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 $\Delta T_c$

Collaborators:
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References:
BEC of homogeneous ideal Bose gas

Grand canonical partition function:

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

Equation of state:

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

Thermodynamic limit \( V \to \infty \):

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

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

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

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:

$$\frac{\Delta T_c}{T_c^0} = -1.3 \frac{a}{a_{ho}} N^{1/6} \quad a_{ho}: \text{ size of BEC cloud}$$

- $\Rightarrow$ interactions lead to smaller $T_c$
Results for $\Delta T_c$

Historical results for $\Delta T_c$:

- $\Delta T_c \propto a^{1/2}$
  - 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 $c_1$ ($\Delta T_c/T_c^0 \approx c_1 an^{1/3}$)

![Graph showing results for $\Delta T_c$ and $T_c / n^{2/3}$ vs. $n^{1/3} a$]
Mean field analysis

- Hartree Fock self-energy:
  \[ \Sigma_{HF} = 4a\lambda_T^2 n \]

- modified relation between density and chemical potential:
  \[ n = \frac{1}{\lambda_T^3 g_{3/2}}(z = e^{\beta(\mu - \Sigma_{HF})}) \]

- at transition \( \mu - \Sigma_{HF} = 0 \)
- \( \Rightarrow T_{c}^{HF} = T_{c}^{0} \)
- shift in \( T_{c} \) is correlation effect!
How to calculate $\Delta T_c$

- Calculate change in density $\Delta n_c$ 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:

$$n = -T \sum \nu \int \frac{d^3k}{(2\pi)^3} G(k, i\omega_\nu)$$

$$G(k, i\omega_\nu) = \frac{1}{i\omega_\nu + \mu - \varepsilon_k - \Sigma(k, i\omega_\nu)}$$

- 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

Need only consider $\omega = 0$ sector
IR breakdown of perturbation theory

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

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

- $n^{th}$ 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:

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

- 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:

\[ \sigma\left(\frac{k}{k_c}\right) \approx \left(\frac{k}{k_c}\right)^{2-\eta} \quad \text{for } k \ll k_c \quad \text{critical regime} \]

\[ \sigma\left(\frac{k}{k_c}\right) \approx \ln\left(\frac{k}{k_c}\right) \quad \text{for } k \gg k_c \quad \text{“perturbative” regime} \]
Renormalization group approach: two versions

Field theoretical RG:

- renormalizability required: physical quantities can be expressed in terms of a finite number of couplings, defined at arbitrary scale $\lambda$
- 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 finite due to lattice)
- best method for one-loop calculations, but difficult beyond one loop
Functional RG (=”exact” RG)

Modern implementation of Wilsonian RG:

- **Wilsonian effective action**: integrate over short wavelength modes and rescale
- **partition field**: \( \phi = \phi_\uparrow + \phi_\downarrow = \Theta(\Lambda_0 > |k| > \Lambda)\phi_\uparrow(k) + \Theta(\Lambda > |k|)\phi_\downarrow(k) \)
- **integrate over short-wavelength part**:

\[
\exp[ -S_\Lambda \{ \phi' \} ] = \int \mathcal{D}\{ \phi_\uparrow \} \exp[ -S_{\Lambda_0} \{ \phi_\downarrow + \phi_\uparrow \} ]
\]

formally: use cutoff-dependent propagator: \( G_{0,\Lambda_0}^\Lambda (k) = \frac{\Theta(\Lambda < |k| < \Lambda_0)}{k^2 + m_0^2} \)

- rescale field and momenta: \( \phi'_\downarrow(k') = \zeta \phi_\downarrow(e^{-i}k') \).

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

technical problem: ambiguities for sharp cutoff:

\[
\delta(x)\Theta(x) \to \frac{1}{2}\delta(x) , \quad \delta(x)\Theta^2(x) \to \frac{1}{3}\delta(x)
\]
One-particle irreducible version of exact RG

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

1. generating functional $G_c\{J\}$ of connected correlation functions.
2. generating functional of amputated connected correlation functions.

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

technical advantage: \(\Theta\)-functions appear under integral \(\implies\) no ambiguities!

several recent applications to interacting fermions:

( Wetterich-group; Honerkamp-Salmhofer collaboration; Göttingen-Stuttgart collaboration (Metzner-Meden-Schönhammer); P.K.-group; Katanin-Kampf collaboration; ... )
Effective action for interacting bosons

Effective action with cutoff $\Lambda_0$

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

$$S_{\Lambda_0}^0\{\bar{\psi}, \psi\} = \int_{k<\Lambda_0,\omega_n} [-i\omega_n + \varepsilon_k - \mu + \Sigma(0, i0)] \bar{\psi}_K \psi_K$$

$$S_{\Lambda_0}^{\text{int}}\{\bar{\psi}, \psi\} = \int_{k<\Lambda_0,\omega_n} [\Sigma_{\Lambda_0}(K) - \Sigma(0, i0)] \bar{\psi}_K \psi_K$$

$$+ \frac{1}{(2!)^2} \int_{K_1', K_2', K_2, K_1} \delta_{K_1' + K_2' + K_2 + K_1} \Gamma_{\Lambda_0}^{(4)}(K_1', K_2'; K_2, K_1) \bar{\psi}_{K_1'} \bar{\psi}_{K_2'} \psi_{K_2} \psi_{K_1} + \ldots$$

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 $l = -\ln(\Lambda/\Lambda_0)$):

$$\tilde{\Gamma}^{(2n)}_l(q_1', \ldots, q_n', q_n, \ldots, q_1) = (KDT)^{n-1} \Lambda^{D(n-1)-2n} \left(\frac{2mZ_l}{\hbar^2}\right)^n \Gamma^{(2n)}_\Lambda \{k_i = \Lambda q_i, \omega_{ni} = 0\}$$
Exact flow equation for irreducible vertices

General hierarchical structure of flow equations:
Two contributions: rescaling and integrating out high momentum slice

\[ \partial_t \tilde{\Gamma}_l^{(2n)}(\{q_i\}) = \left[ 2n - D(n-1) - n\eta_l - \sum_{i=1}^{2n} q_i \cdot \nabla q_i \right] \tilde{\Gamma}_l^{(2n)}(\{q_i\}) + \dot{\Gamma}_l^{(2n)}(\{q_i\}) \]

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

![Diagram of flow equation](image)
More exact flow equations:

**six-point vertex:**

\[ \begin{align*}
6 & = 8 + 3 \left[ 4 + 4 + 4 \right] \\
& + 9 \left[ 4 + 4 + 4 \right] \\
& + 9 \left[ 4 + 4 \right] \\
\end{align*} \]

and eight-point vertex:

\[ \begin{align*}
8 & = 16 \left[ 6 + 6 \right] + 9 \left[ 6 + 6 \right] \\
\end{align*} \]

and so on...

need truncation!!
Simplest truncation: relevant couplings

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

\( u_l = \tilde{\Gamma}_l^{(4)}(0,0;0,0) \): relevant part of four point vertex \( \tilde{\Gamma}_l^{(4)}(q'_1, q'_2; q_1, q_2) \)

Flow equations:

\[
\partial_l u_l = u_l - \frac{5}{2} u_l^2 \\
\partial_l r_l = 2r_l + u_l
\]

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 \( u_0 \propto a/\lambda_T \)

Wilson-Fisher fixed point:

\[
u_* = \frac{2}{5} \\
r_* = -u_*/2
\]

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:

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

with

\[ \dot{\Gamma}_l^{(2)}(q) = \int_{q'} \tilde{G}_l(q') \tilde{\Gamma}_l^{(4)}(q, q'; q', q) \]

\[ \tilde{G}_l(q) = \frac{\delta(|q| - 1)}{Z_l q^2 + \tilde{\Gamma}_l^{(2)}(q)} \]

⇒ dimensionless self-energy at RG fixed point \((l \rightarrow \infty)\):

\[ \sigma(x) = \int_0^\infty dl \, e^{-2(l-l_c)} \int_0^l d\tau \, \eta_l \left[ \tilde{\Gamma}_l^{(2)}(e^{l-l_c}x) - \tilde{\Gamma}_l^{(2)}(0) \right] \quad ; \quad x = k/k_c \]

Need “only” to calculate 4-point vertex and \(\eta_l\)
Approximation for $\tilde{\Gamma}_l^{(4)}$

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

\[
\begin{align*}
\tilde{\Gamma}_l^{(4)} &= \text{BCS} + \text{ZS} + \text{ZS}'
\end{align*}
\]

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

\[
\tilde{\Gamma}_l^{(4)}(q'_1, q'_2; q_2, q_1) \approx -u_l^2 \left[ \frac{1}{2} \dot{\chi}_l(|q_1 + q_2|) + \dot{\chi}_l(|q_1 - q'_1|) + \dot{\chi}_l(|q_1 - q'_2|) \right]
\]

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

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

Momentum-dependent self-energy: RG result

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

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

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

\[
= \int_0^\infty dl \ e^{-2(l-l_c)} \int_0^l d\tau \eta_{\tau} \left[ \hat{\Gamma}^{(2)}_l (e^{l-l_c} x) - \hat{\Gamma}^{(2)}_l (0) \right]
\]

\[
\approx \frac{3u_*^2}{2} x^{2-\eta_*} \int_{xe^{-l_c}}^\infty dy y^{-3+2\varepsilon} \frac{F(x,y;\eta_*,l_c)}{[x^\varepsilon + y^\varepsilon]^{2-2\eta_*/\varepsilon}}
\]

with \(\varepsilon = 4 - D\) and

\[
F(x,y;\eta_*,l_c) = \int_0^1 dz \frac{z^{1-\varepsilon}}{[x^\varepsilon + (y/z)^\varepsilon]^{\eta_*/\varepsilon} \left[ 1 + r_{l_c + \ln \frac{y}{z^x}} \right]}
\]

\[
\times \langle \hat{\chi}_{l_c + \ln \frac{y}{x}}(z) - \hat{\chi}_{l_c + \ln \frac{y}{x}}(\parallel \hat{q}' + y\hat{q} \parallel) \rangle \hat{q}' .
\]
Self energy: scaling function

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

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 ± 0.02
- Kashurnikov, 2001 (Lattice): 1.29 ± 0.05
- Kastening, 2004 (VPT): 1.27 ± 0.11
- Kleinert, 2003 (VPT): 1.23 ± 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
  \[ \tilde{\Gamma}_l^{(4)}(q_1', q_2'; q_2, q_1) = u_l + a_l (|q_1 - q_2'| + |q_1 - q_1'|) + b_l |q_1 + q_2| + O(q^2) \]

- Momentum independent part of 6-point vertex
  \[ \tilde{\Gamma}_l^{(6)}(q_1', q_2', q_3'; q_3, q_2, q_1) = v_l + O(q) \]
Including the 6-point vertex – results for $\eta$:

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

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

$\eta^{MC} = 0.038$

so far: $\eta_* = 0.104$

two loop $\varepsilon$-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. Schütz, L. Bartosch, cond-mat/0409404)
  3. Quantum impurity models (with F. Schütz)