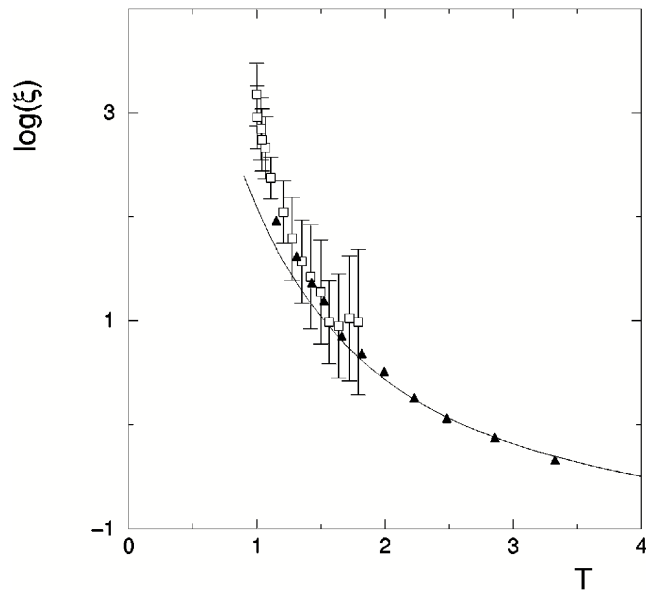
## QHRT Equation

$$\frac{d\mathcal{A}_Q}{dQ} = -\frac{D_d(Q)}{2} \left\{ 4 \ln \left[ \frac{\sinh\left(\frac{1}{2}\beta m \alpha_{\perp Q}\right)}{\sinh\left(\frac{1}{2}\beta m \sqrt{\alpha_{\perp Q}^2 - 4J^2(d^2 - Q^2)}\right)} \right] + \ln \left[ \frac{\alpha_{\parallel Q}^2}{\alpha_{\parallel Q}^2 - 4J^2(d^2 - Q^2)} \right] \right\}$$

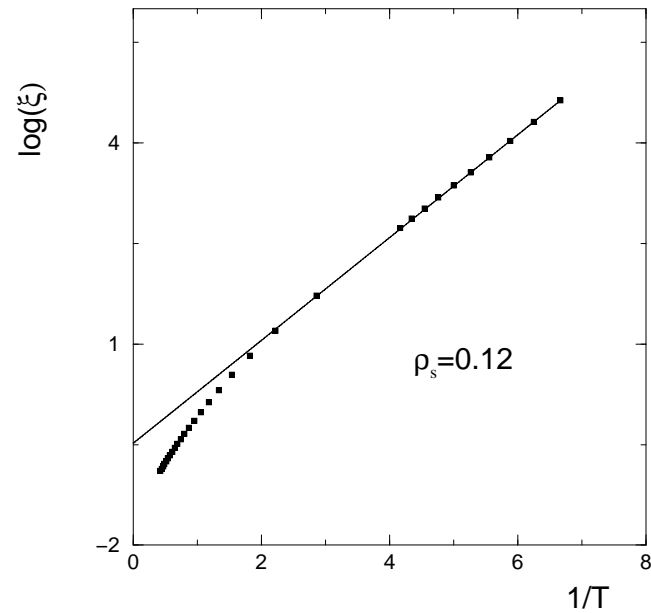
$$Q \in (0, d) \quad m \in (0, 1)$$

# Numerical results in two dimensions

## Spin-1 model



## Spin- $\frac{1}{2}$ model



$$\xi(T) \sim \xi_0 e^{\frac{2\pi\bar{\rho}_s}{T}}$$

The Heisenberg model always falls in the renormalized classical regime

## Non Linear $\sigma$ -Model

$$S[\Omega] = \frac{\rho_s}{2} \int d^d \mathbf{r} \int_0^\beta d\tau \left\{ |\nabla \Omega|^2 + \frac{1}{c_s^2} \left( \frac{\partial \Omega}{\partial \tau} \right)^2 \right\} \quad |\Omega| = 1$$

### One loop RG equations

$$Q \frac{dg}{dQ} = (d-1)g - \frac{K_d}{2} g^2 \coth(g/2T)$$

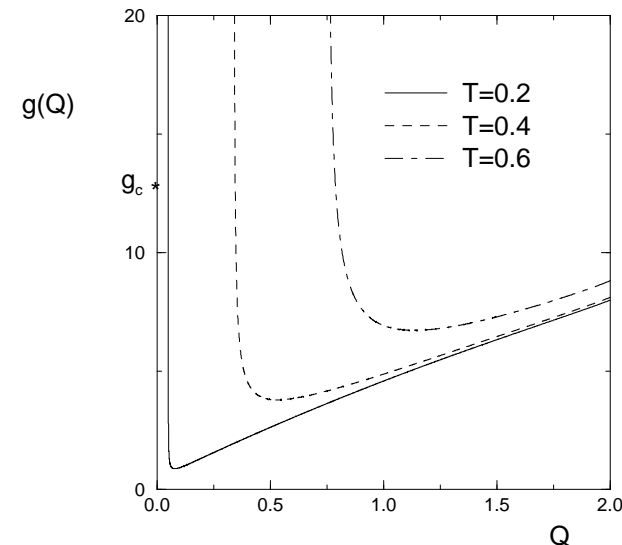
$$\frac{d}{dQ} \left( \frac{g}{T} \right) = \frac{g}{T}$$

### Effective coupling constant

$$g = \left( \frac{Q}{\sqrt{d}} \right)^{d-1} \frac{\sqrt{4d}}{m_Q}$$

### QHRT evolution of the spontaneous magnetization

$$\frac{dm_Q}{dQ} = K_d \left( \frac{Q}{\sqrt{d}} \right)^{d-2} \coth(\beta Q m_Q)$$



# Outlook

## Closures

- Beyond LPA: the second equation of the hierarchy
  - $\eta$  at two loop order
- Better representation of short range physics
  - Repulsive interactions
  - Classical and Quantum Heisenberg models

## Order parameters

- Beyond the  $O(n)$  model: inhomogeneous systems
- Competing interactions: more complex order parameters
- The Fermi surface in QHRT
- The Coulomb gas (primitive model)

# BMW approach

$c(r) = \exp[-\beta\{v_R(r) + w(r)\}]$  for the Ornstein-Zernike direct correlation function. From the free energy Eq. (2) one then finds the correct first virial coefficient. If in the hierarchy we approximate  $\tilde{\epsilon}_n^Q$  with its ideal-gas value starting from  $n = m$  then the truncated system gives the correct low-density expansion for  $c(r)$  up to order  $m - 2$ .

In the opposite limit of high density the effect of the many-particle correlations becomes essentially irrelevant. In fact the strong effect of screening of  $w(r)$  by the repulsive forces is manifest in (4) because  $\tilde{F}(p)$  is very small in the region of small  $p$  where  $\tilde{\phi}(p)$  is significant. Therefore to lowest order  $M^Q$  can be considered as a negligible quantity so

$$\left(\frac{\partial}{\partial \ln Q} + x \frac{\partial}{\partial x} - 2 + \eta\right) u_2^Q(x) = \frac{1}{2} (2\pi)^{-d} \int d\Omega_y \{u_4^Q(\bar{x}, -\bar{x}, \bar{y}, -\bar{y}) - 2[u_2^Q(\bar{x}, \bar{y} - \bar{x} - \bar{y})]^2 / u_2^Q(\bar{y} + \bar{x})\} / u_2^Q(y), \quad (7)$$

where the momentum integration is over the surface  $|\bar{y}| = 1$  with the limitation  $|y + x| > 1$ . Here we have introduced the scaled functions

$$u_n^Q(\bar{x}_1, \dots, \bar{x}_n) = -Q^{n(d-2+n)/2-d} \tilde{\epsilon}_n^Q(\bar{x}_1 Q, \dots, \bar{x}_n Q) \quad \left(\sum_i \bar{x}_i = 0\right) \quad (8)$$

for  $n > 2$  and  $u_2^Q(x)$  is defined in the same way in term of  $\tilde{\epsilon}^Q$ . The exponent  $\eta$  is defined as the constant for which  $\lim_{Q \rightarrow 0} Q^{-2+\eta} [\tilde{\epsilon}^Q(xQ) - \tilde{\epsilon}^Q(0)]$  is finite at the critical point. The evolution equation (7) for  $u_2^Q$  and those for the  $u_n^Q$  are equivalent to the RG equations which can be deduced from the theory of Nicoll and Chang.<sup>5</sup> This can be shown by recasting our approximate hierarchy in the form of a differential generator for the free energy  $\tilde{A}$  of an inhomogeneous system. In our case this generator involves the second functional derivative of  $\beta\tilde{A}$  with respect to the local density, this being equal to  $\tilde{\epsilon}$ , in place of the local magnetization as in the case of Nicoll and Chang. The characteristic momentum  $Q$  corresponds to the momentum shell of integration in the RG. Thus the existence of a fixed point for our approximate hierarchy implies a scaling form for the correlation functions in the critical region.<sup>6</sup> The critical behavior given by our approximate hierarchy can be analyzed in the framework of the  $\epsilon = 4 - d$  expansion and in fact, because of the equivalence already discussed, we recover the  $\epsilon$  expansion for the critical exponents as obtained by RG technique for a one-component order parameter. It is known that to first order in  $\epsilon$  the presence of vertices of odd order does not modify the Ising universality class.<sup>7</sup>

So far we have not considered the effect of the core condition. When we use (6) in place of (3) we find that the extra term introduced by the core con-

dition vanishes in the  $Q \rightarrow 0$  limit faster than the other terms provided that

$$\begin{aligned} \tilde{\epsilon}_4^Q(\bar{q}, -\bar{q}, 0, 0) &= \partial^2 \tilde{\epsilon}^Q(q) / \partial \rho^2, \\ \tilde{\epsilon}_3^Q(\bar{q}, 0, -\bar{q}) &= \partial \tilde{\epsilon}^Q(q) / \partial \rho. \end{aligned} \quad (9)$$

These relations are satisfied by the exact correlation functions and we can construct simple decoupling schemes for the full  $\tilde{\epsilon}_n^Q$  and  $\tilde{\epsilon}_n^Q$  compatible with (9), for instance

$$\begin{aligned} \tilde{\epsilon}_4^Q(\bar{q}, -\bar{q}, \bar{k}, -\bar{k}) \\ = \frac{1}{2} [\partial^2 \tilde{\epsilon}^Q(q + \bar{k}) / \partial \rho^2 + \partial^2 \tilde{\epsilon}^Q(q - \bar{k}) / \partial \rho^2] \end{aligned}$$

and

$$\tilde{\epsilon}_3^Q(\bar{q}, \bar{k}, -\bar{q} - \bar{k}) = \partial \tilde{\epsilon}^Q(q + \bar{k}) / \partial \rho.$$

When we use this closure in (4) we obtain a closed equation for  $\tilde{\epsilon}^Q$  from which we can deduce the critical exponents in the framework of the  $\epsilon$  expansion. These turn out to be

$$\begin{aligned} \gamma &= 1 + \frac{1}{6} \epsilon + O(\epsilon^2); \\ \nu &= \frac{1}{2} + \frac{1}{12} \epsilon + O(\epsilon^2); \\ \eta &= \frac{1}{34} \epsilon^2 + O(\epsilon^3), \end{aligned} \quad (10)$$

and these are equal to the Ising values to leading order. An open question is if the basin of attraction of this fixed point also encompasses initial condi-

PRL, 53, 2417 (1984)

⇐ Equation for  $\Gamma^{(2)}(k)$

⇐ BMW approximation