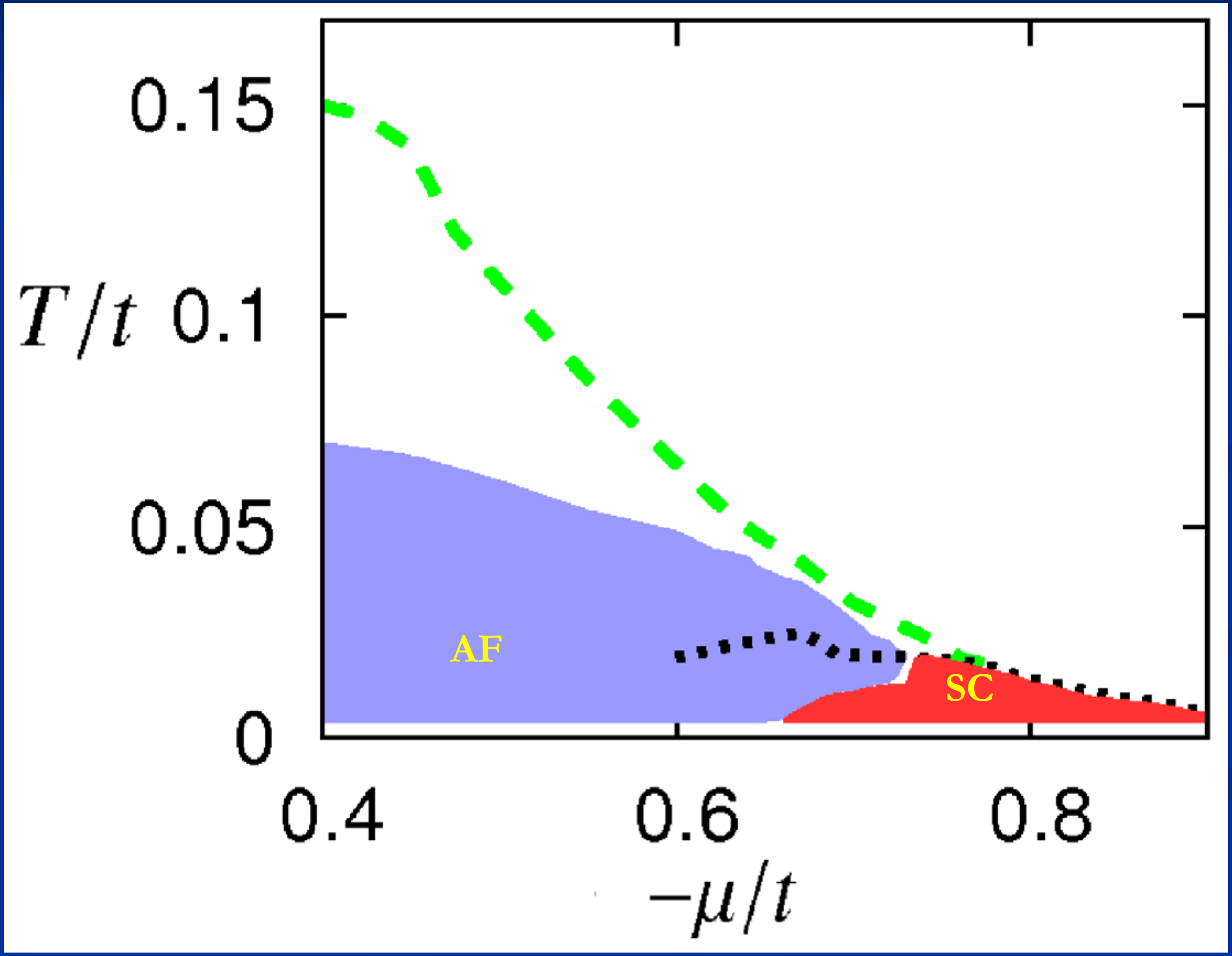
Phase transitions in Hubbard Model

Anti-ferromagnetic and superconducting order in the Hubbard model

A functional renormalization group study

T.Baier, E.Bick, …
C.Krahl, J.Mueller, S.Friederich

Phase diagram

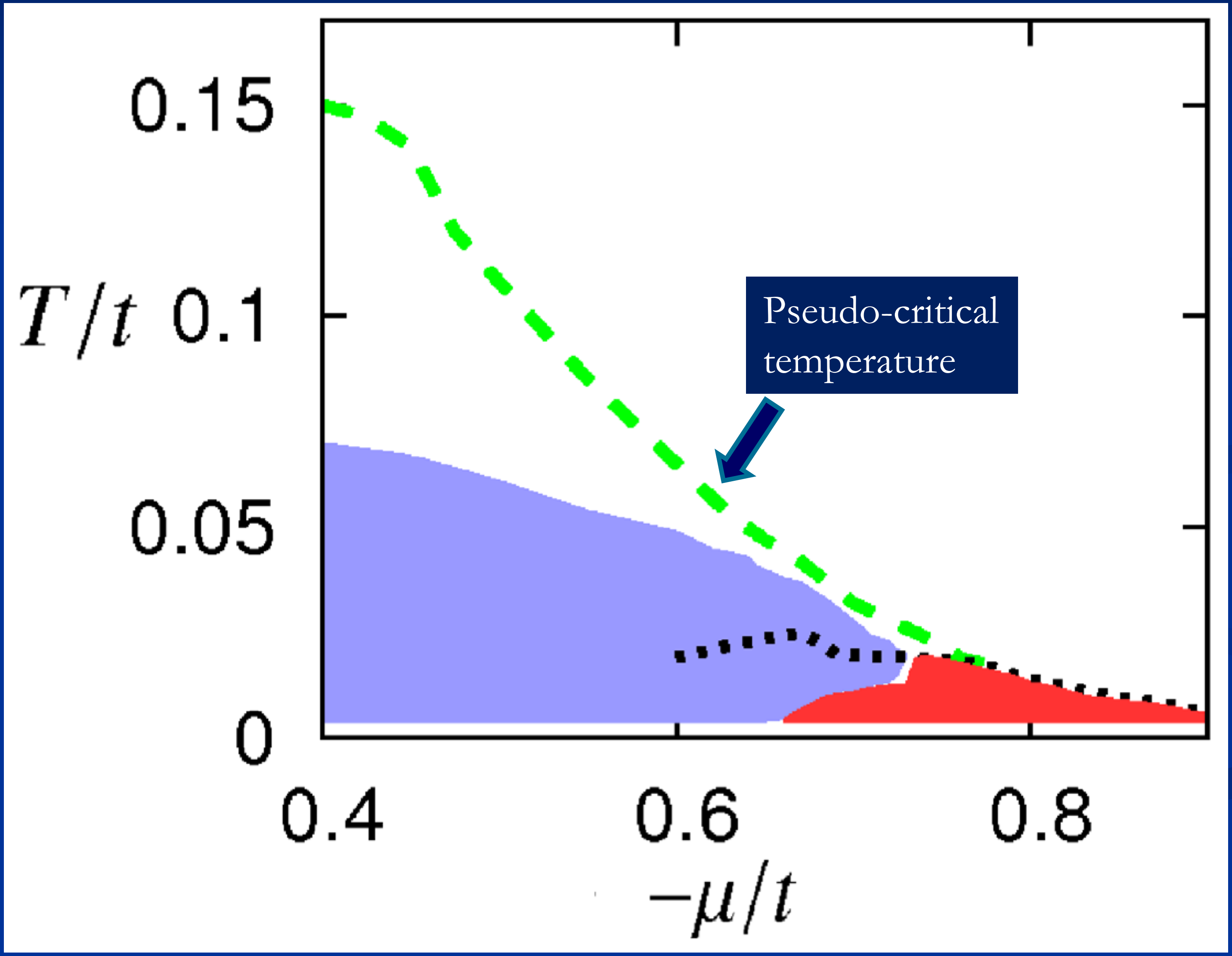


Mermin-Wagner theorem ?

No spontaneous symmetry breaking of continuous symmetry in $d=2$!

not valid in practice !

Phase diagram



Goldstone boson fluctuations

- spin waves (anti-ferromagnetism)
- electron pairs (superconductivity)

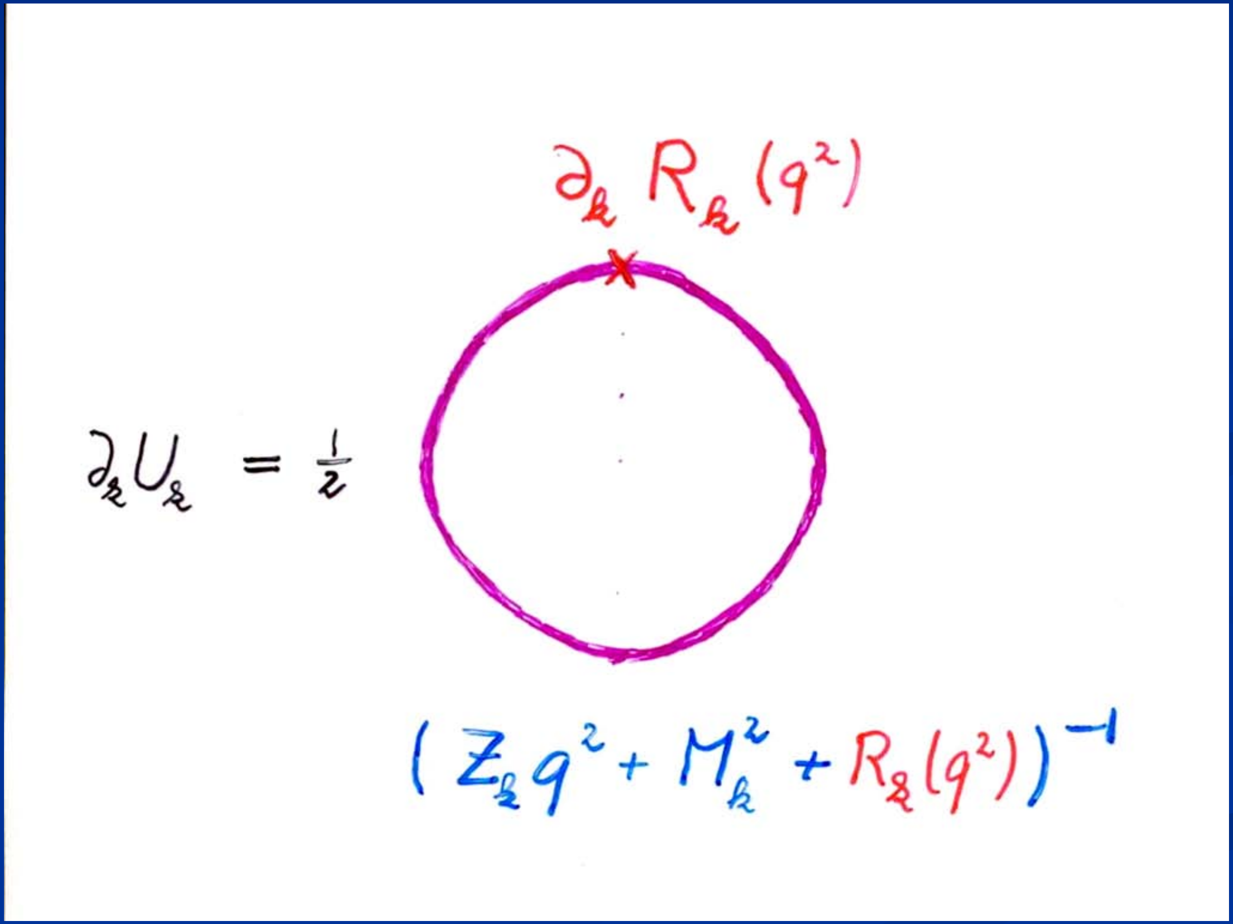
Flow equation for average potential

$$\partial_k U_k(\varphi) = \frac{1}{2}\sum_i \int \frac{d^d q}{(2\pi)^d} \frac{\partial_k R_k(q^2)}{Z_k q^2 + R_k(q^2) + \bar{M}^2_{k,i}(\varphi)}$$

$\bar{M}^2_{k,ab} = \frac{\partial^2 U_k}{\partial\varphi_a \partial\varphi_b}$: Mass matrix

$\bar{M}^2_{k,i}$: Eigenvalues of mass matrix

Simple one loop structure – nevertheless (almost) exact



Scaling form of evolution equation

$$u = \frac{U_k}{k^d}$$
$$\tilde{\rho} = Z_k k^{2-d} \rho$$
$$u' = \frac{\partial u}{\partial \tilde{\rho}} \quad \text{etc.}$$

$$\partial_t u|_{\tilde{\rho}} = -du + (d-2+\eta)\tilde{\rho}u' + 2v_d\{l_0^d(u' + 2\tilde{\rho}u''; \eta) + (N-1)\, l_0^d(u'; \eta)\}$$

$$v_d^{-1} = 2^{d+1}\pi^{d/2}\Gamma\left(\frac{d}{2}\right)$$

linear cutoff:

$$l_0^d(w;\eta) = \frac{2}{d}\left(1 - \frac{\eta}{d+2}\right)\frac{1}{1+w}$$

On r.h.s. :
neither the scale k
nor the wave function
renormalization Z
appear explicitly.

Scaling solution:
no dependence on t;
corresponds
to second order
phase transition.

Tetradis …

Solution of partial differential equation :

yields highly nontrivial non-perturbative results despite the one loop structure !

Example:
Kosterlitz-Thouless phase transition

Anti-ferromagnetism in Hubbard model

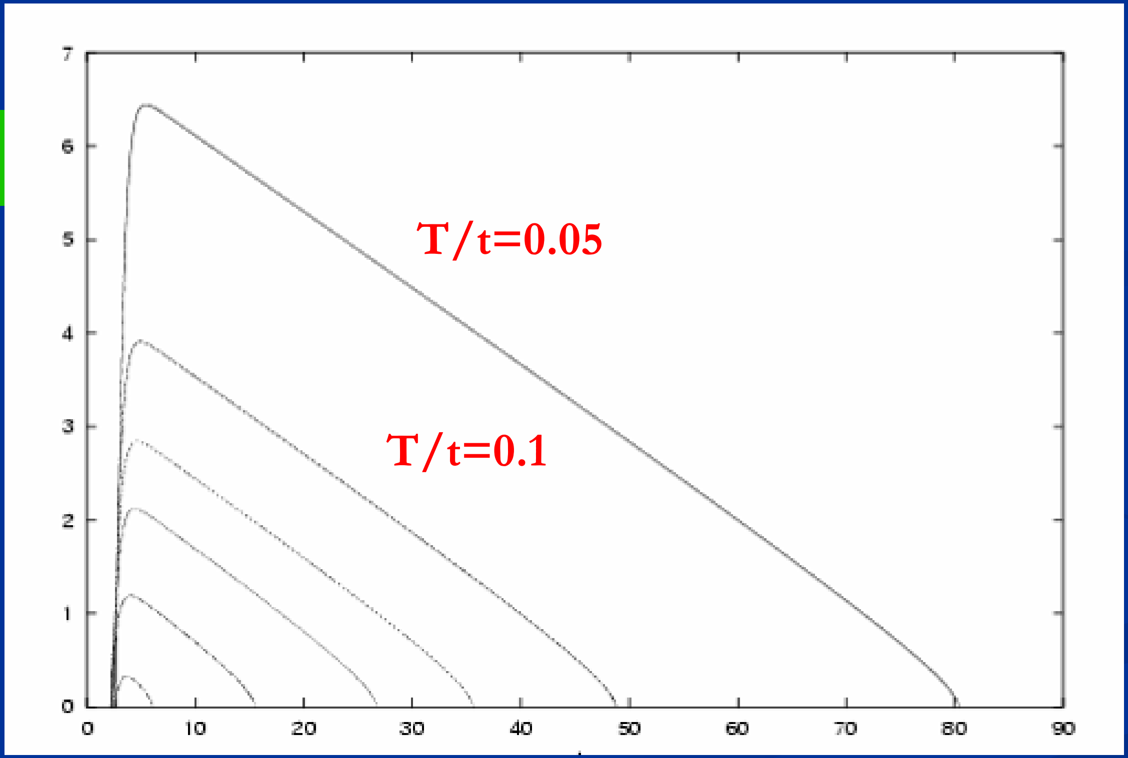
- SO(3) – symmetric scalar model coupled to fermions
- For low enough k : fermion degrees of freedom decouple effectively
- crucial question : running of $\varkappa$ (location of minimum of effective potential , renormalized , dimensionless)

Critical temperature

For $T<T_c$: $\varkappa$ remains positive for $k/t > 10^{-9}$

size of probe > 1 cm

$\varkappa$



local disorder
pseudo gap

SSB

-ln(k/t)

$$\kappa_a = \frac{Z_a t^2}{T} \alpha_0$$

T_c=0.115

Below the pseudocritical temperature

the reign of the goldstone bosons

effective nonlinear O(3) – σ - model

critical behavior

for interval $T_c < T < T_{pc}$
evolution as for classical Heisenberg model

cf. Chakravarty,Halperin,Nelson

$$k\partial_k\kappa = \frac{1}{4\pi} + \frac{1}{16\pi^2\kappa} + 0(\kappa^{-2})$$

critical correlation length

$$\xi t = c(T) \exp\left\{20.7\beta(T)\frac{T_c}{T}\right\}$$

c,β : slowly varying functions

exponential growth of correlation length
compatible with observation !

at T_c : correlation length reaches sample size !

Mermin-Wagner theorem ?

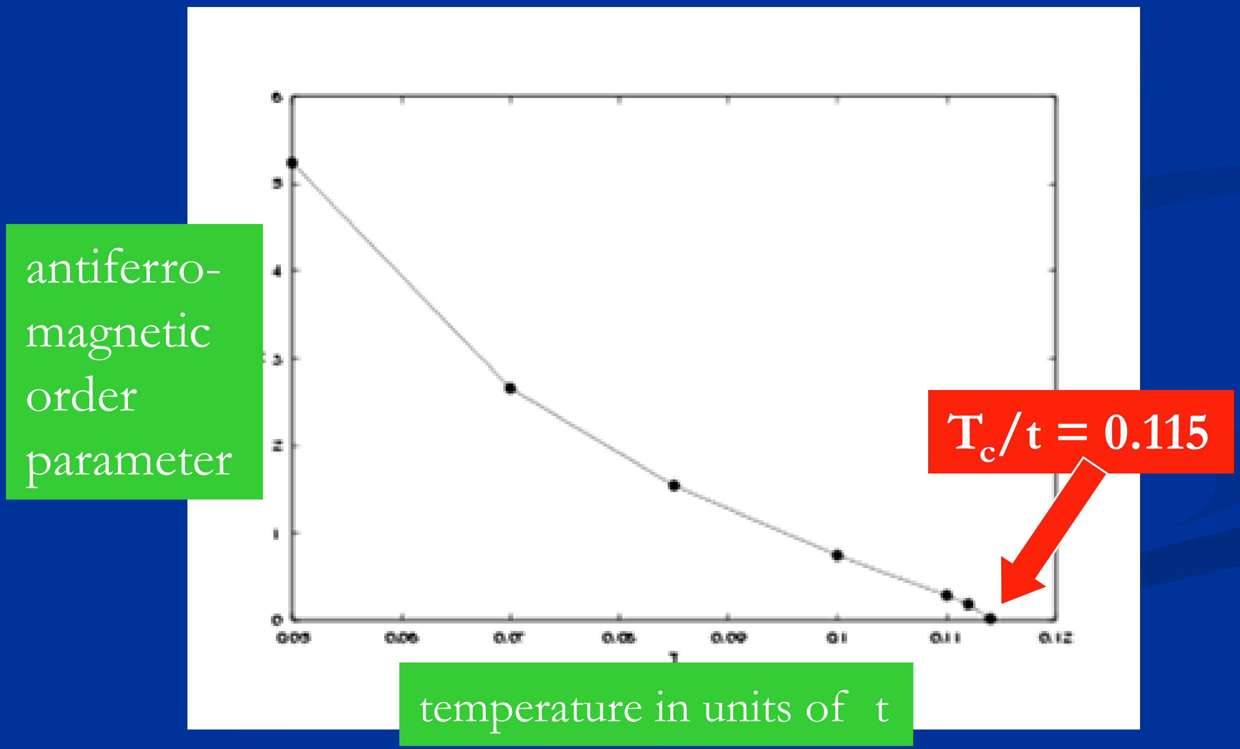
No spontaneous symmetry breaking of continuous symmetry in d=2 !

not valid in practice !

Below the critical temperature :

Infinite-volume-correlation-length becomes larger than sample size

finite sample ≈ finite k : order remains effectively



Action for Hubbard model

$$
\begin{aligned}
S &= \sum_Q \hat{\psi}^\dagger(Q)[i\omega_Q + \xi_Q]\hat{\psi}(Q) \\
&\quad + \frac{U}{2} \sum_{K_1,K_2,K_3,K_4} [\hat{\psi}^\dagger(K_1)\hat{\psi}(K_2)]\,[\hat{\psi}^\dagger(K_3)\hat{\psi}(K_4)] \\
&\quad \times \delta\,(K_1 - K_2 + K_3 - K_4)\ ,
\end{aligned}
$$

$$
\hat{\psi}(Q) = \left(\hat{\psi}_\uparrow(Q), \hat{\psi}_\downarrow(Q)\right)^T
$$

$$
\xi(\mathbf{q}) = -\mu - 2t(\cos q_x + \cos q_y) - 4t' \cos q_x \cos q_y
$$

$$
\sum_Q = T \sum_{n=-\infty}^{\infty} \int_{-\pi}^{\pi} \frac{d^2q}{(2\pi)^2}\ ,
$$

$$
\delta(Q - Q') = T^{-1}\delta_{n,n'}(2\pi)^2\delta^{(2)}(\mathbf{q} - \mathbf{q}')
$$

Truncation for flowing action

$$\Gamma_k[\chi] = \Gamma_{F,k} + \Gamma_{Fm,k} + \Gamma_{F\rho,k} + \Gamma_{Fs,k} + \Gamma_{Fd,k} + \Gamma_{a,k} + \Gamma_{\rho,k} + \Gamma_{s,k} + \Gamma_{d,k} + \sum_X U_{B,k}(\mathbf{a}, \rho, s, d)$$

$$\Gamma_F = \Gamma_{F\mathrm{kin}} + \Gamma_F^U$$

$$\Gamma_{F\mathrm{kin}} = \sum_Q \psi^\dagger(Q) P_F(Q) \psi(Q)$$

$$P_F(Q) = Z_F(\omega_Q)\left(i\omega_Q + \xi(\mathbf{q})\right)$$

$$\Gamma_F^U = \frac{1}{2} \sum_{K_1,K_2,K_3,K_4} U\,\delta\,(K_1 - K_2 + K_3 - K_4) \times [\psi^\dagger(K_1)\psi(K_2)]\,[\psi^\dagger(K_3)\psi(K_4)]\,.$$

Additional bosonic fields

- anti-ferromagnetic
- charge density wave
- s-wave superconducting
- d-wave superconducting

initial values for flow : bosons are decoupled auxiliary fields (microscopic action)

Effective potential for bosons

$$\sum_X U_B(\mathbf{a},\rho,s,d) = \sum_Q \frac{1}{2}\Big(\bar{m}_a^2\,\mathbf{a}^T(-Q)\mathbf{a}(Q) + \bar{m}_\rho^2\,\rho(-Q)\rho(Q)\Big)$$
$$+\bar{m}_s^2\,s^*(Q)s(Q) + \bar{m}_d^2\,d^*(Q)d(Q)$$
$$+\frac{1}{2}\sum_{Q_1,Q_2,Q_3,Q_4}\delta\,(Q_1+Q_2+Q_3+Q_4)$$
$$\times\Big(\bar{\lambda}_a\,\alpha(Q_1,Q_2)\alpha(Q_3,Q_4) \qquad (23)$$
$$+\bar{\lambda}_d\,\delta(Q_1,Q_2)\delta(Q_3,Q_4)$$
$$+2\bar{\lambda}_{ad}\,\alpha(Q_1,Q_2)\delta(Q_3,Q_4)\Big)\,,$$

SYM

microscopic :
only "mass terms"

$$\sum_X U_B(\mathbf{a},d) = \frac{1}{2}\sum_{Q_1,Q_2,Q_3,Q_4}\delta\,(Q_1+Q_2+Q_3+Q_4)$$
$$\Big(\bar{\lambda}_a\{\alpha(Q_1,Q_2)-\alpha_0\delta(Q_1)\delta(Q_2)\}$$
$$\times\{\alpha(Q_3,Q_4)-\alpha_0\delta(Q_3)\delta(Q_4)\}$$
$$+\bar{\lambda}_d\{\delta(Q_1,Q_2)-\delta_0\delta(Q_1)\delta(Q_2)\} \qquad (24)$$
$$\times\{\delta(Q_3,Q_4)-\delta_0\delta(Q_3)\delta(Q_4)\}$$
$$+2\bar{\lambda}_{ad}\{\alpha(Q_1,Q_2)-\alpha_0\delta(Q_1)\delta(Q_2)\}$$
$$\times\{\delta(Q_3,Q_4)-\delta_0\delta(Q_3)\delta(Q_4)\}\Big)\,.$$

SSB

Yukawa coupling between fermions and bosons

$$
\begin{aligned}
\Gamma_{Fa} &= -\sum_{K,Q,Q'} \bar{h}_a(K)\, \mathbf{a}(K) \cdot [\psi^\dagger(Q)\boldsymbol{\sigma}\psi(Q')] \\
&\qquad\qquad \delta(K - Q + Q' + \Pi)\,, \\
\Gamma_{F\rho} &= -\sum_{K,Q,Q'} \bar{h}_\rho(K)\, \rho(K)\, [\psi^\dagger(Q)\psi(Q')]\, \delta(K - Q + Q')\,, \\
\Gamma_{Fs} &= -\sum_{K,Q,Q'} \bar{h}_s(K) \left(s^*(K)\, [\psi^T(Q)\epsilon\psi(Q')] \right. \qquad (12) \\
&\qquad \left. - s(K)\, [\psi^\dagger(Q)\epsilon\psi^*(Q')] \right) \delta(K - Q - Q')\,, \\
\Gamma_{Fd} &= -\sum_{K,Q,Q'} \bar{h}_d(K) f_d\, ((Q - Q')/2) \left(d^*(K)\, [\psi^T(Q)\epsilon\psi(Q')] \right. \\
&\qquad \left. - d(K)\, [\psi^\dagger(Q)\epsilon\psi^*(Q')] \right) \delta(K - Q - Q')\,,
\end{aligned}
$$

$$
f_d(Q) = f_d(\mathbf{q}) = \frac{1}{2}\left(\cos(q_x) - \cos(q_y)\right)
$$

Microscopic Yukawa couplings vanish !

Kinetic terms for bosonic fields

$$\Gamma_a = \frac{1}{2}\sum_Q \mathbf{a}^T(-Q)P_a(Q)\mathbf{a}(Q)\,,$$

$$\Gamma_\rho = \frac{1}{2}\sum_Q \rho(-Q)P_\rho(Q)\rho(Q)\,,$$

$$\Gamma_s = \sum_Q s^*(Q)P_s(Q)s(Q)\,,$$

$$\Gamma_d = \sum_Q d^*(Q)P_d(Q)d(Q)\,.$$

anti-ferromagnetic boson

d-wave superconducting boson

$$\mathbf{a}(Q) = \mathbf{m}(Q+\Pi)$$

incommensurate anti-ferromagnetism

$$P_a(Q) = Z_a \omega_Q^2 + A_a F(\mathbf{q})$$

commensurate regime :

$$F_c(\mathbf{q}) = \frac{D_a^2 \cdot [\mathbf{q}]^2}{D_a^2 + [\mathbf{q}]^2}$$

$$[\mathbf{q}]^2 = q_x^2 + q_y^2 \text{ for } q_{x,y} \in [-\pi, \pi]$$

incommensurate regime :

$$F_i(\mathbf{q}, \hat{q}) = \frac{D_a^2 \tilde{F}(\mathbf{q}, \hat{q})}{D_a^2 + \tilde{F}(\mathbf{q}, \hat{q})},$$

$$\tilde{F}(\mathbf{q}, \hat{q}) = \frac{1}{4\hat{q}^2}((\hat{q}^2 - [\mathbf{q}]^2)^2 + 4[q_x]^2[q_y]^2)$$

$$D_a = \frac{1}{A_a}\left(\tilde{P}_a(0, \pi, \pi) - \tilde{P}_a(0, \hat{q}, 0)\right)$$

infrared cutoff

$$R_k^F(Q) = \mathrm{sgn}(\xi(\mathbf{q}))\,(\mathrm{k} - |\xi(\mathbf{q})|)\,\Theta(\mathrm{k} - |\xi(\mathbf{q})|)$$

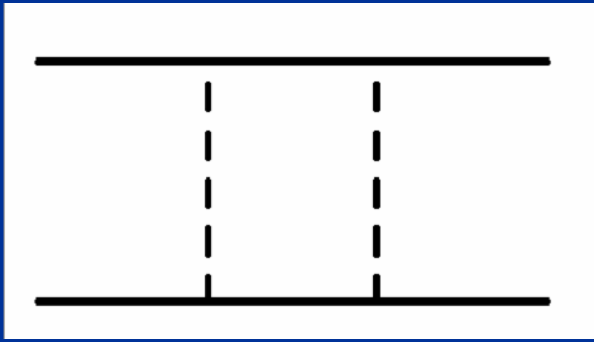
$$R_k^{a/\rho}(Q) = A_{a/\rho} \cdot (k^2/t^2 - F_{c/i}(\mathbf{q},\hat{q}))\Theta(k^2/t^2 - F_{c/i}(\mathbf{q},\hat{q}))$$

linear cutoff (Litim)

flowing bosonisation

effective four-fermion coupling

in appropriate channel



is translated to bosonic

interaction at every scale k

H.Gies , …

$$\Gamma_k[\psi,\psi^*,\phi] = \sum_Q \psi^*(Q)P_{\psi,k}\psi(Q) + \frac{1}{2}\sum_Q \phi(-Q)P_{\phi,k}(Q)\phi(Q) - \sum_Q h_k(Q)\phi(Q)\tilde{\phi}(-Q) + \sum_Q \lambda_{\psi,k}(Q)\tilde{\phi}(Q)\tilde{\phi}(-Q)$$

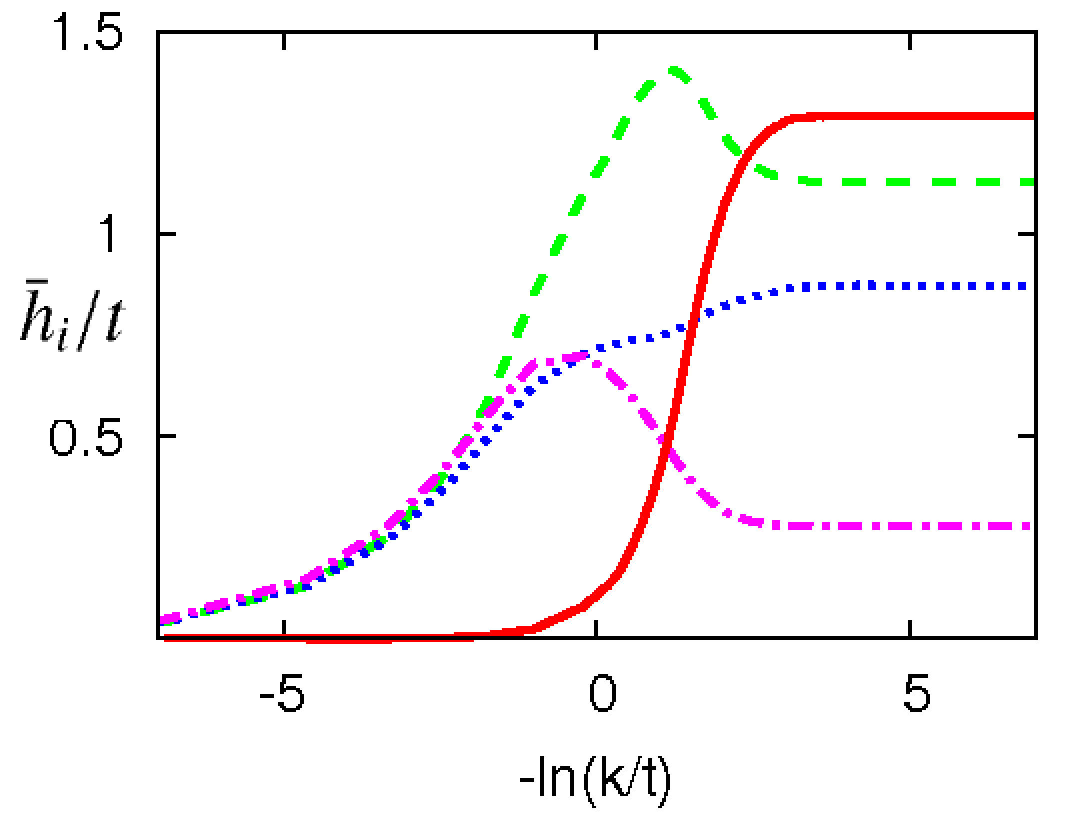
k-dependent field redefinition

$$\phi_k(Q) = \phi_{\bar{k}}(Q) + \Delta\alpha_k(Q)\tilde{\phi}(Q)$$

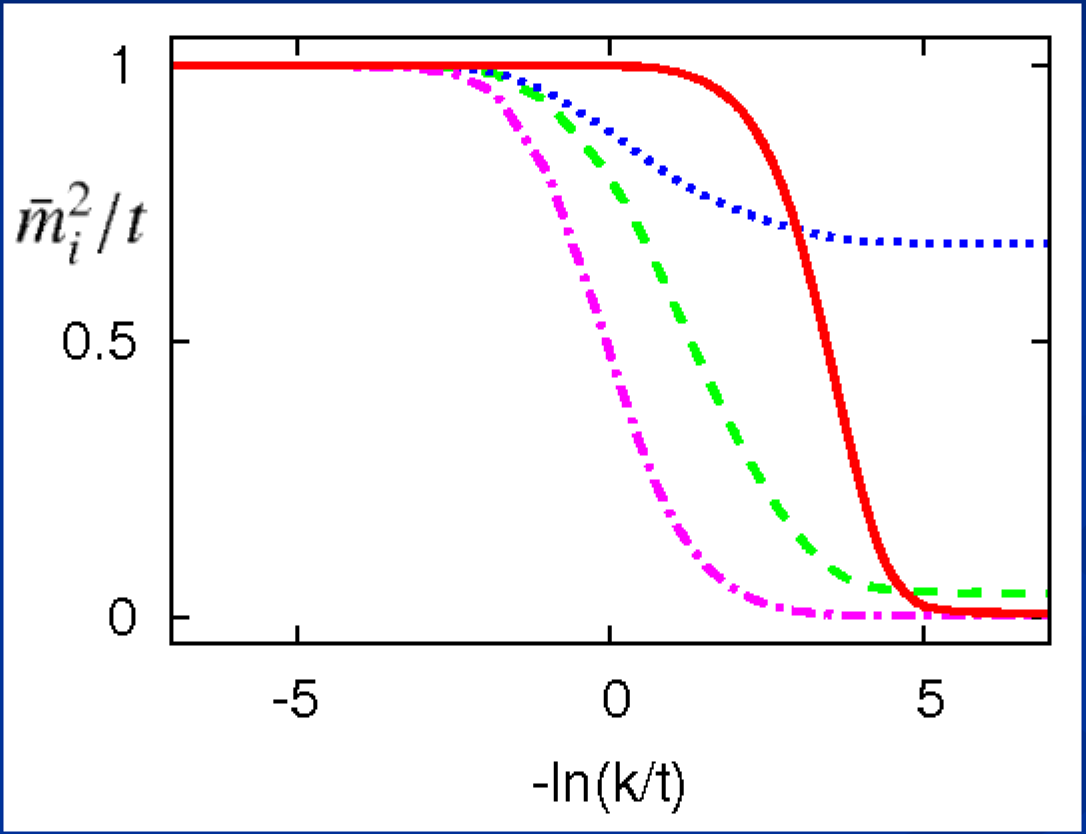
$$\partial_k\phi_k(Q) = -\,\partial_k\alpha_k(Q)\tilde{\phi}(Q)$$

absorbs four-fermion coupling

running Yukawa couplings



flowing boson mass terms



SYM : close to phase transition

Pseudo-critical temperature T_{pc}

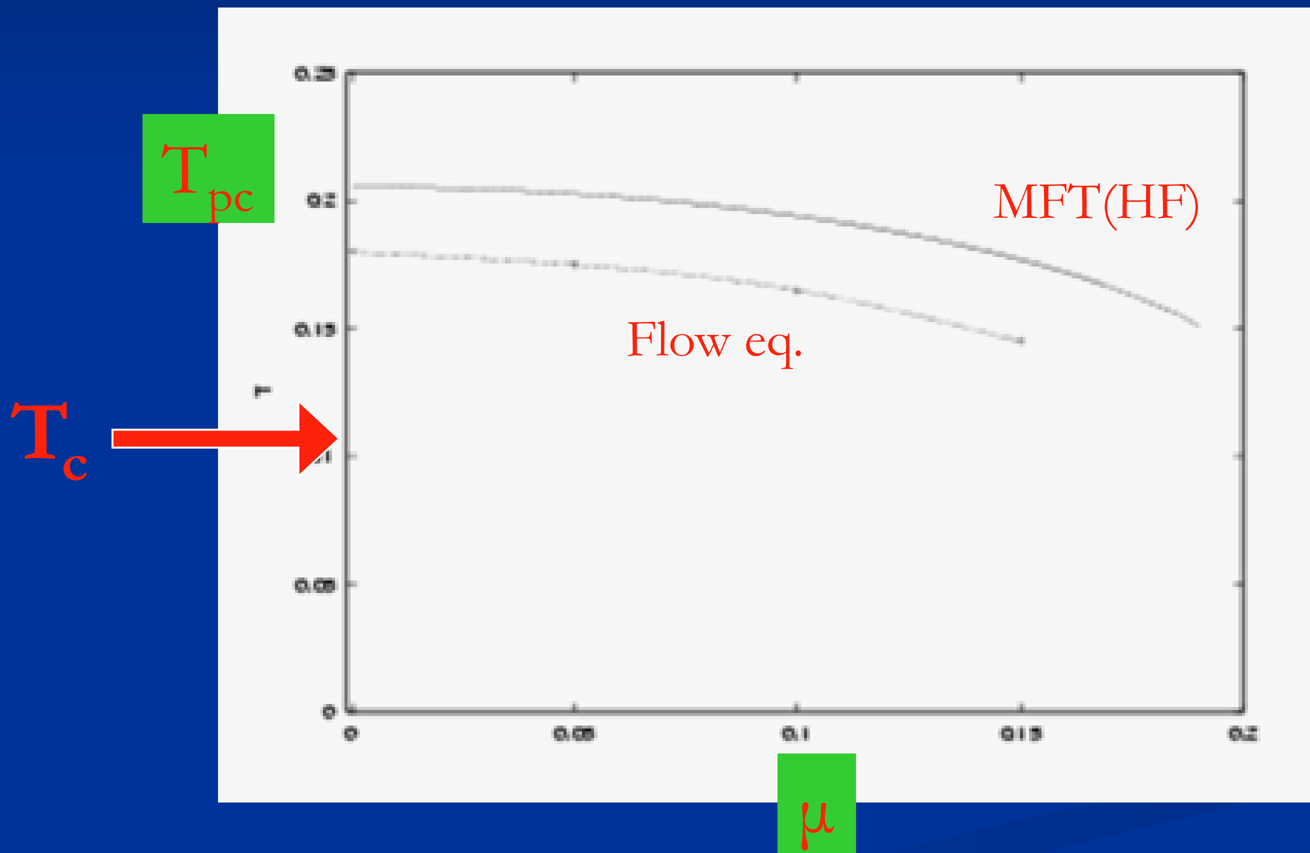
Limiting temperature at which bosonic mass term vanishes ($\varkappa$ becomes nonvanishing)

It corresponds to a diverging four-fermion coupling

This is the "critical temperature" computed in MFT !

Pseudo-gap behavior below this temperature

Pseudocritical temperature

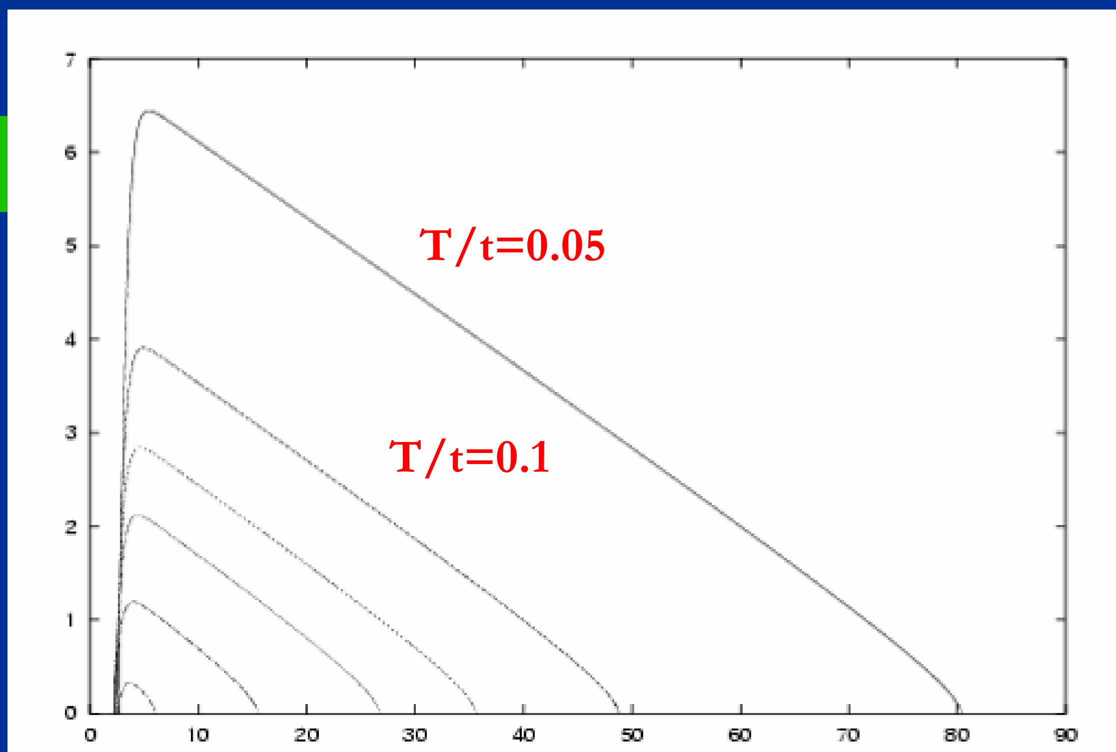


Critical temperature

For $T<T_c$: $\varkappa$ remains positive for $k/t > 10^{-9}$

size of probe > 1 cm

$\varkappa$



-ln(k/t)

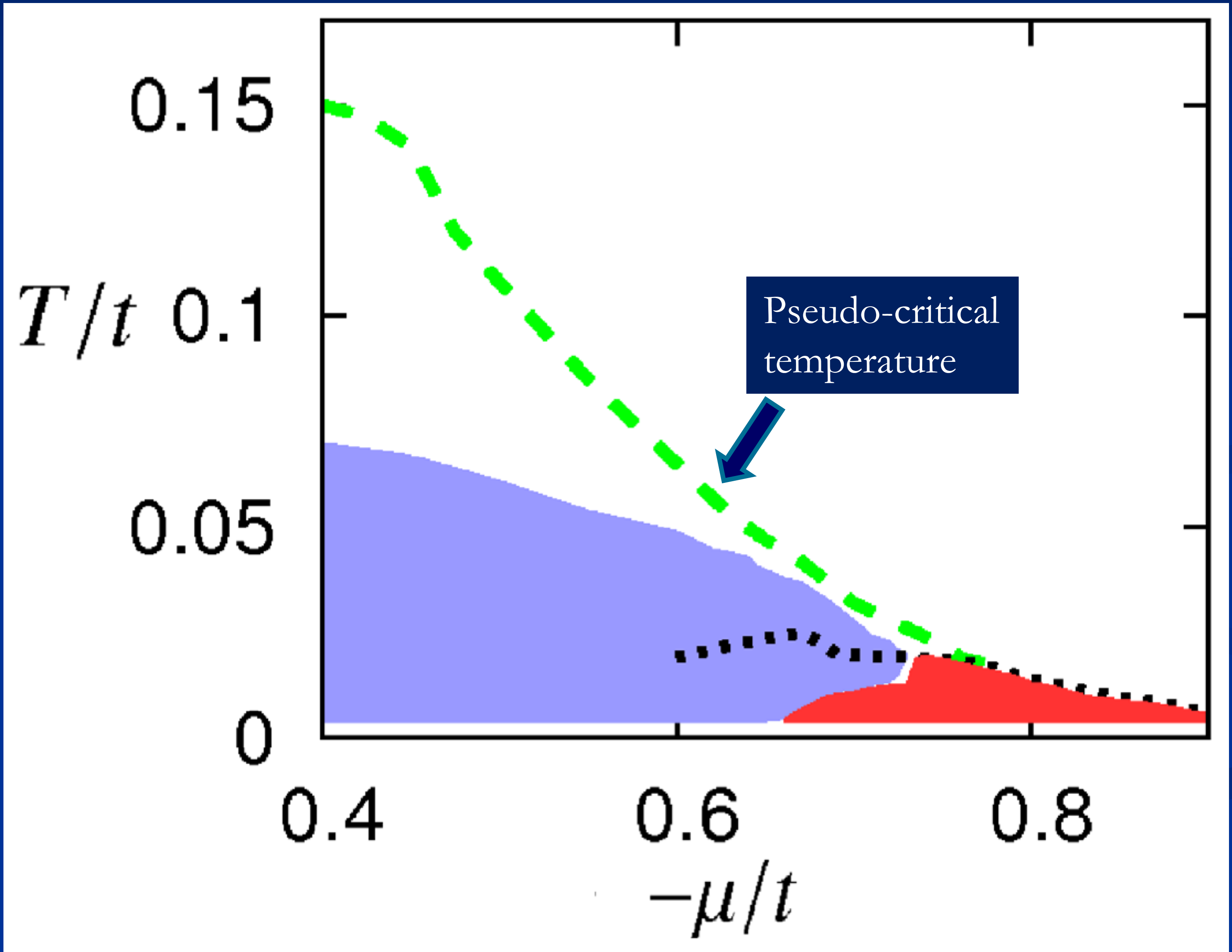
local disorder
pseudo gap

SSB

$$\kappa_a = \frac{Z_a t^2}{T} \alpha_0$$

T_c=0.115

Phase diagram



spontaneous symmetry breaking of abelian continuous symmetry in d=2

$$u = \frac{U_k}{k^d}$$
$$\tilde{\rho} = Z_k k^{2-d} \rho$$
$$u' = \frac{\partial u}{\partial \tilde{\rho}} \quad \text{etc.}$$

$$\partial_t u|_{\tilde{\rho}} = -du + (d - 2 + \eta)\tilde{\rho}u' + 2v_d\{l_0^d(u' + 2\tilde{\rho}u''; \eta) + (N-1)\, l_0^d(u';\eta)\}$$

$$v_d^{-1} = 2^{d+1}\pi^{d/2}\,\Gamma\left(\frac{d}{2}\right)$$

linear cutoff:

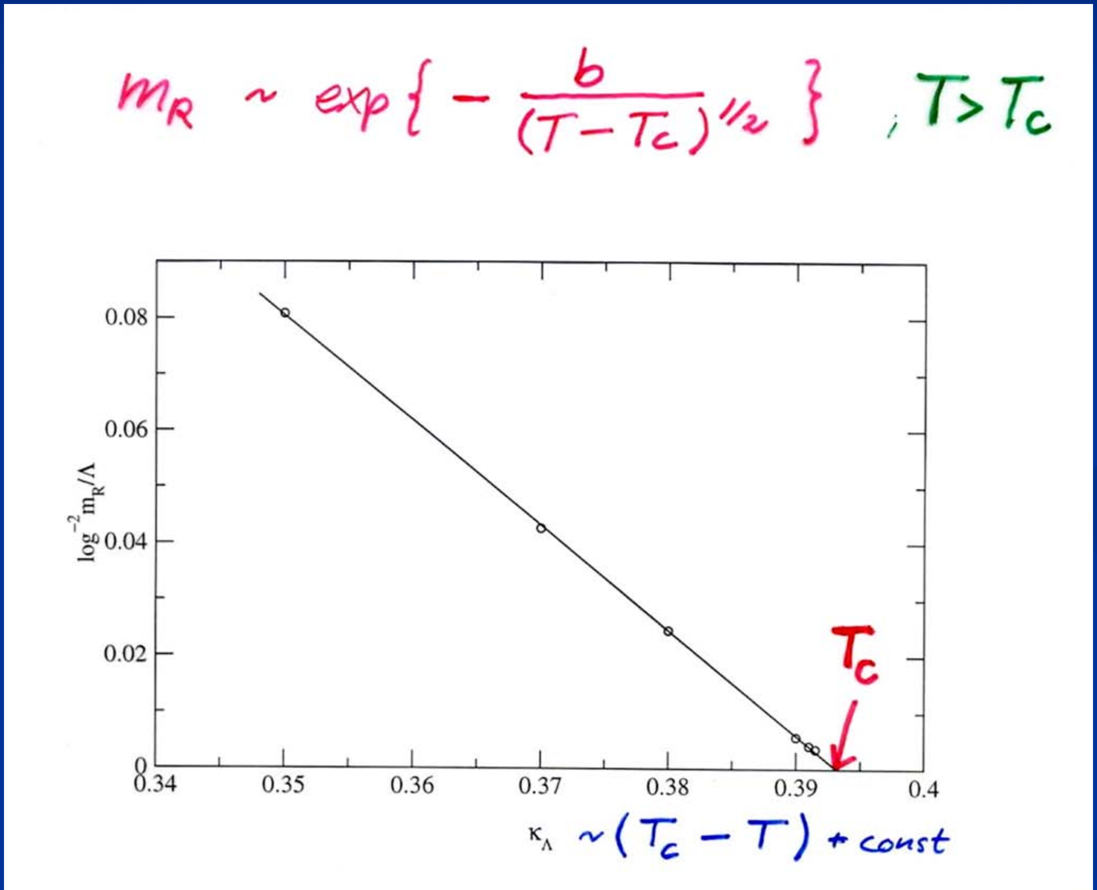
$$l_0^d(w;\eta) = \frac{2}{d}\left(1 - \frac{\eta}{d+2}\right)\frac{1}{1+w}$$

Bose –Einstein condensate

Superconductivity in Hubbard model

Kosterlitz – Thouless phase transition

Essential scaling : d=2,N=2



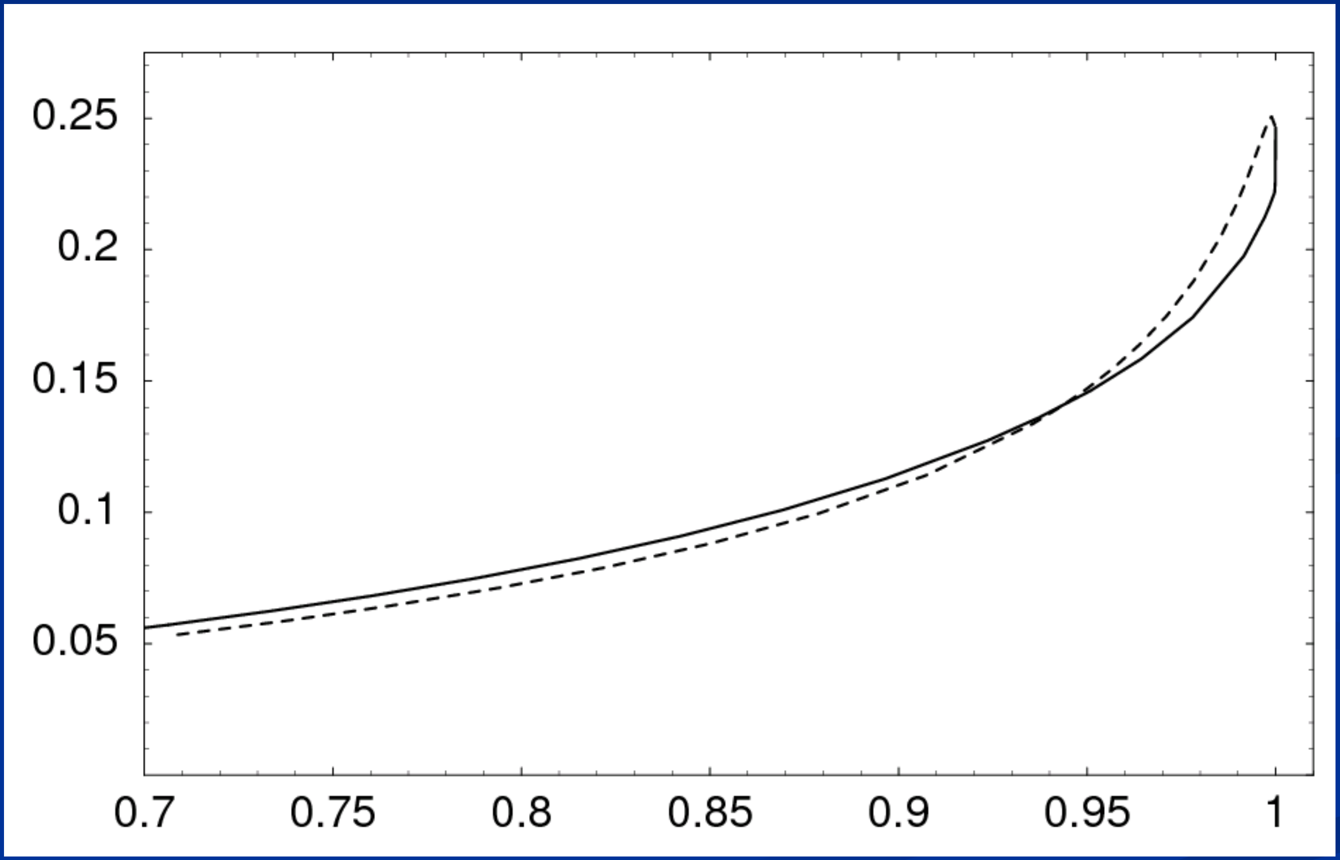
- Flow equation contains correctly the non-perturbative information !
- (essential scaling usually described by vortices)

Von Gersdorff …

Kosterlitz-Thouless phase transition (d=2,N=2)

Correct description of phase with
Goldstone boson
(infinite correlation length)
for $T<T_c$

Temperature dependent anomalous dimension η



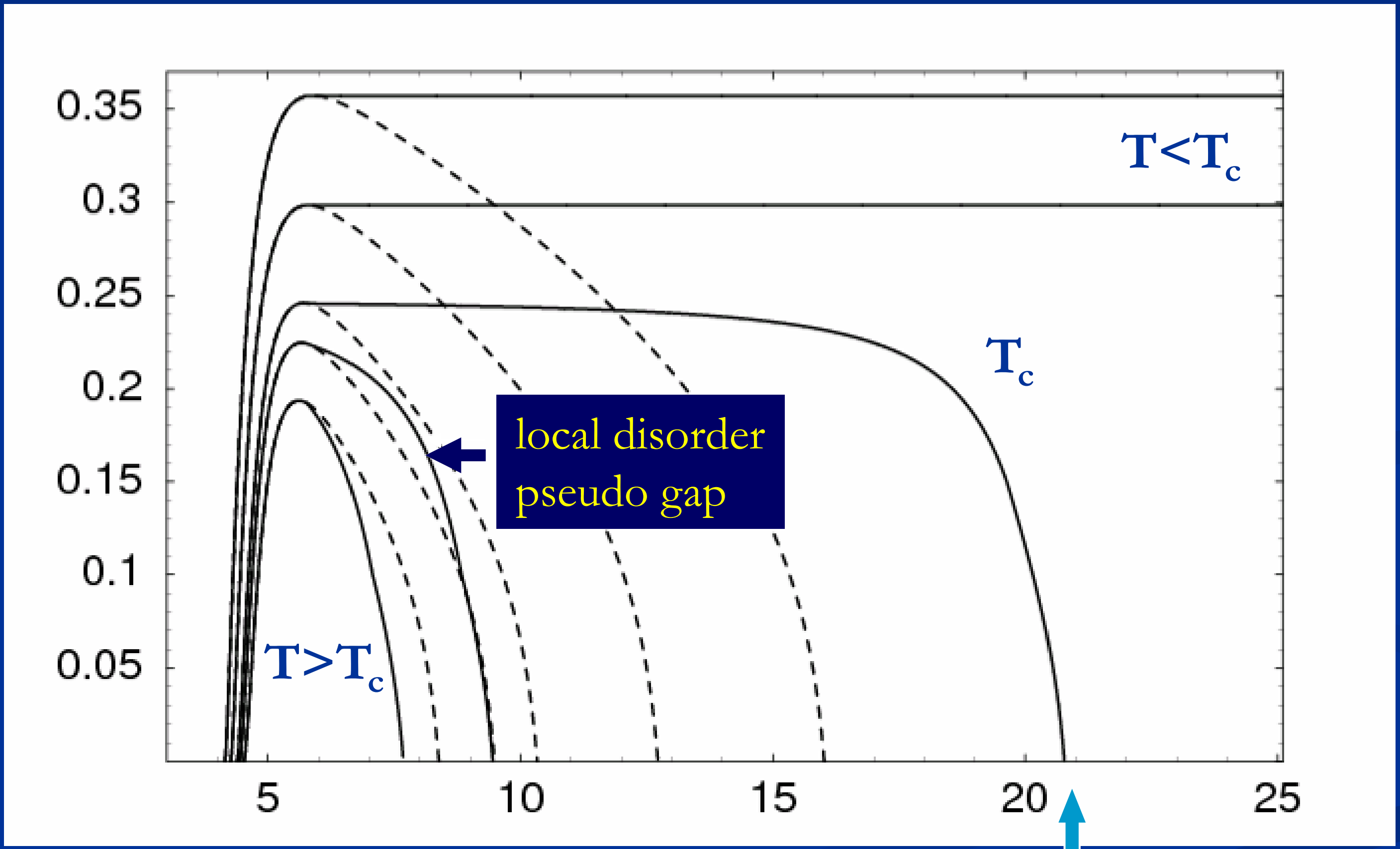
η

T/T_c

Running renormalized d-wave superconducting order parameter $\varkappa$ in doped Hubbard (-type) model

$\varkappa$

location of minimum of u

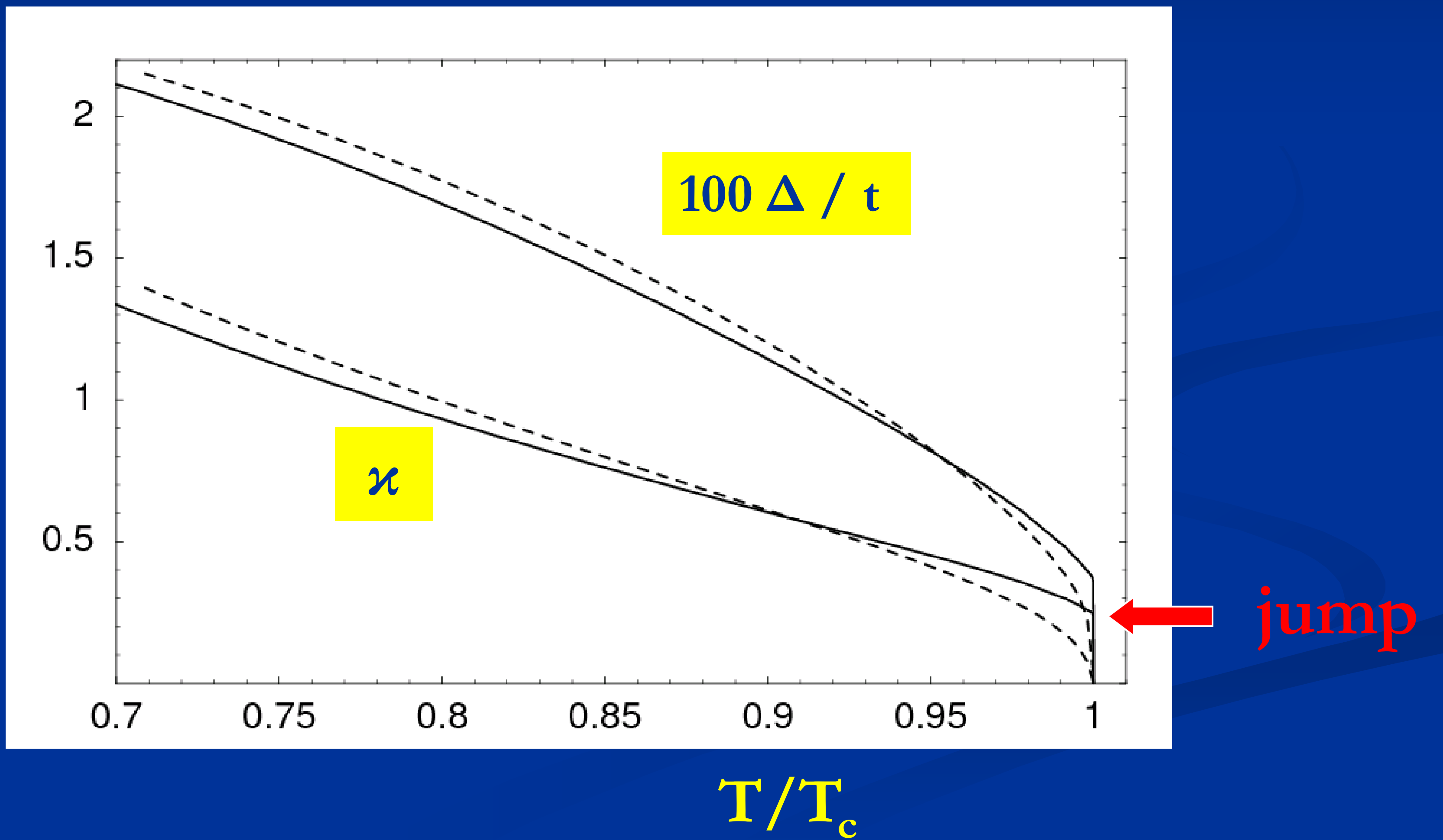


C.Krahl,…

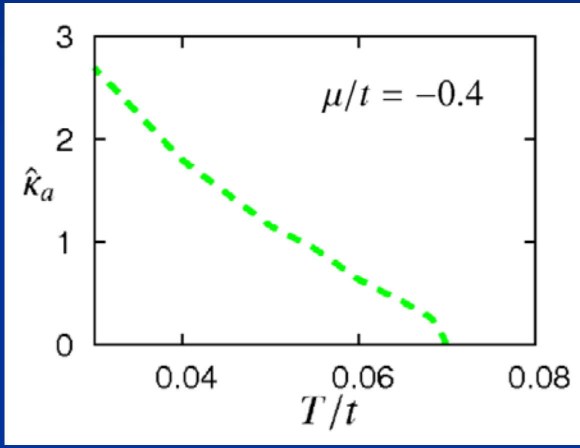
- ln (k/Λ)

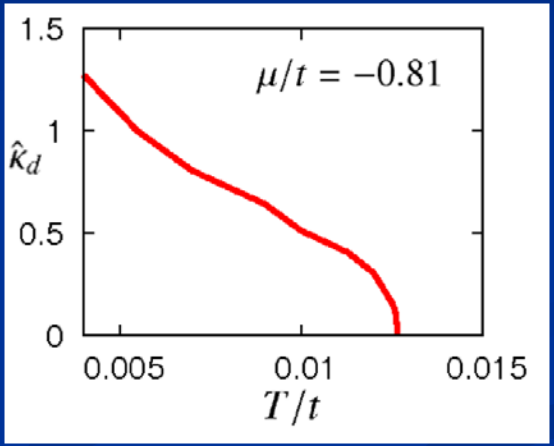
macroscopic scale 1 cm

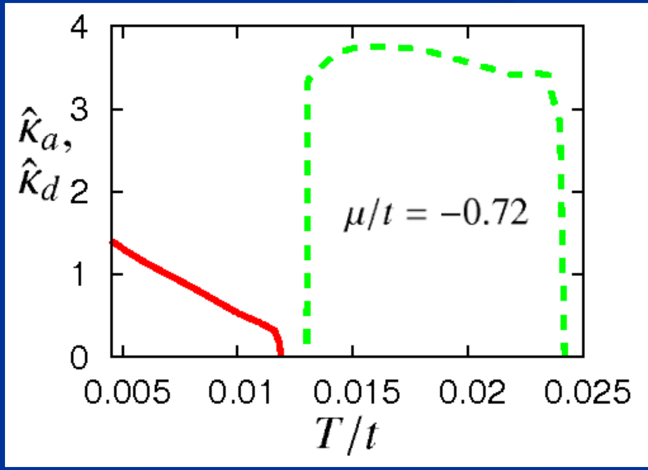
Renormalized order parameter $\varkappa$ and gap in electron propagator Δ in doped Hubbard-type model



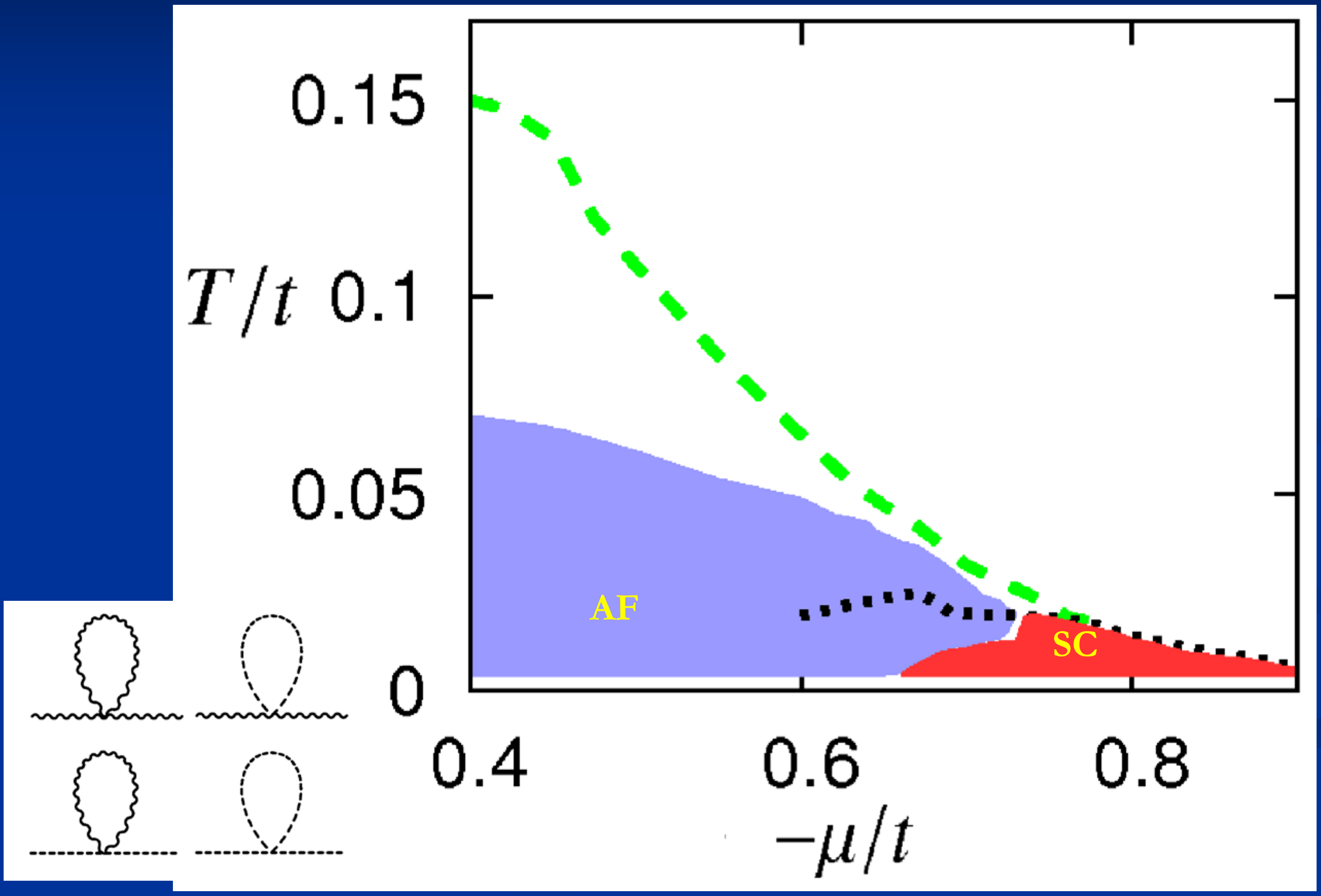
order parameters in Hubbard model



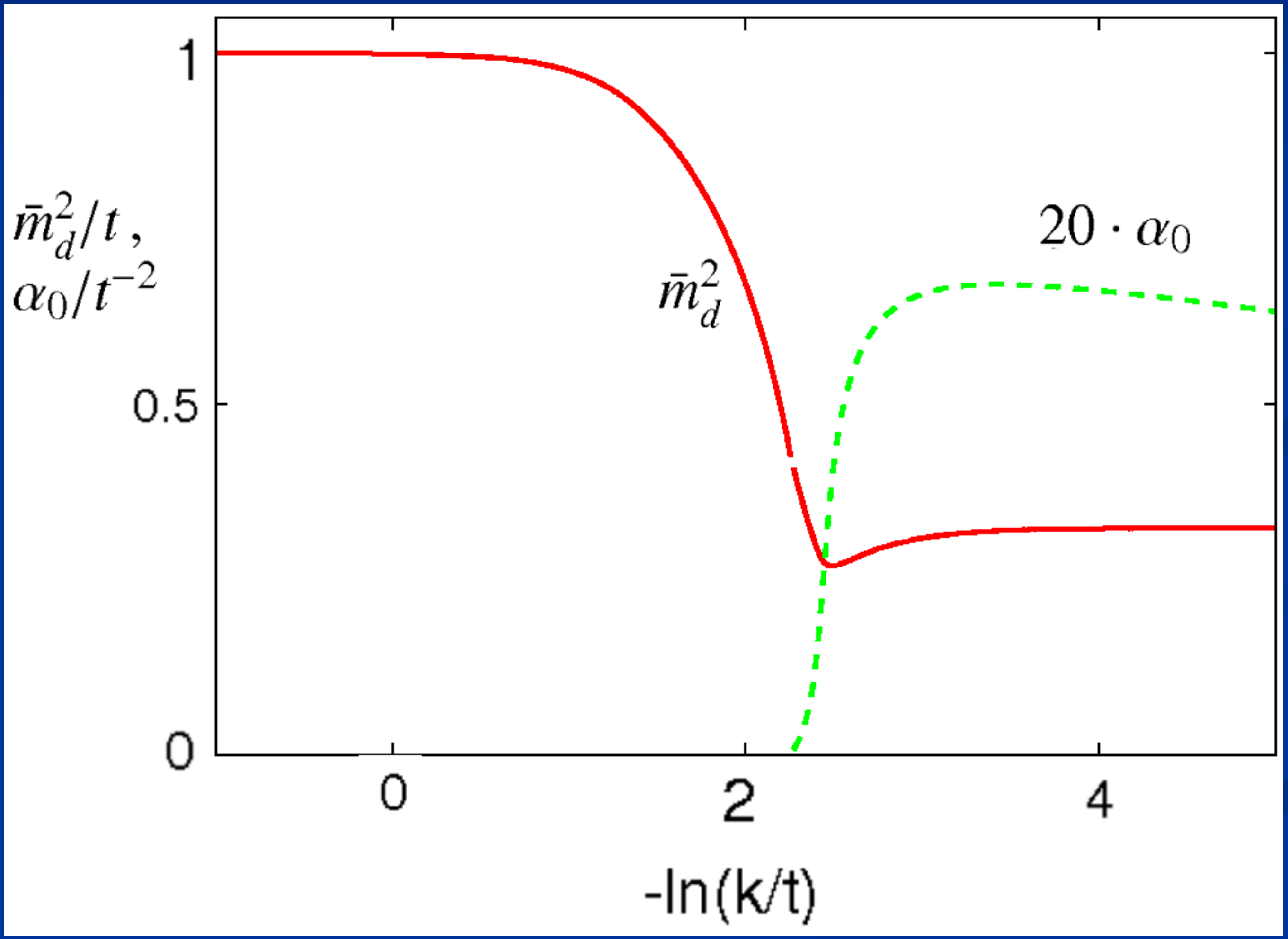




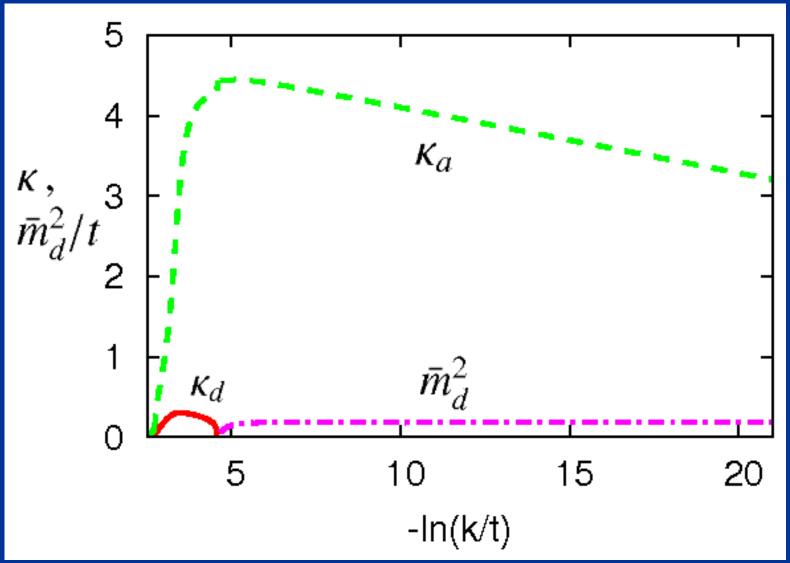
Competing orders

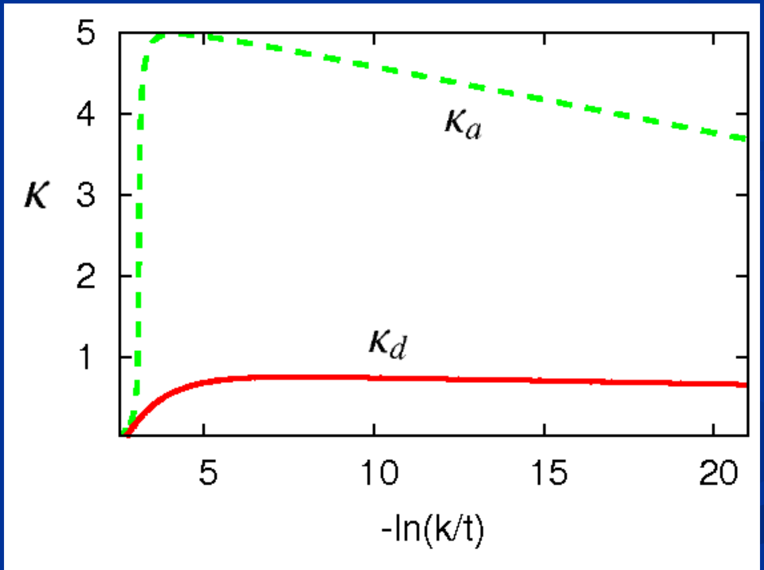


Anti-ferromagnetism suppresses superconductivity

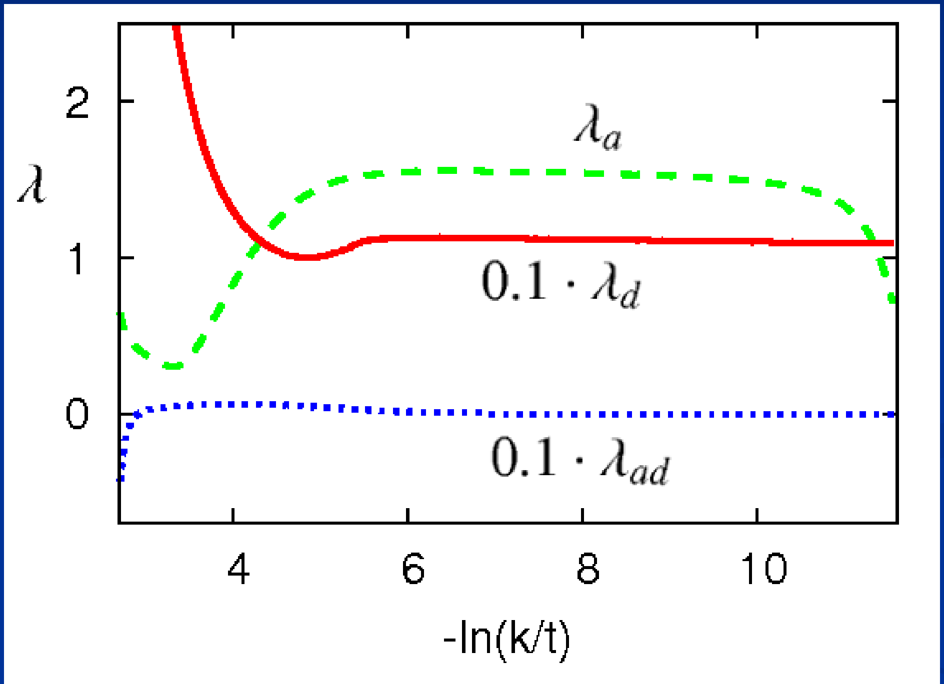


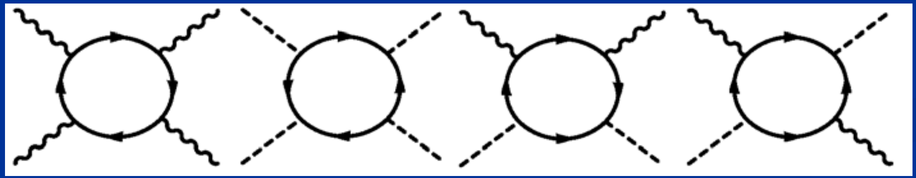
coexistence of different orders ?

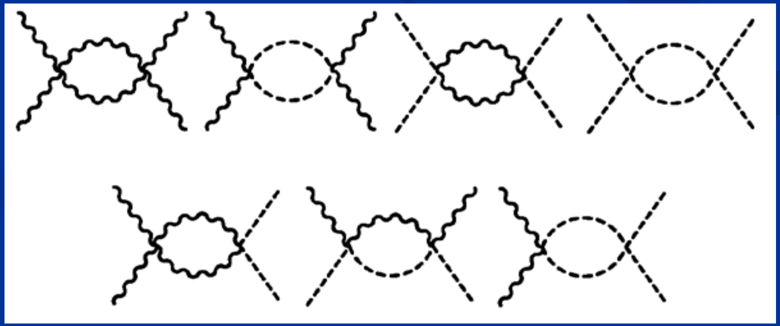




quartic couplings for bosons







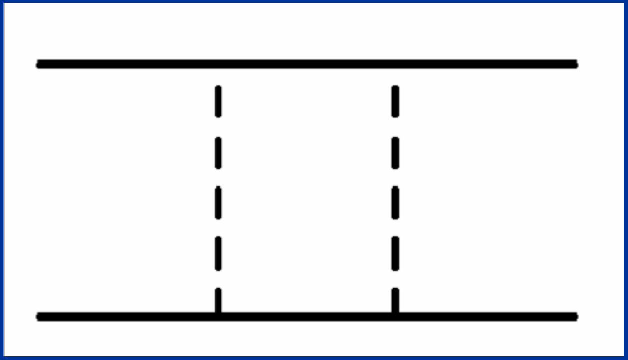
conclusions

- functional renormalization gives access to low temperature phases of Hubbard model
- order parameters can be computed as function of temperature and chemical potential
- competing orders
- further quantitative progress possible

changing degrees of freedom

flowing bosonisation

- adapt bosonisation to every scale k such that



is translated to bosonic interaction

H.Gies , …

$$\begin{aligned}\Gamma_k[\psi,\psi^*,\phi] &= \sum_Q \psi^*(Q)P_{\psi,k}\psi(Q)\\ &+\frac{1}{2}\sum_Q \phi(-Q)P_{\phi,k}(Q)\phi(Q)\\ &-\sum_Q h_k(Q)\phi(Q)\tilde{\phi}(-Q)\\ &+\sum_Q \lambda_{\psi,k}(Q)\tilde{\phi}(Q)\tilde{\phi}(-Q)\end{aligned}$$

k-dependent field redefinition

$$\phi_k(Q) = \phi_{\bar{k}}(Q) + \Delta\alpha_k(Q)\tilde{\phi}(Q)$$

$$\partial_k\phi_k(Q) = -\,\partial_k\alpha_k(Q)\tilde{\phi}(Q)$$

absorbs four-fermion coupling

flowing bosonisation

Evolution with k-dependent field variables

$$\partial_k \Gamma_k[\psi,\psi^*,\phi_k] = \partial_k \Gamma_k[\psi,\psi^*,\phi_k]|_{\phi_k} + \sum_Q \left(\frac{\delta}{\delta \phi_k}\Gamma[\psi,\psi^*,\phi_k]\right)\partial_k \phi_k$$
$$= \partial_k \Gamma_k[\psi,\psi^*,\phi_k]|_{\phi_k} + \sum_Q \big(-\partial_k \alpha_k(Q) P_{\phi,k}(Q)\phi_k(Q)\tilde{\phi}(-Q) + h_k(Q)\partial_k \alpha_k(Q)\tilde{\phi}(Q)\tilde{\phi}(-Q)\big)$$

modified flow of couplings

$$\begin{aligned}\partial_k h_k(Q) &= \partial_k h_k(Q)|_{\phi_k} + \partial_k \alpha_k(Q) P_{\phi,k}(Q),\\ \partial_k \lambda_{\psi,k}(Q) &= \partial_k \lambda_{\psi,k}(Q)|_{\phi_k} + h_k(Q)\,\partial_k \alpha_k(Q).\end{aligned}$$

Choose α_k in order to absorb the four fermion coupling in corresponding channel ➡

$$\partial_k h_k(Q) = \partial_k h_k(Q)|_{\phi_k} - \frac{P_{\phi,k}(Q)}{h_k(Q)}\partial_k \lambda_{\psi,k}(Q)|_{\phi_k}$$

Mean Field Theory (MFT)

Evaluate Gaussian fermionic integral
in background of bosonic field , e.g.

$$\hat{\rho}(Q) \rightarrow \rho\delta(Q)$$
$$\hat{\vec{m}}(Q) \rightarrow \vec{a}\delta(Q-\Pi)$$

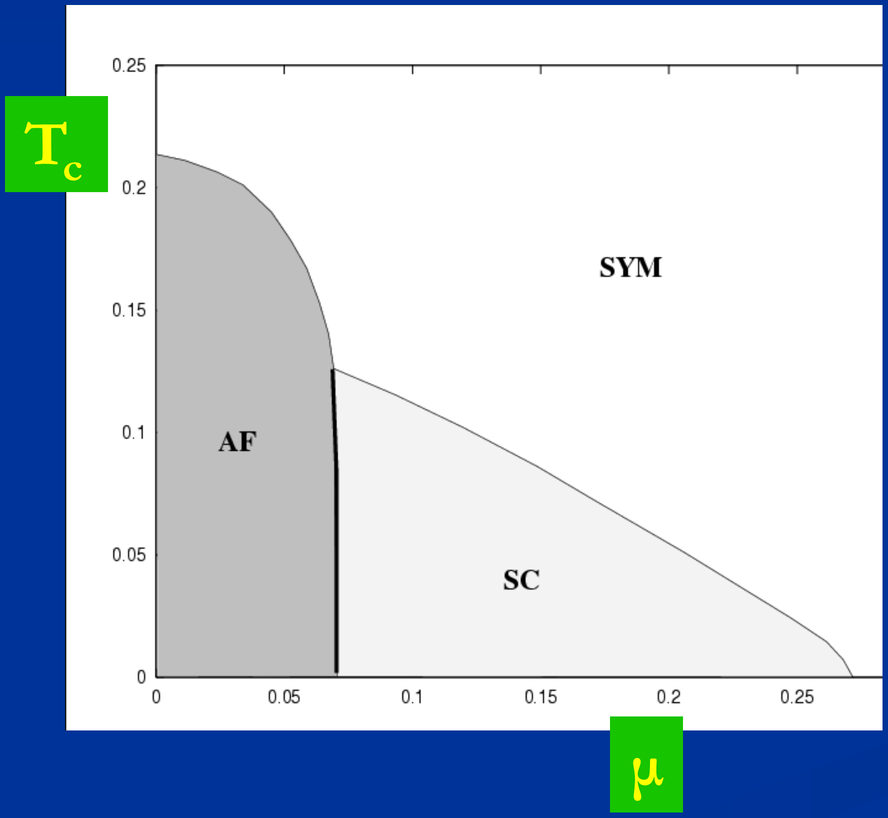
$$\begin{aligned} Z_{\rm MF} &= \int \mathcal{D}(\hat{\psi}^*, \hat{\psi}) \exp(-S_{\rm MF}), \\ S_{\rm MF} &= \sum_Q \hat{\psi}^\dagger(Q)(i\omega_F - \mu - 2t(\cos q_1 + \cos q_2))\hat{\psi}(Q) \\ &\quad - \sum_Q (U_\rho \rho \hat{\psi}^\dagger(Q)\hat{\psi}(Q) + U_m \vec{a}\hat{\psi}^\dagger(Q+\Pi)\vec{\sigma}\hat{\psi}(Q)) \\ &\quad + \frac{V_2}{2T}(U_\rho \rho^2 + U_m \vec{a}^2) - J_\rho(0)\rho - \vec{J}_m(-\Pi)\vec{a} \end{aligned}$$

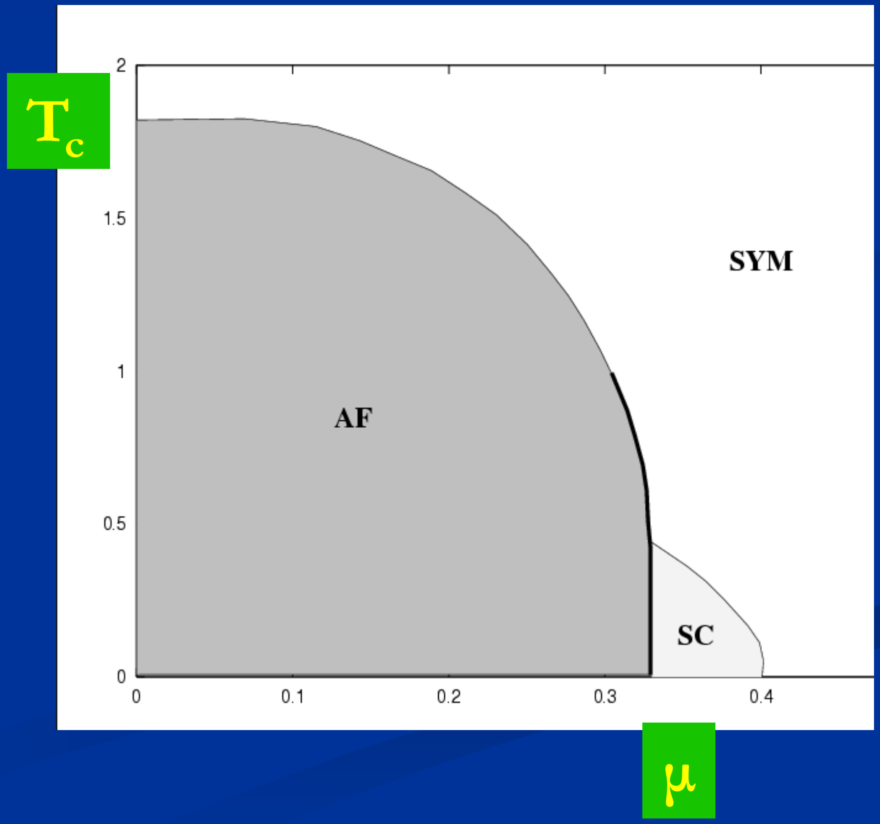
$$U = -U_\rho + 3U_m$$

$$\Gamma_{\rm MF} = -\ln Z_{\rm MF} + J_\rho(0)\rho + \vec{J}_m(-\Pi)\vec{a}$$

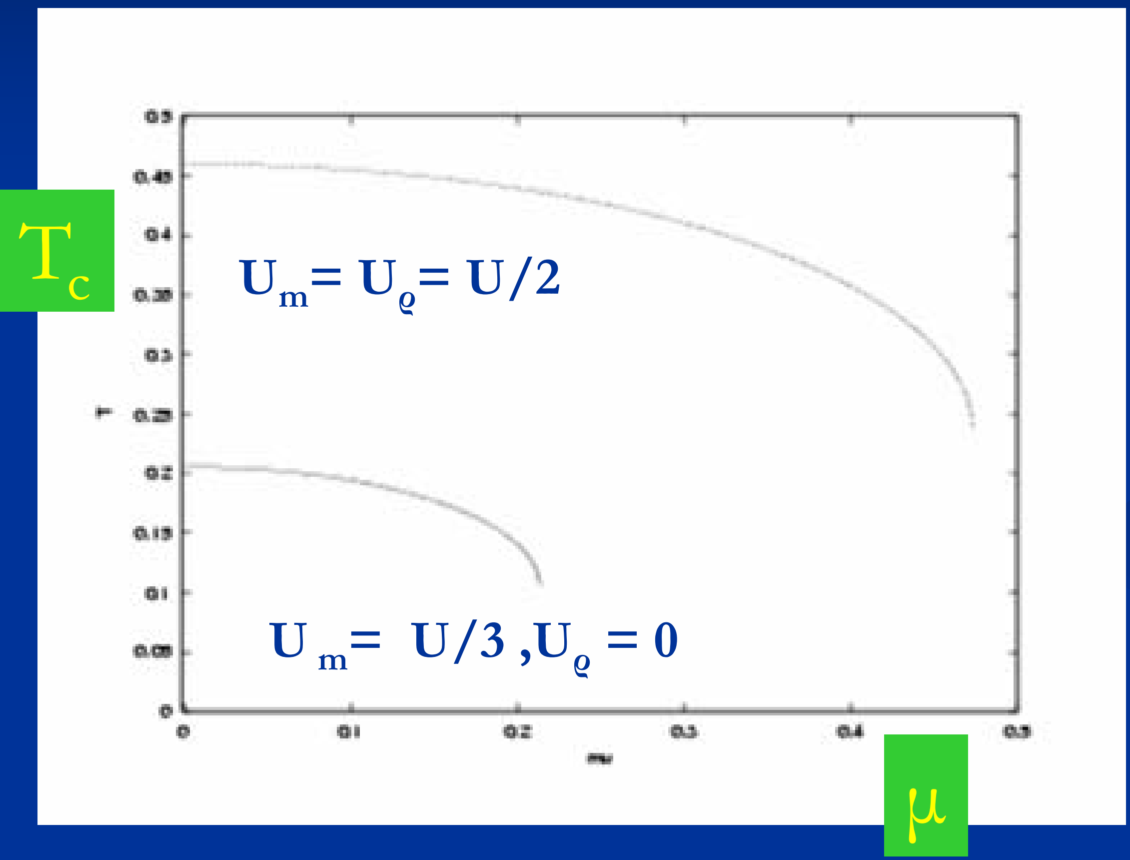
Mean field phase diagram

for two different choices of couplings – same U !





Mean field ambiguity



mean field phase diagram

Artefact of approximation …

cured by inclusion of bosonic fluctuations

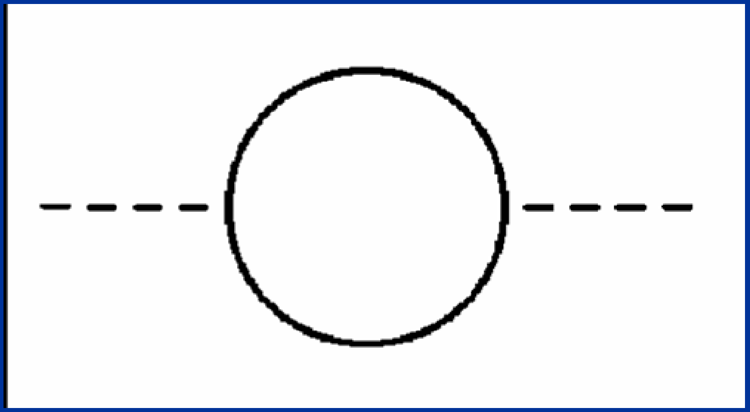
J.Jaeckel,…

$$U = -U_\rho + 3U_m$$

Bosonisation and the mean field ambiguity

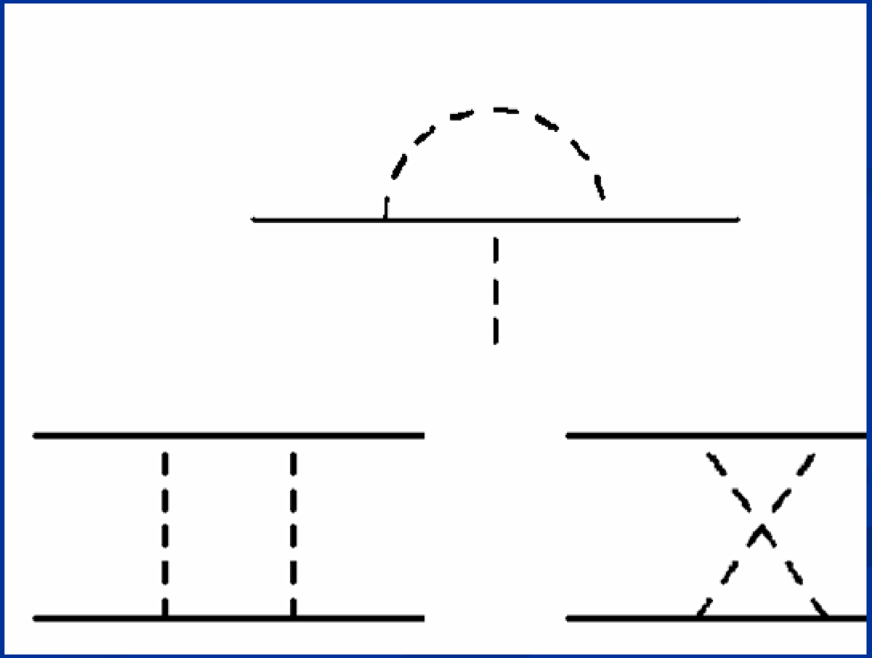
Bosonic fluctuations

fermion loops

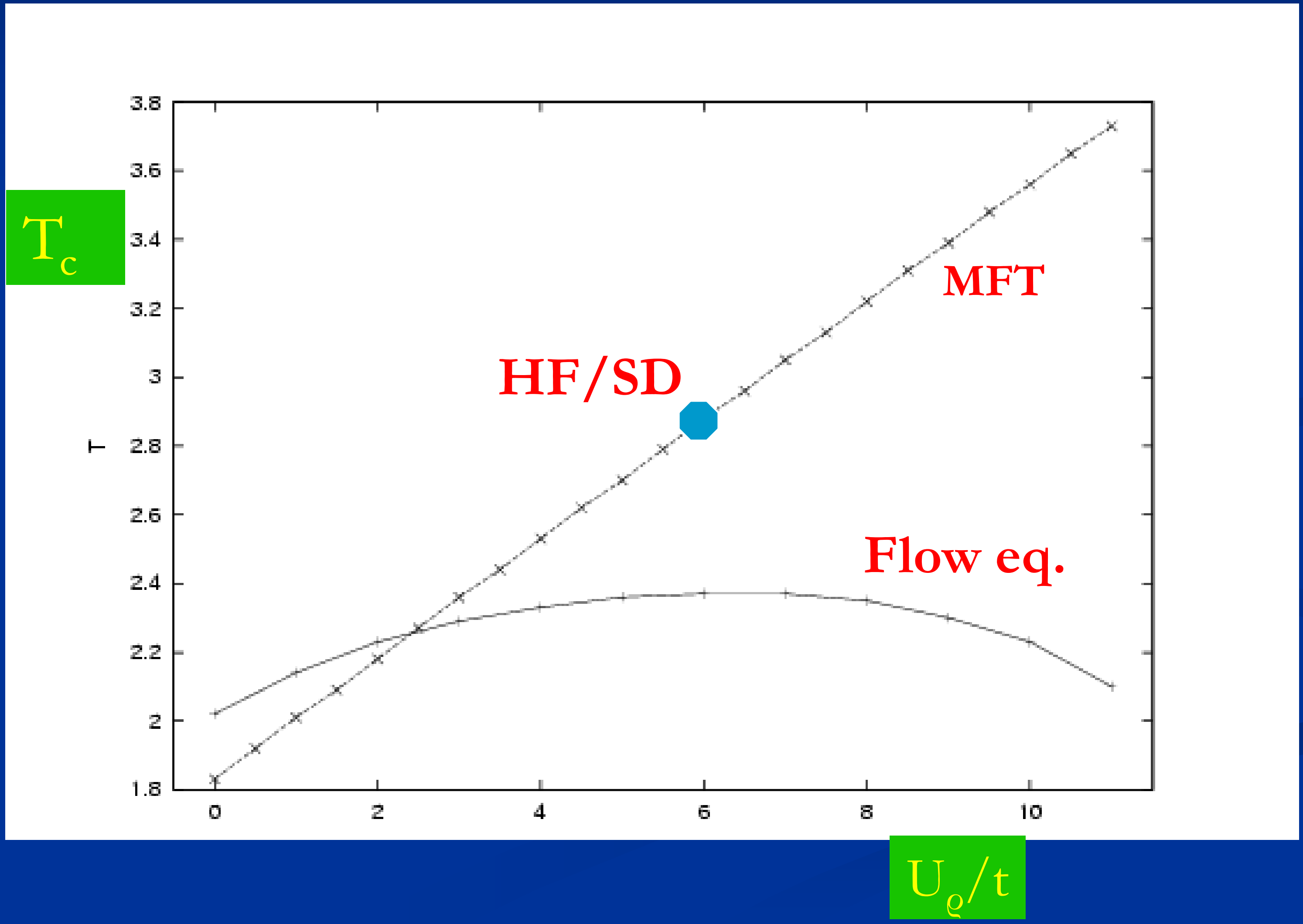


mean field theory

boson loops

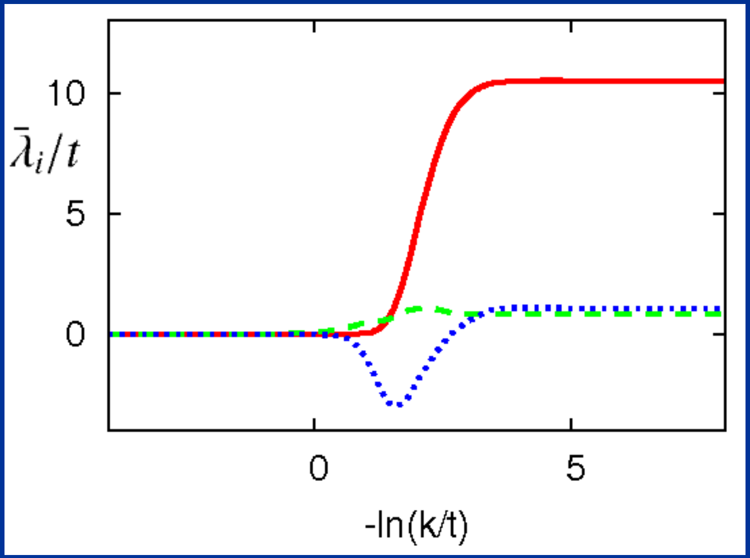


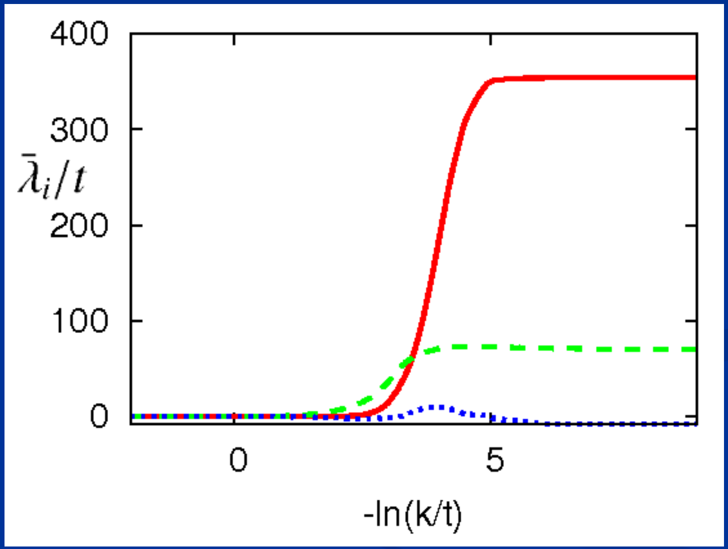
Bosonisation cures mean field ambiguity



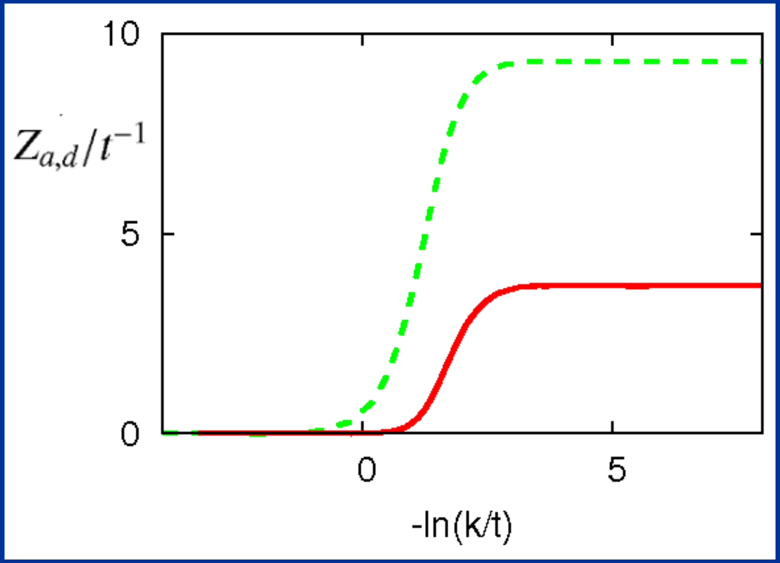
end

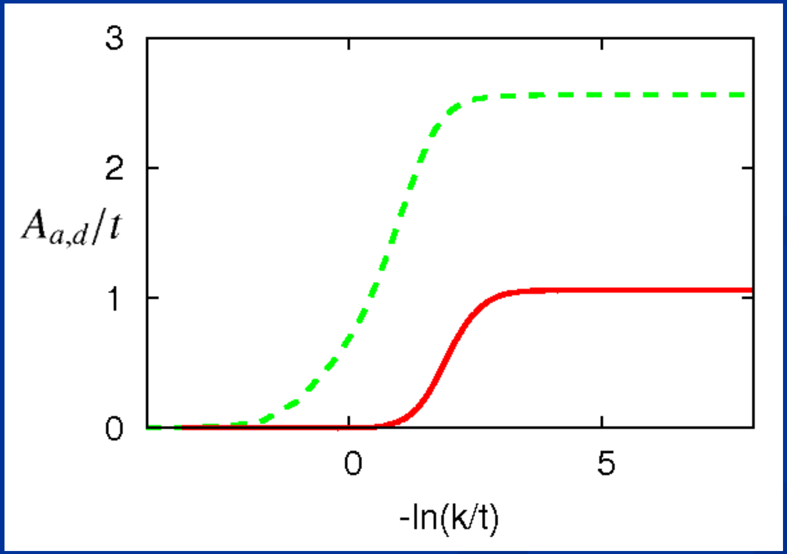
quartic couplings for bosons



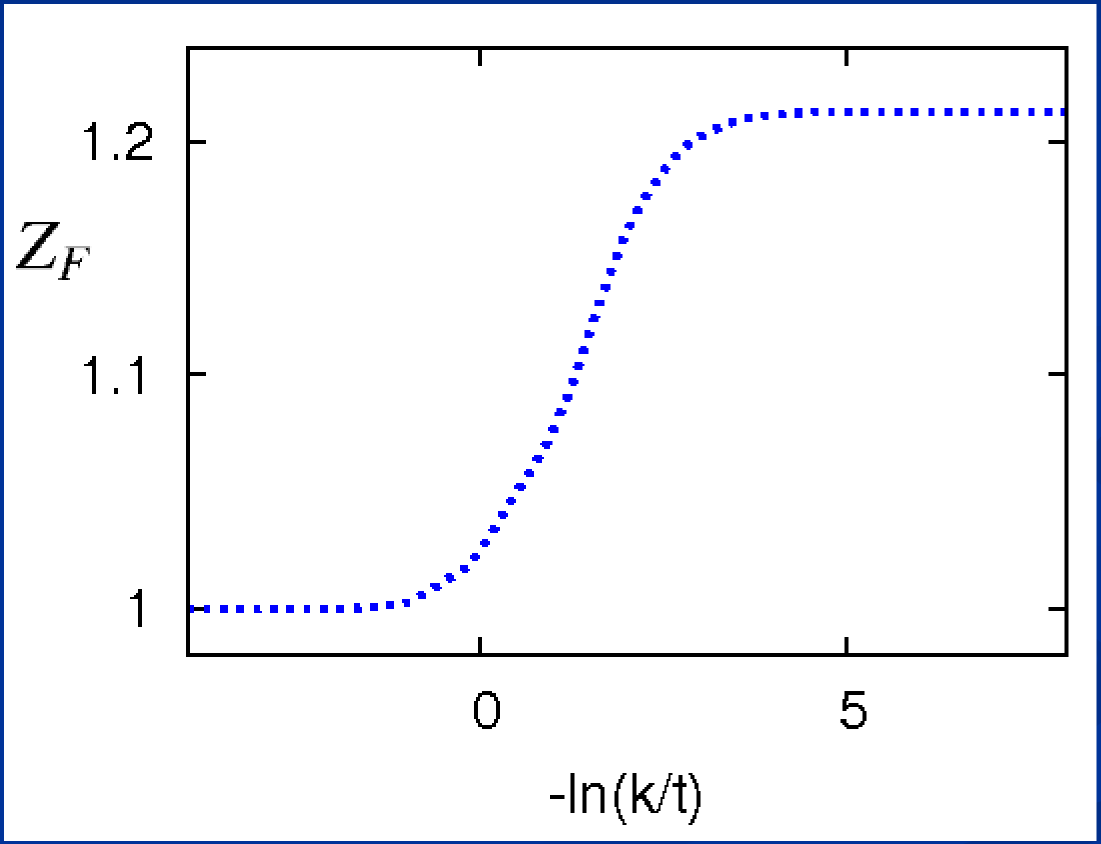


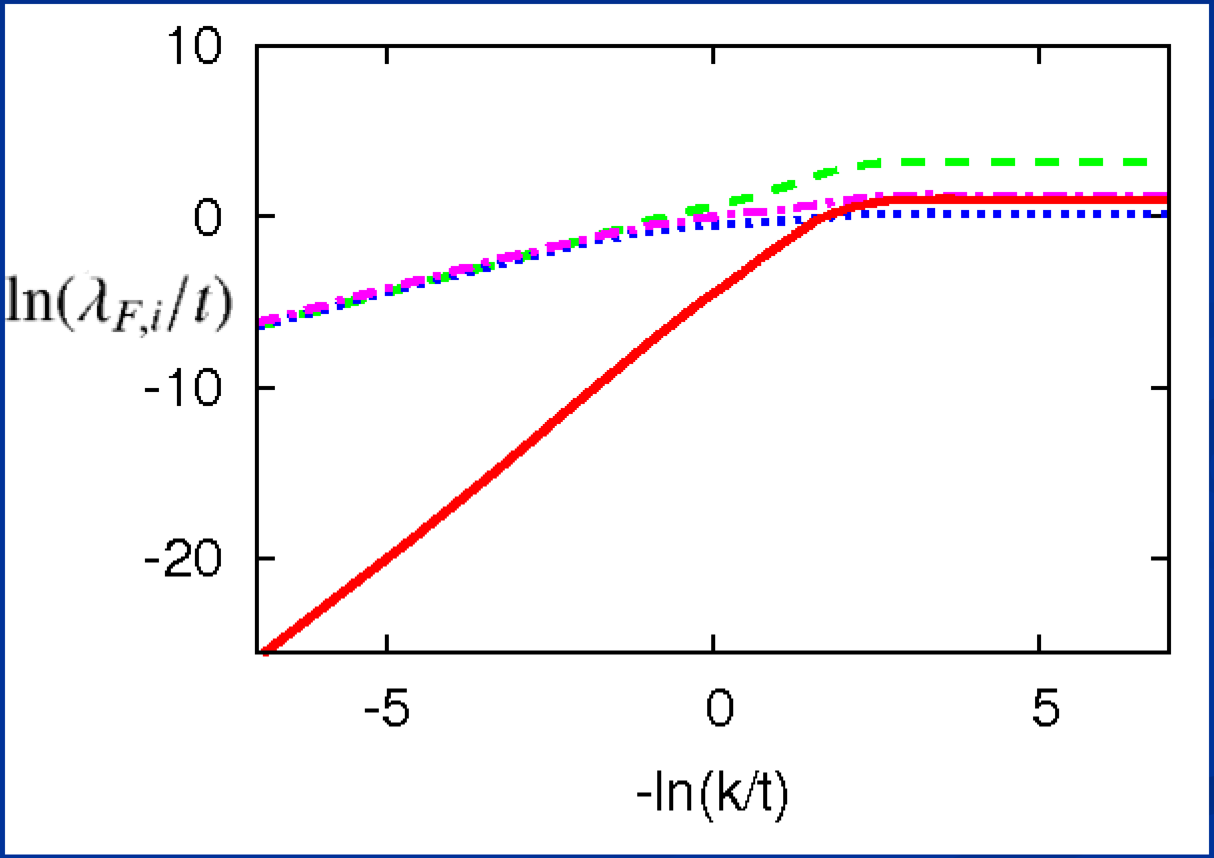
kinetic and gradient terms for bosons



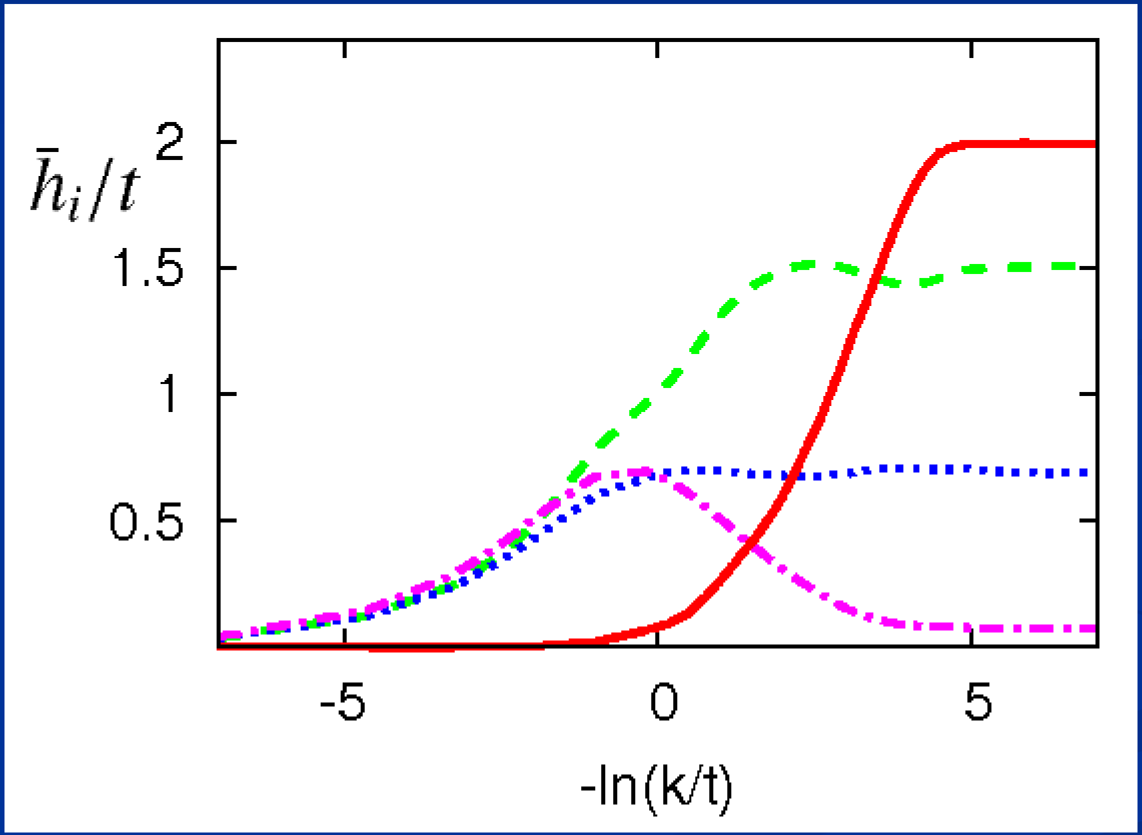


fermionic wave function renormalization

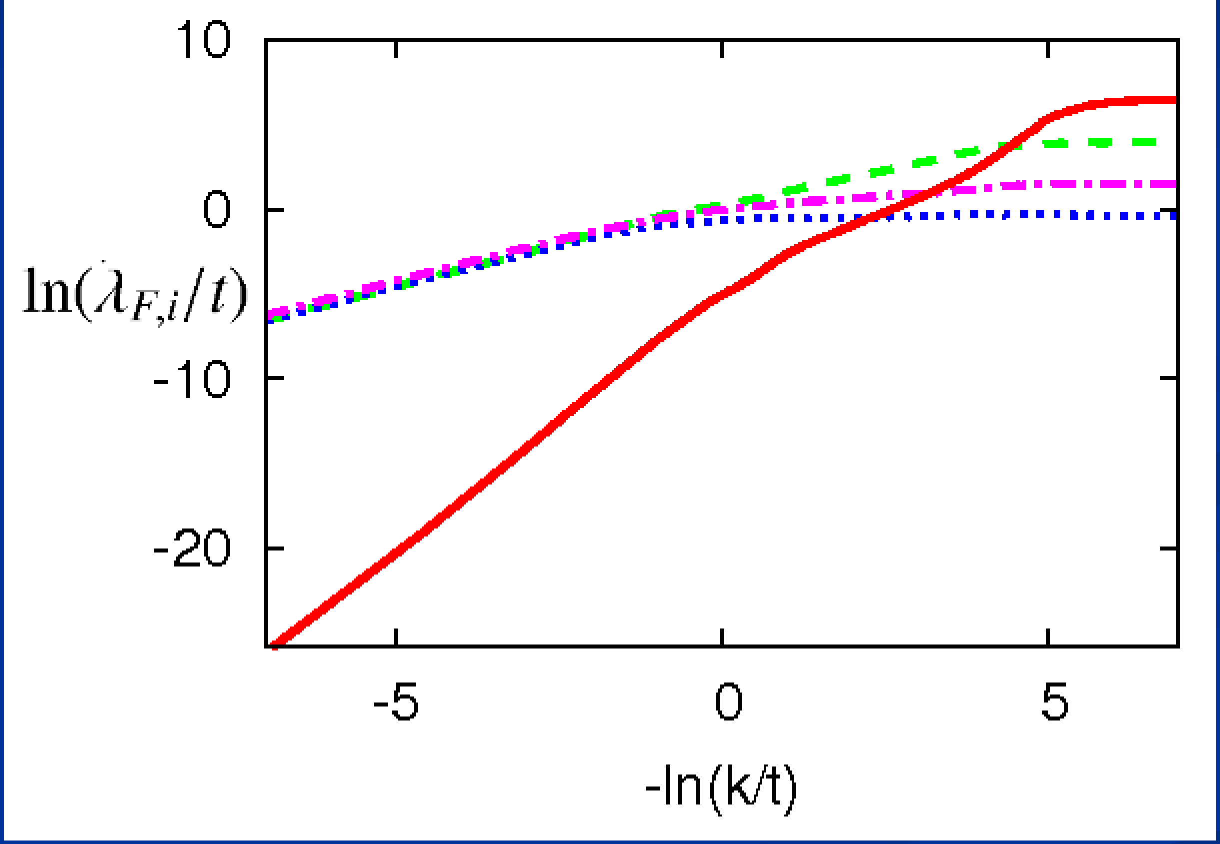




10
0
$\ln(\lambda_{F,i}/t)$
-10
-20
-5
0
5
-ln(k/t)



$\bar{h}_i/t$
2
1.5
1
0.5
-5
0
5
-ln(k/t)



10
0
-10
-20
$\ln(\lambda_{F,i}/t)$
-5
0
5
-ln(k/t)