Self-Energy and Critical Temperature of Weakly Interacting Bosons

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Outline

- Bose-Einstein-Condensation: Introduction
- Weak interactions: Shift of T_c
- Functional RG formalism
- Calculation of the self energy
- Calculation of ΔT_c

Collaborators:

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References:
Phys. Rev. A 69, 061601 (R) (2004).

Phys. Rev. A 70, 063621 (2004).

BEC of homogeneous ideal Bose gas

Grand canonical partition function:

$$\mathcal{Z}(\mu,V,T)=\prod_{\mathbf{k}}\frac{1}{1-\exp[-\beta(\varepsilon_k-\mu)]};\quad \varepsilon_k=\hbar^2k^2/(2m)$$

Equation of state:

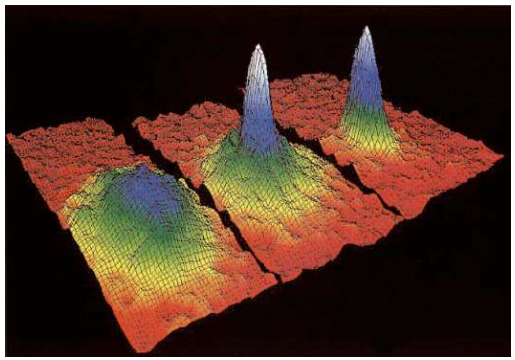
$$N=z\frac{\partial}{\partial z}\ln\mathcal{Z}=\sum_{\mathbf{k}}\frac{\exp[-\beta(\varepsilon_k-\mu)]}{1-\exp[-\beta(\varepsilon_k-\mu)]};\quad z=\exp(\beta\mu)$$

Thermodynamic limit $V\to\infty$:

$$n=\frac{N}{V}=\frac{1}{\lambda_T^3}g_{3/2}(z)+\frac{1}{V}\frac{z}{1-z};\quad g_{3/2}(z)=\sum_{\ell=1}^{\infty}\frac{z^\ell}{\ell^{3/2}},\quad N_0=\frac{z}{1-z},\quad \lambda_T=\sqrt{\frac{2\pi}{mk_BT}}\hbar$$

At critical temperature: $\mu=0,\ g_{3/2}(1)=\zeta(3/2)$

$$n_c=\frac{1}{\lambda_T^3}\zeta(3/2);\quad T_c=\frac{2\pi\hbar^2n^{2/3}}{m\zeta(3/2)^{2/3}}$$



Dalfovo *et al.*

RMP 99

Effect of weak interactions on T_c

- Weak interactions : $an^{1/3} \ll 1$ with s-wave scattering length a
- Correct result established only in 1999 Baym *et al.*

$$\frac{\Delta T_c}{T_c^0} = c_1\, an^{1/3} + O[(an^{1/3})^2] \text{ with } c_1 > 0$$

- non-perturbative result
- $\Rightarrow$ interactions lead to larger T_c
- for atoms in harmonic trap: mean-field calculation sufficient:

$$\frac{\Delta T_c}{T_c^0} = -1.3 \frac{a}{a_{\rm ho}} N^{1/6}$$

a_{ho}: size of BEC cloud

- $\Rightarrow$ interactions lead to smaller T_c

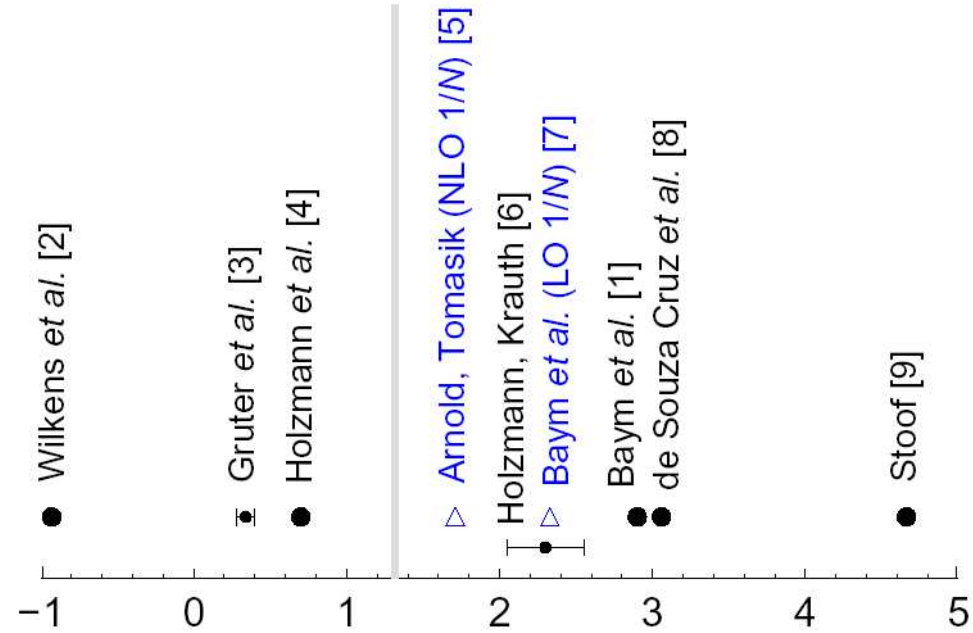
Results for ΔT_c

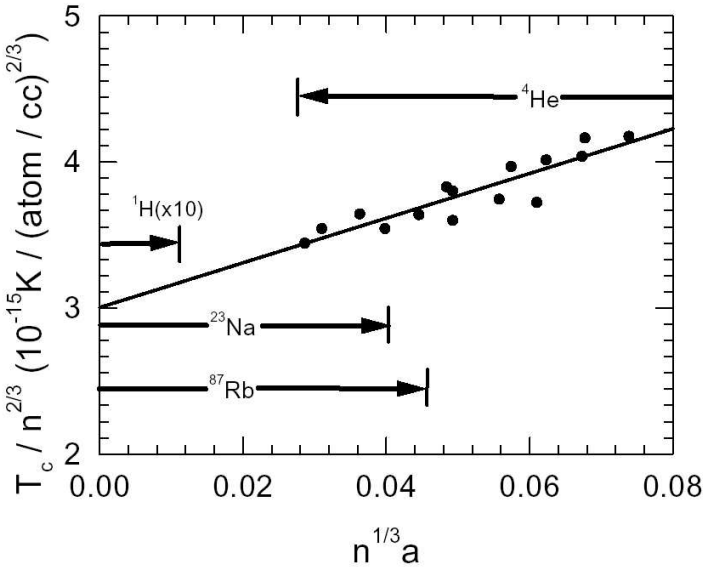
Historical results for ΔT_c:

- $\Delta T_c \propto a^{1/2}$
  Lee and Yang 57
  Glassgold *et al.* 60
  Toyoda 82
  Huang 99
- $\Delta T_c \propto a^{3/2}$
  Huang 64
- $\Delta T_c \propto a \ln a$
  Bijlsma and Stoof 96

Experiment: He-Vycor system
Reppy *et al.* 2000

Results for c_1 ($\Delta T_c / T_c^0 \approx c_1\, a n^{1/3}$)





Mean field analysis

- Hartree Fock self-energy:

$$\Sigma_{HF} = 4a\lambda_T^2 n$$

- modified relation between density and chemical potential:

$$n = \frac{1}{\lambda_T^3} g_{3/2}\left(z = e^{\beta(\mu - \Sigma_{HF})}\right)$$

- at transition $\mu - \Sigma_{HF} = 0$
- $\Rightarrow T_c^{HF} = T_c^0$
- shift in T_c is correlation effect!

How to calculate ΔT_c

- Calculate change in density Δn_c at critical point: $\frac{\Delta T_c}{T_c^0} = -\frac{2}{3}\frac{\Delta n_c}{n_c^0}$
- Greens-function expression for density:

$$n = -T\sum_{\nu}\int \frac{d^3k}{(2\pi)^3} G(k, i\omega_\nu) \qquad G(k, i\omega_\nu) = \frac{1}{i\omega_\nu + \mu - \varepsilon_k - \Sigma(k, i\omega_\nu)}$$

- At T_c one has $\Sigma(0,0) = \mu \Rightarrow$

$$\Delta n_c = n_c - n_c^0 = -\frac{2}{\pi\lambda_T^2}\int_0^\infty dk \frac{U(k)}{k^2 + U(k)} + \sum_{\nu\neq 0}\cdots$$

$$U(k) = 2m[\Sigma(k,0) - \Sigma(0,0)]$$

- Contribution from $\nu \neq 0$ terms is $O(a^2) \rightarrow$ neglect

$$\boxed{\textit{Need only consider } \omega = 0 \textit{ sector}}$$

IR breakdown of perturbation theory

- Second order perturbation theory for $\Sigma(k,0)$:

$$\Sigma^{(2)}(k,0) - \Sigma^{(2)}(0,0) \propto T\left(\frac{a}{\lambda_T}\right)^2 \ln(k\xi) \ , \ \text{IR cutoff: } \xi^2 = -\frac{1}{2m(\mu - \Sigma_{HF})}$$

- n^{th} order: : $\Sigma^{(n)}(k,0) - \Sigma^{(n)}(0,0) \propto T\left(\frac{a}{\lambda_T}\right)^2 \left(\frac{a\xi}{\lambda_T^2}\right)^{n-2} F(k\xi)$
- breakdown of perturbation theory at scale $\xi \approx \lambda_T^2/a$
- $\xi \to \infty$ for $T \to T_c \Rightarrow$ only length scale left is $k_c^{-1} = \lambda_T^2/a$
- Scaling ansatz:

$$\boxed{U(k) = 2m[\Sigma(k,0) - \Sigma(0,0)] \equiv k_c^2 \sigma(k/k_c)}$$

- Shift of n_c:

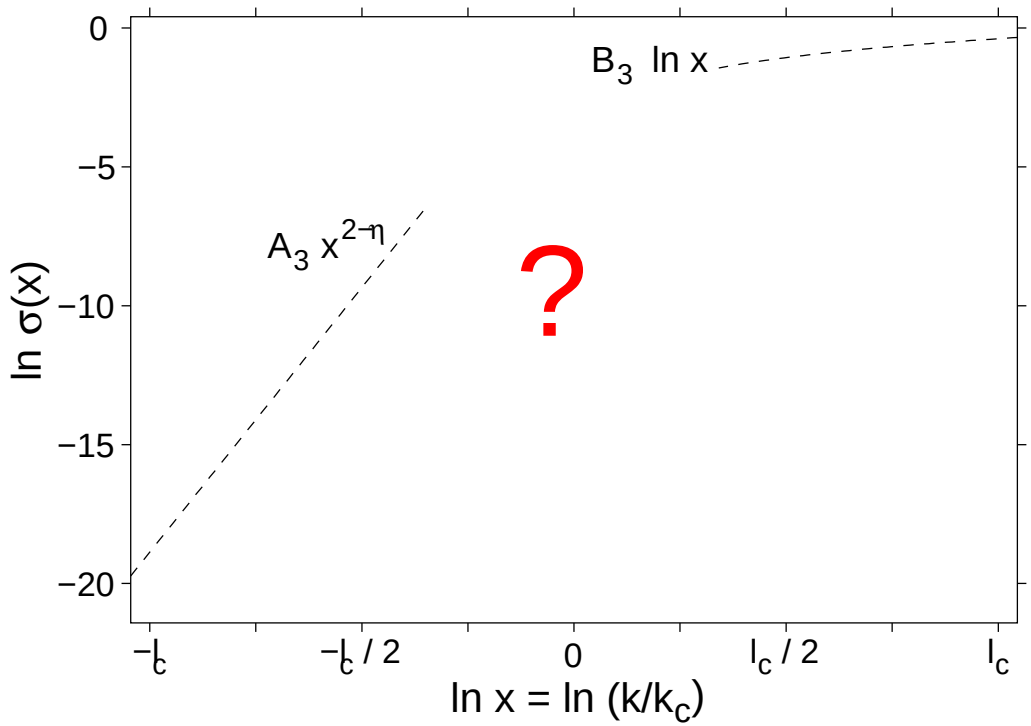
$$\Delta n_c = -\frac{2k_c}{\pi\lambda_T^2}\int_0^\infty dx \frac{\sigma(x)}{x^2 + \sigma(x)} \propto a$$

Scaling form of the self energy

Limiting behavior of self energy:

$$\sigma(k/k_c) \approx \left(\frac{k}{k_c}\right)^{2-\eta} \qquad \text{for } k \ll k_c \qquad \text{critical regime}$$

$$\sigma(k/k_c) \approx \ln\left(\frac{k}{k_c}\right) \qquad \text{for } k \gg k_c \qquad \text{“perturbative” regime}$$



Renormalization group approach: two versions

Field theoretical RG:

- renormalizability required: physical quantities can be expressed in terms of a fi nite number of couplings, defi ned at arbitrary scale λ
- bare correlations functions independent of $\lambda \Rightarrow$ connection between renormalized correlation functions and renormalized couplings
- very successful in calculation of critical exponents
- effectively sets $k_c = \infty \Rightarrow$ cannot describe short-wavelength regime $k \gg k_c$

"Wilsonian" RG:

- idea: integrate out degrees of freedom in steps and rescale.
- renormalizability not required (UV cutoff fi nite due to lattice)
- best method for one-loop calculations, but difficult beyond one loop
- application to Bose gas: Bijlsma, Stoof (1996); Anderson, Strickland (1999)

Functional RG (="exact" RG)

Modern implementation of Wilsonian RG:
original idea: Wegner, Houghton (1973); Polchinski (1984).

- Wilsonian effective action: integrate over short wavelength modes and rescale
- partition field: $\phi = \phi_> + \phi_< = \Theta(\Lambda_0 > |\mathbf{k}| > \Lambda)\phi_>(\mathbf{k}) + \Theta(\Lambda > |\mathbf{k}|)\phi_<(\mathbf{k})$
- integrate over short-wavelength part:

$$\exp[-S_\Lambda\{\phi'_<\}] = \int \mathcal{D}\{\phi_>\} \exp[-S_{\Lambda_0}\{\phi_< + \phi_>\}]$$

formally: use cutoff-dependent propagator: $G_0^{\Lambda,\Lambda_0}(\mathbf{k}) = \frac{\Theta(\Lambda<|\mathbf{k}|<\Lambda_0)}{\mathbf{k}^2+m_0^2}$

- rescale fi eld and momenta: $\phi'_<(\mathbf{k}') = \zeta\phi_<(e^{-l}\mathbf{k}')$.

change of $S_\Lambda\{\phi'\}$ due to infinitesimal change in Λ leads to formally exact functional equation for momentum-dependent vertices of effective action

technical problem: ambiguities for sharp cutoff:

$$\delta(x)\Theta(x) \to \frac{1}{2}\delta(x) \quad , \quad \delta(x)\Theta^2(x) \to \frac{1}{3}\delta(x)$$

One-particle irreducible version of exact RG

several alternative formulations of exact RG,
using different types of generating functionals:

1. generating functional $\mathcal{G}_c\{J\}$ of connected correlation functions.
2. generating functional of amputated connected correlation functions.
3. Legendre effective action: generating functional of one-particle irreducible vertices (Di Castro, Jona-Lasinio, Peliti (1974); Nicoll, Chang, Stanley (1976); Wetterich (1993); Morris (1994))

$$\frac{1}{2}(\varphi, G_0^{-1}\varphi) + \Gamma\{\varphi\} \quad = \quad (\varphi, J) - \mathcal{G}_c\{J\{\varphi\}\} \ , \ \varphi(\mathbf{r}) = \langle\phi(\mathbf{r})\rangle_c = \frac{\delta\mathcal{G}_c\{J\}}{\delta J(\mathbf{r})} \ .$$

technical advantage: Θ-functions appear under integral $\Longrightarrow$ no ambiguities!

several recent applications to interacting fermions:

(Wetterich-group; Honerkamp-Salmhofer collaboration; Göttingen-Stuttgart collaboration (Metzner-Meden-Schönhammer); P.K.-group; Katanin-Kampf collabotation; ...)

Effective action for interacting bosons

Effective action with cutoff Λ_0

$$S_{\Lambda_0}\{\bar{\psi},\psi\} \quad = \quad S^0_{\Lambda_0}\{\bar{\psi},\psi\} + S^{\rm int}_{\Lambda_0}\{\bar{\psi},\psi\} \ , \ \text{with } K = (k, i\omega_n)$$

$$\begin{aligned}
S^0_{\Lambda_0}\{\bar{\psi},\psi\} &= \int_{k<\Lambda_0,\omega_n} [-i\omega_n + \varepsilon_{\mathbf{k}} - \mu + \Sigma(0,i0)]\bar{\psi}_K\psi_K \\
S^{\rm int}_{\Lambda_0}\{\bar{\psi},\psi\} &= \int_{k<\Lambda_0,\omega_n} [\Sigma_{\Lambda_0}(K) - \Sigma(0,i0)]\bar{\psi}_K\psi_K \\
&\quad + \frac{1}{(2!)^2}\int_{K_1',K_2',K_2,K_1} \delta_{K_1'+K_2',K_2+K_1}\Gamma^{(4)}_{\Lambda_0}(K_1',K_2';K_2,K_1)\bar{\psi}_{K_1'}\bar{\psi}_{K_2'}\psi_{K_2}\psi_{K_1} + \ldots
\end{aligned}$$

Quantum mechanics is irrelevant for classical critical phenomena

$\Rightarrow$ only $i\omega_n = 0$ component relevant (classical $O(2)$ model)

rescaled classical one-particle irreducible vertices (with $l = -\ln(\Lambda/\Lambda_0)$):

$$\tilde{\Gamma}^{(2n)}_l(\mathbf{q}_1',\ldots,\mathbf{q}_n';\mathbf{q}_n,\ldots,\mathbf{q}_1) \quad = \quad (K_D T)^{n-1}\Lambda^{D(n-1)-2n}\left(\frac{2mZ_l}{\hbar^2}\right)^n \Gamma^{(2n)}_{\Lambda}(\{\mathbf{k}_i = \Lambda\mathbf{q}_i, \omega_{n_i} = 0\})$$

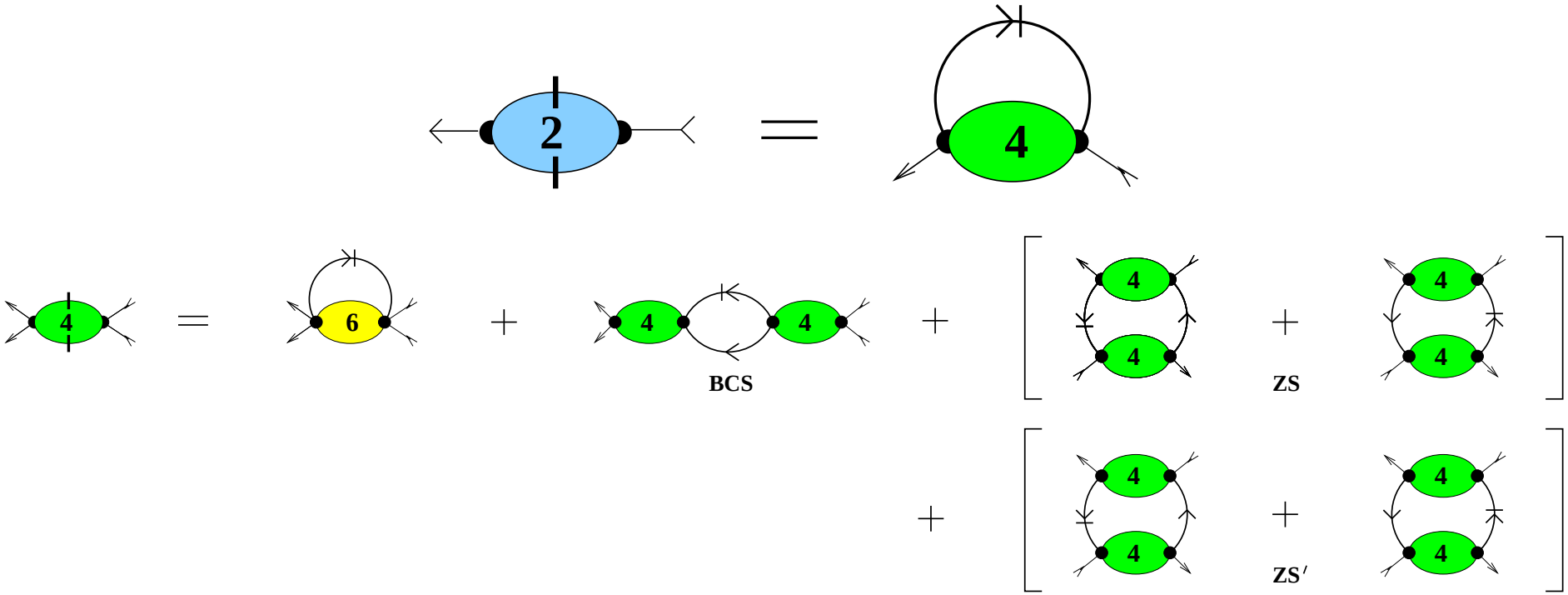
Exact flow equation for irreducible vertices

General hierachical structure of flow equations:

Two contributions: rescaling and integrating out high momentum slice

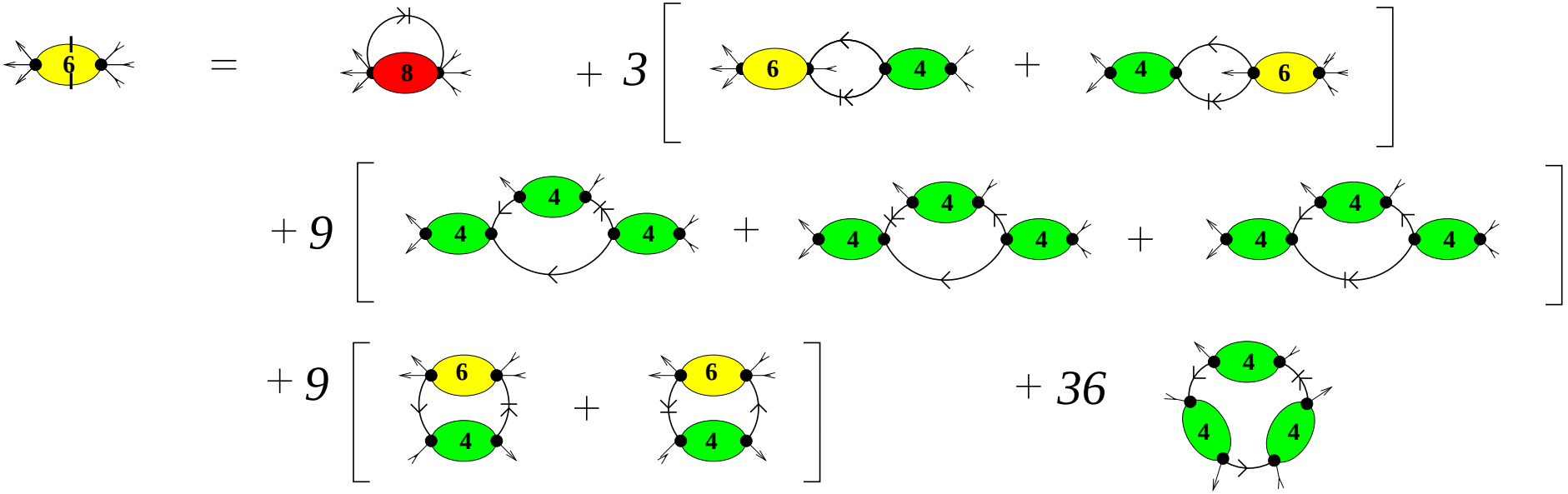
$$\partial_l \tilde{\Gamma}_l^{(2n)}(\{\mathbf{q}_i\}) = \left[2n - D(n-1) - n\eta_l - \sum_{i=1}^{2n} \mathbf{q}_i \cdot \nabla_{\mathbf{q}_i}\right] \tilde{\Gamma}_l^{(2n)}(\{\mathbf{q}_i\}) + \dot{\Gamma}_l^{(2n)}(\{\mathbf{q}_i\})$$

$\dot{\Gamma}_l^{(2n)}$ depends on $2m$-point vertices with $m = n+1, n, \ldots, 1$

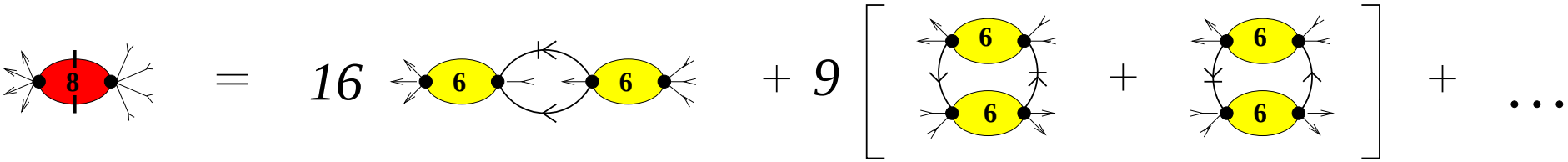


More exact flow equations:

six-point vertex:



and eight-point vertex:



and so on...

need truncation!!

Simplest truncation: relevant couplings

$r_l = \tilde{\Gamma}_l^{(2)}(0)$: relevant part of self-energy $\tilde{\Gamma}_l^{(2)}(\mathbf{q}) = \frac{2mZ_l}{\Lambda^2}\left[\Sigma_\Lambda(\mathbf{q}\Lambda) - \Sigma(0)\right]$

$u_l = \tilde{\Gamma}_l^{(4)}(0,0;0,0)$: relevant part of four point vertex $\tilde{\Gamma}_l^{(4)}(\mathbf{q}_1', \mathbf{q}_2'; \mathbf{q}_1, \mathbf{q}_2)$

flow equations:

$$\begin{aligned} \partial_l u_l &= u_l - \frac{5}{2}u_l^2 \\ \partial_l r_l &= 2r_l + u_l \end{aligned}$$

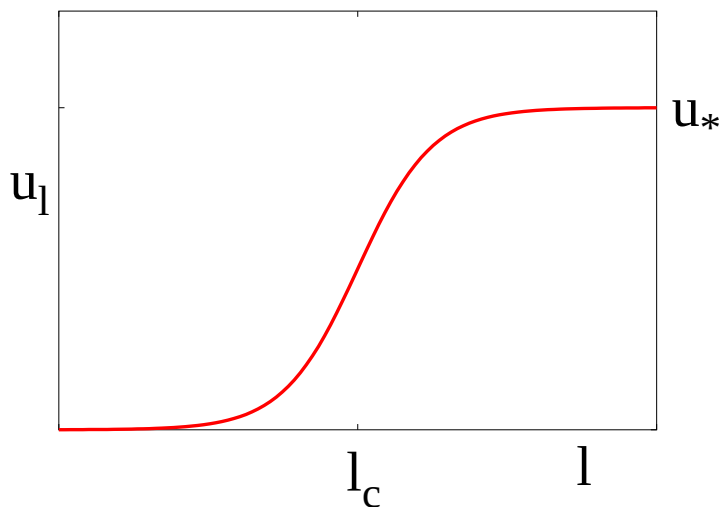
Wilson-Fisher fixed point:

$$\begin{aligned} u_* &= \frac{2}{5} \\ r_* &= -u_*/2 \end{aligned}$$

flow of u_l is Fermi function

$$u_l = \frac{u_*}{\exp[l - l_c] + 1}$$

with $l_c \approx \ln(u_*/u_0)$ and $u_0 \propto a/\lambda_T$



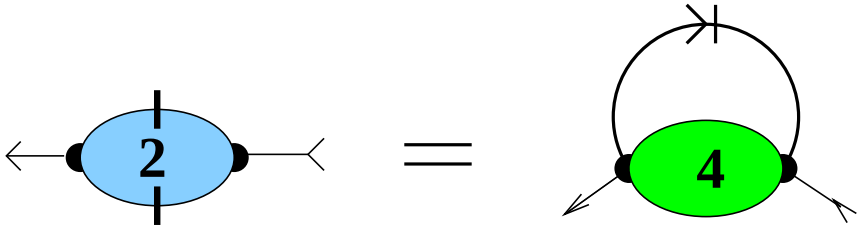
Cross-over scale: $k_c = \Lambda_0 \exp[-l_c] \propto a/\lambda_T^2$ ✔

Exact RG equation for self-energy

Need: momentum-dependence of self-energy. Exact flow equation:

$$\partial_l \tilde{\Gamma}_l^{(2)}(\mathbf{q}) \quad = \quad [2-\eta_l-\mathbf{q}\cdot\nabla_{\mathbf{q}}]\tilde{\Gamma}_l^{(2)}(\mathbf{q})+\dot{\Gamma}_l^{(2)}(\mathbf{q})$$

with $\dot{\Gamma}_l^{(2)}(\mathbf{q}) \quad = \quad \int_{\mathbf{q}'} \dot{G}_l(\mathbf{q}')\tilde{\Gamma}_l^{(4)}(\mathbf{q},\mathbf{q}';\mathbf{q}',\mathbf{q})$ $\qquad \dot{G}_l(\mathbf{q}) = \dfrac{\delta(|\mathbf{q}|-1)}{Z_l\mathbf{q}^2+\tilde{\Gamma}_l^{(2)}(\mathbf{q})}$



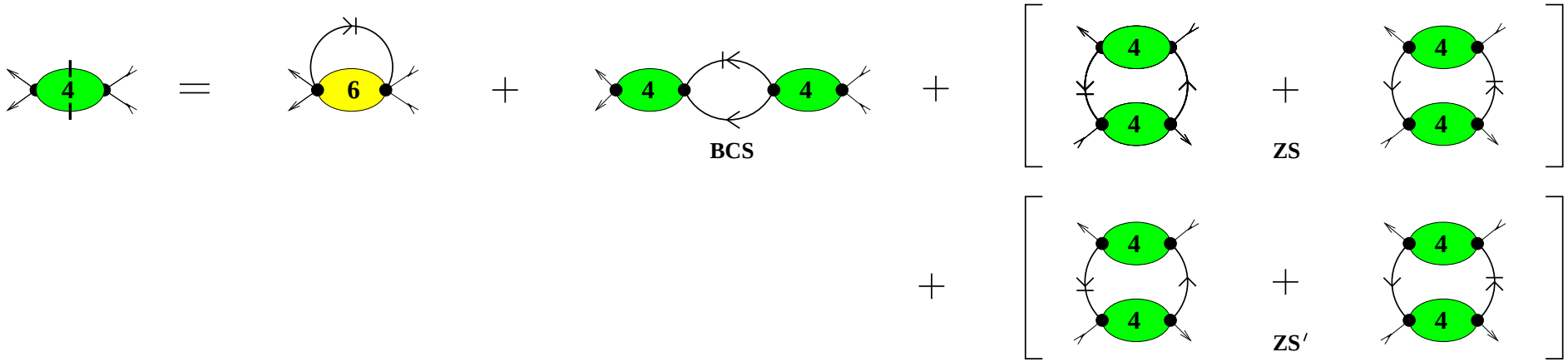
$\Rightarrow$ dimensionless self-energy at RG fixed point $(l \to \infty)$:

$$\sigma(x) \quad = \quad \int_0^\infty dl\; e^{-2(l-l_c)+\int_0^l d\tau\;\eta_\tau}\left[\dot{\Gamma}_l^{(2)}(e^{l-l_c}x)-\dot{\Gamma}_l^{(2)}(0)\right] \qquad ; \quad x=k/k_c$$

Need “only” to calculate 4-point vertex and η_l

Approximation for $\tilde{\Gamma}_l^{(4)}$

To calculate $\tilde{\Gamma}_l^{(4)}$, need $\dot{\Gamma}_l^{(4)}$



simplest approximation: ignore six-point vertex, keep only u_l^2 terms:

$$\dot{\Gamma}_l^{(4)}(\mathbf{q}_1', \mathbf{q}_2'; \mathbf{q}_2, \mathbf{q}_1) \approx -u_l^2 \left[\frac{1}{2}\dot{\chi}_l(|\mathbf{q}_1 + \mathbf{q}_2|) + \dot{\chi}_l(|\mathbf{q}_1 - \mathbf{q}_1'|) + \dot{\chi}_l(|\mathbf{q}_1 - \mathbf{q}_2'|) \right]$$

$$\dot{\chi}_l(|\mathbf{q}|) \quad = \quad 2\int_{\mathbf{q}'} \dot{G}_l(|\mathbf{q}'|)\tilde{G}_l(|\mathbf{q}+\mathbf{q}'|) \ ,$$ full momentum dependence: irrelevant couplings

now can calculate $\sigma(x)$: $\dot{\Gamma}_l^{(4)} \Rightarrow \tilde{\Gamma}_l^{(4)} \Rightarrow \dot{\Gamma}_l^{(2)} \Rightarrow \sigma(x)$.

Momentum-dependent self-energy: RG result

dimensionless self-energy at RG fixed point ($l \to \infty$):

flowing anomalous dimension: $\eta_l \approx \eta_* \frac{u_l}{u_*}$, $\eta_* \approx 0.104$.

$$
\begin{aligned}
\sigma(x) &= \frac{2m}{k_c^2}\left[\Sigma(k_c x) - \Sigma(0)\right] \qquad ; \quad x = k/k_c \\
&= \int_0^\infty dl\; e^{-2(l-l_c)+\int_0^l d\tau\, \eta_\tau} \left[\dot{\Gamma}_l^{(2)}(e^{l-l_c}x) - \dot{\Gamma}_l^{(2)}(0)\right] \\
&\approx \frac{3u_*^2}{2} x^{2-\eta_*} \int_{xe^{-l_c}}^\infty dy \frac{y^{-3+2\varepsilon} F(x,y;\eta_*,l_c)}{\left[x^\varepsilon + y^\varepsilon\right]^{2-2\eta_*/\varepsilon}}
\end{aligned}
$$

with $\varepsilon = 4 - D$ and

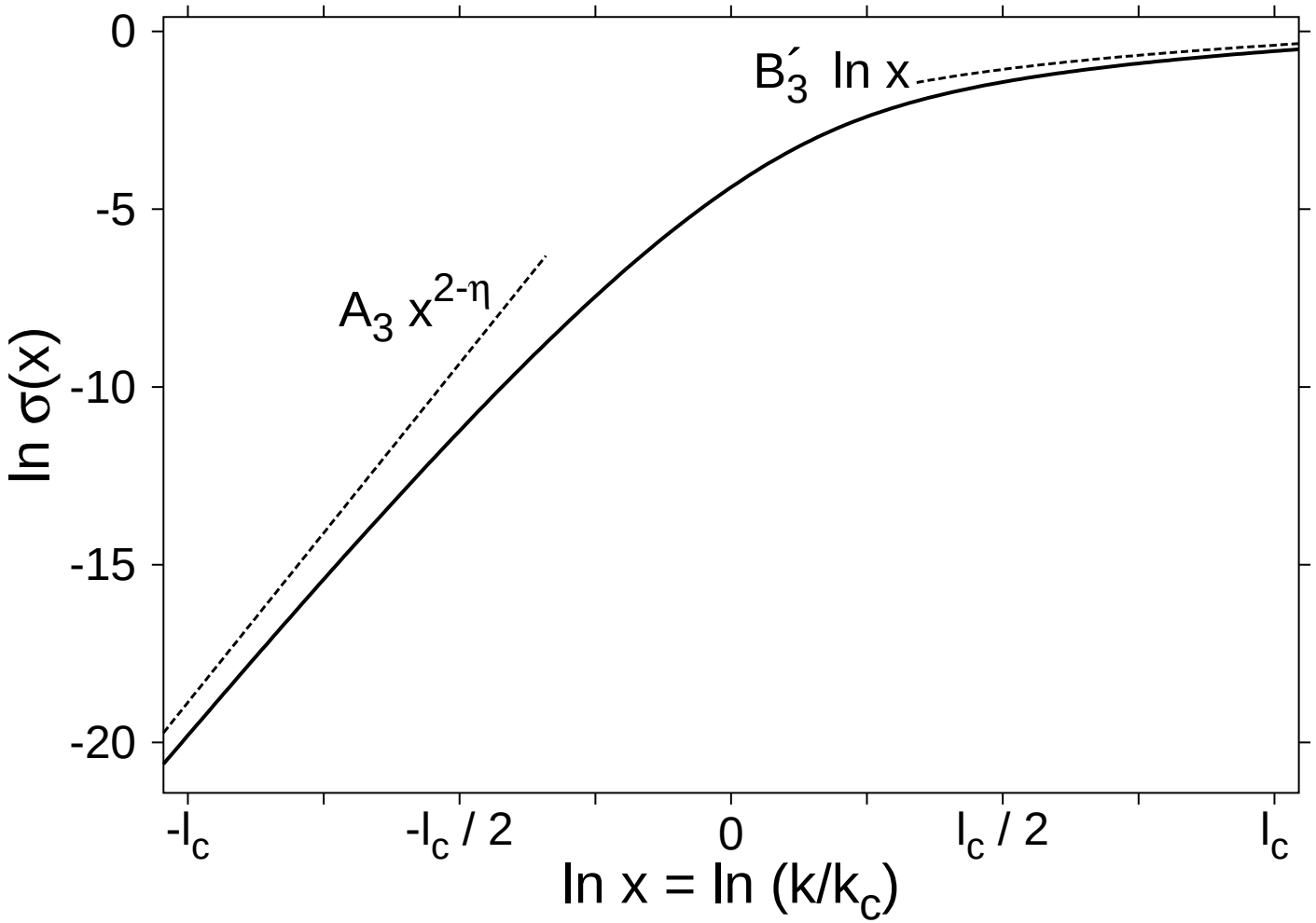
$$
\begin{aligned}
F(x,y;\eta_*,l_c) &= \int_0^1 dz \frac{z^{1-\varepsilon}}{\left[x^\varepsilon + (y/z)^\varepsilon\right]^{\eta_*/\varepsilon}\left[1 + r_{l_c + \ln\frac{y}{zx}}\right]} \\
&\quad \times \langle \dot{\chi}_{l_c+\ln\frac{y}{x}}(z) - \dot{\chi}_{l_c+\ln\frac{y}{x}}(|z\hat{\mathbf{q}}' + y\hat{\mathbf{q}}|)\rangle_{\hat{\mathbf{q}}'} \; .
\end{aligned}
$$

Self energy: scaling function

$\sigma(x) = \frac{2m}{k_c^2}\left[\Sigma(k_c x) - \Sigma(0)\right]$

our results: $\eta_* = 0.104$, $A_3 \approx 1.20$, $B_3' = 3\pi^2 u_*^2/24$

best Monte Carlo results: $\eta_* = 0.038$, $A_3 = 0.980$



Result for T_c shift

$$\frac{\Delta T_c}{T_c} = \frac{4k_c^2}{3\pi\lambda_T^2}\int_0^\infty dx \frac{\sigma(x)}{x^2+\sigma(x)} \approx 1.23an^{1/3}$$

In very good agreement with

- Arnold and Moore, 2001 (Lattice): 1.32 $\pm$ 0.02
- Kashurnikov, 2001 (Lattice): 1.29 $\pm$ 0.05
- Kastening, 2004 (VPT): 1.27 $\pm$ 0.11
- Kleinert, 2003 (VPT): 1.23 $\pm$ 0.10

Why is RG so accurate?

- Both the critical regime $x \ll 1$ and the perturbative regime $x \geq 1$ contribute to c_1
- main contribution from $x \approx 1$
- error due to $\eta_* \approx 0.104$ (as compared with $\eta_*^{MC} \approx 0.038$) negligible

Improvement: keep all marginal parameters

Relevant parameters in $3 \leq D < 4$:

- Momentum independent part of 2-point vertex
  $\tilde{\Gamma}_l^{(2)}(0) = r_l$
- Momentum independent part of 4-point vertex
  $\tilde{\Gamma}_l^{(4)}(0,0;0,0) = u_l$

Marginal parameter:

- Wavefunction renormalization Z_l:
  $\partial_l Z_l = -\eta_l Z_l$

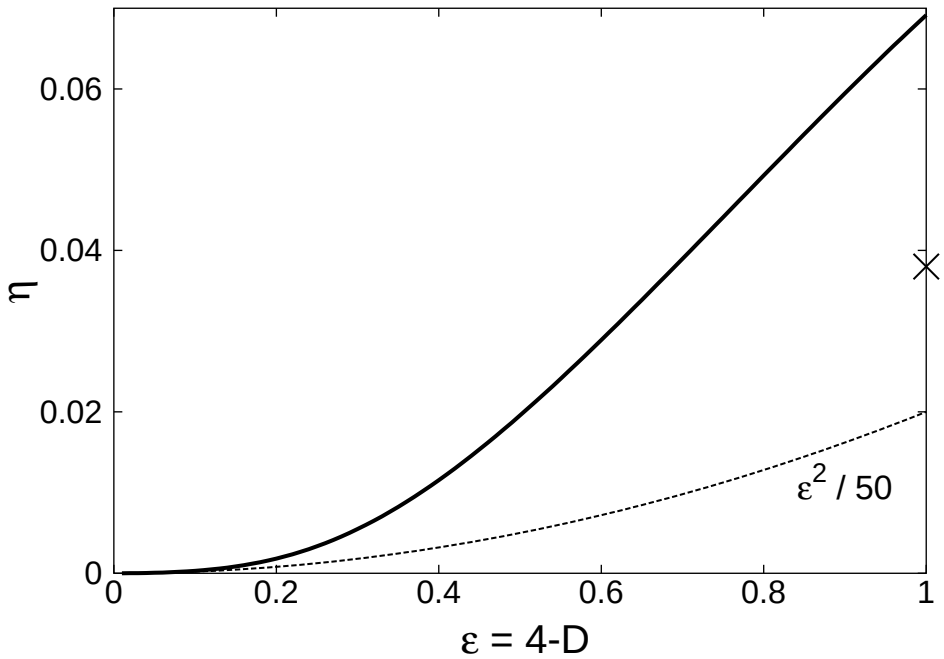
Marginal parameters in $D = 3$:

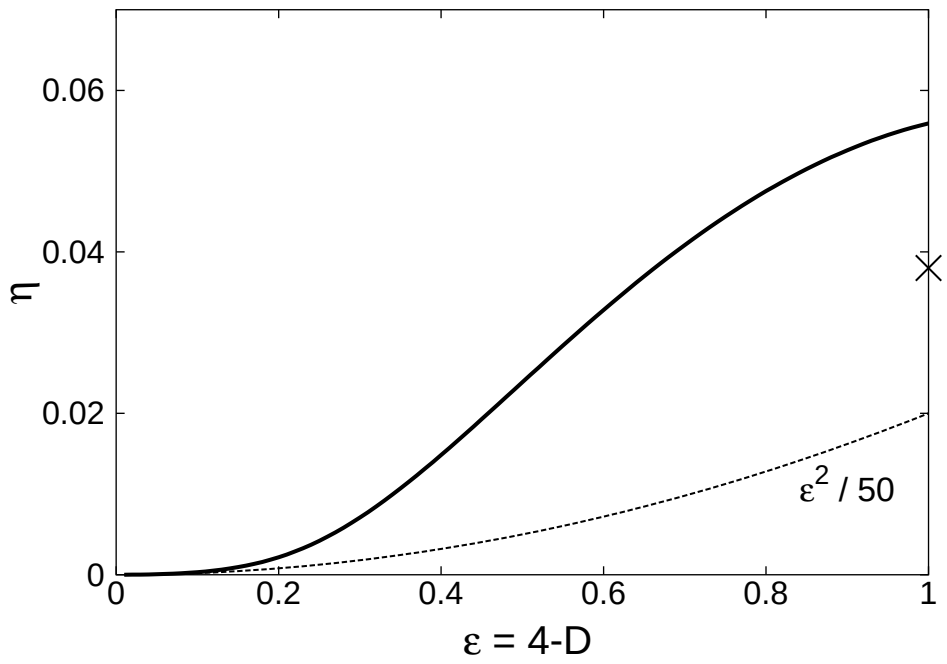
- First order momentum expansion of 4-point vertex
  $\tilde{\Gamma}_l^{(4)}(\mathbf{q}_1', \mathbf{q}_2'; \mathbf{q}_2, \mathbf{q}_1) = u_l + a_l\left(|\mathbf{q}_1 - \mathbf{q}_2'| + |\mathbf{q}_1 - \mathbf{q}_1'|\right) + b_l|\mathbf{q}_1 + \mathbf{q}_2| + O(q^2)$
- Momentum independent part of 6-point vertex
  $\tilde{\Gamma}_l^{(6)}(\mathbf{q}_1', \mathbf{q}_2', \mathbf{q}_3'; \mathbf{q}_3, \mathbf{q}_2, \mathbf{q}_1) = v_l + O(q)$

Including the 6-point vertex – results for η:

include 6-point vertex but ignore momentum dependence of $\dot{\Gamma}_l^{(6)}$

include 6-point vertex and part of 8-point vertex, include momentum dependence of $\dot{\Gamma}_l^{(6)}$





$\eta_*^{MC} = 0.038$

so far: $\eta_* = 0.104$

two loop ε-expansion: $\eta_* = \varepsilon^2/50$

Conclusions and outlook

Conclusions

- Functional RG formalism well suited to calculate full scaling functions
- Simple truncation scheme leads to good description of self energy
- Very accurate value for T_c shift
- Calculational effort relatively modest

Outlook

- Alternative truncation schemes (Blaizot et al., cond-mat/0412481)
- Quantum antiferromagnets in magnetic fields (with N. Hasselmann)
- Interacting fermions
  1. Fermi surface renormalization (with S. Ledowski, A. Ferraz, cond-mat/0412620)
  2. Fermions with dominant forward scattering (with F. Sch¨utz, L. Bartosch, cond-mat/0409404)
  3. Quantum impurity models (with F. Sch¨utz)