Quantum Phase Diagram for Bose Gases

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1.1. Interaction-Free Bose Gas

Free Energy:

$$
\begin{aligned}
Z &= \oint \mathcal{D}\psi^* \oint \mathcal{D}\psi \, e^{-\mathcal{A}^{(0)}[\psi^*,\psi]/\hbar} = e^{-\beta F}\,, \qquad \beta = \frac{1}{k_B T} \\
\mathcal{A}^{(0)} &= \int_0^{\hbar\beta} d\tau \int d^3x \, \psi^*(\mathbf{x},\tau) \left(\hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2}{2M} \boldsymbol{\Delta} - \mu \right) \psi(\mathbf{x},\tau)
\end{aligned}
$$

Order Parameter:

fluctuation around background field Ψ^*, Ψ:

$$
\begin{aligned}
\psi(\mathbf{x},\tau) &= \Psi + \delta\psi(\mathbf{x},\tau) \\
\psi^*(\mathbf{x},\tau) &= \Psi^* + \delta\psi^*(\mathbf{x},\tau)
\end{aligned}
$$

$\Longrightarrow$ condensate density $n_0 = \Psi^* \Psi$

Effective Potential:

$$
F = \underset{\Psi^*,\,\Psi}{\text{Ext}} \; \mathcal{F}(\Psi^*, \Psi)
$$

$$
\mathcal{F}(\Psi^*, \Psi) = -V\mu\Psi^*\Psi - \frac{V}{\beta\lambda^3} \zeta_{5/2}\left(e^{\beta\mu}\right)
$$

$\lambda = \sqrt{\dfrac{2\pi\hbar^2}{M k_B T}}$ . . . thermodynamic wave length

$\zeta_\nu(z) = \displaystyle\sum_{k=1}^{\infty} \frac{z^k}{k^\nu}$ . . . polylogarithmic function

Extremization:

$$\frac{\partial \mathcal{F}}{\partial \Psi^*} = -V\mu\Psi = 0\,, \qquad \frac{\partial \mathcal{F}}{\partial \Psi} = -V\mu\Psi^* = 0$$

first phase: $\Psi = \Psi^* = n_0 = 0 \qquad \mu \neq 0$

second phase: $\Psi, \Psi^*, n_0 \neq 0 \qquad \mu = 0$

Thermodynamic Consequences:

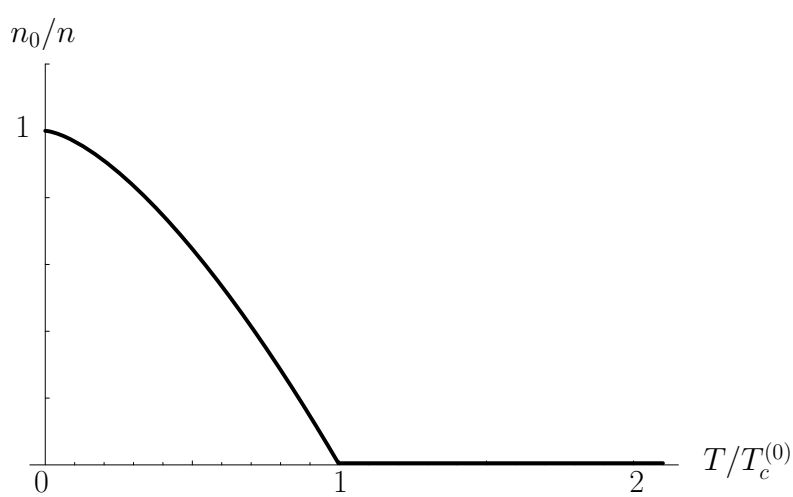
$$n = -\frac{1}{V}\frac{\partial F}{\partial \mu} = \underset{\Psi^*,\,\Psi}{\text{Ext}} \left[n_0 + \frac{1}{\lambda^3}\,\zeta_{3/2}\left(e^{\beta\mu}\right)\right]$$

- critical temperature: $n_0 = \mu = 0$

$$n = \frac{\zeta(3/2)}{\lambda_c^{(0)3}} \quad \Longrightarrow \quad T_c^{(0)} = \frac{2\pi\hbar^2}{Mk_B}\left[\frac{n}{\zeta(3/2)}\right]^{2/3}$$

- condensate density in second phase: $\mu = 0$

$$n = n_0 + \frac{\zeta(3/2)}{\lambda^3} \quad \Longrightarrow \quad n_0 = n\left[1 - \left(\frac{T}{T_c^{(0)}}\right)^{3/2}\right]$$



1.2. Robinson Formula

Definitions:

polylogarithmic function: $\zeta_\nu(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^\nu}$

Riemann zeta function: $\zeta(\nu) = \sum_{k=1}^{\infty} \frac{1}{k^\nu}$

Naive Calculation:

$$\zeta_\nu(e^{\beta\mu}) = \sum_{k=1}^{\infty} \frac{e^{\beta\mu k}}{k^\nu} \neq \sum_{l=0}^{\infty} \frac{(\beta\mu)^l}{l!} \zeta(\nu - l)$$

$\Longrightarrow$ summation order not exchangeable

Correct Calculation:

$$\zeta_\nu(e^{\beta\mu}) = \Gamma(1-\nu)\,(-\beta\mu)^{\nu-1} + \sum_{l=0}^{\infty} \frac{(\beta\mu)^l}{l!} \zeta(\nu - l)$$

$\Uparrow$ singular term

$\Uparrow$ regular term

Proofs:

- Mellin transformation (Robinson, 1951)
- Poisson formula

1.3. Overview

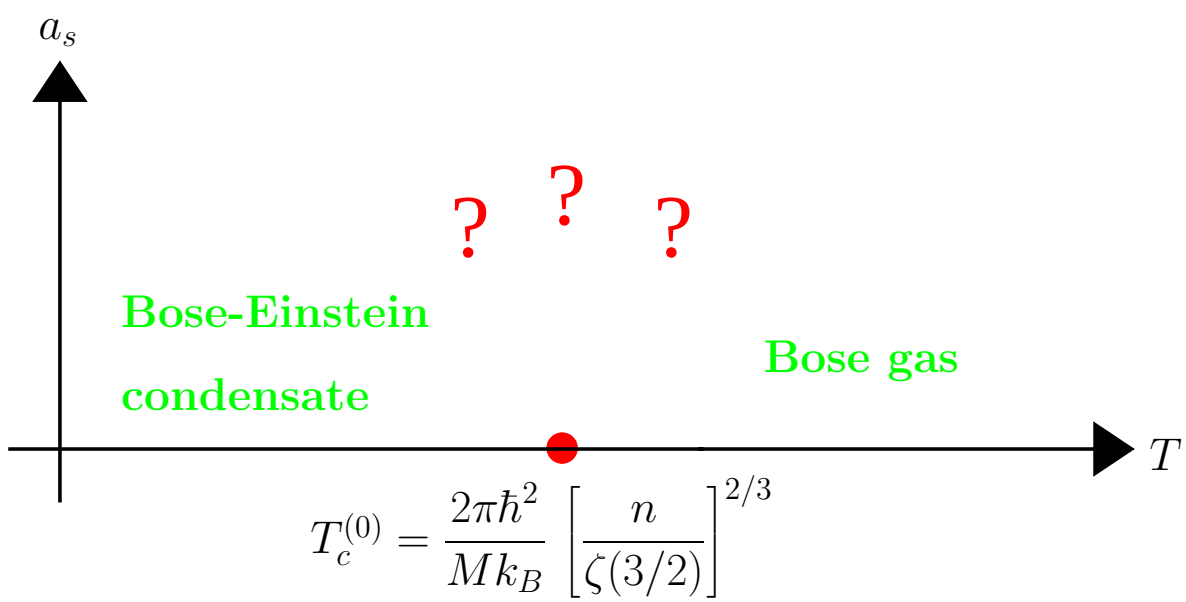
Model:

Bose gas with local repulsive 2-particle interaction

$$\mathcal{L}^{(3+1)} = \psi^* \left(\hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2}{2M} \boldsymbol{\Delta} - \mu \right) \psi + \frac{g}{2} |\psi|^4$$

s-wave scattering length: $\quad a_s = \dfrac{M}{4\pi\hbar^2} g$

Goal: a_s-T-phase diagram



Methods:

- $T > T_c$: perturbation theory with respect to a_s
- $T < T_c$: loop expansion

$\Longrightarrow$ resummation via variational perturbation theory

2.1. Basic Principle

weak-coupling series: $$f_N(g) = \sum_{n=0}^{N} a_n \; g^n$$

strong-coupling limit

strong-coupling series: $$f_M(g) = g^{p/q} \sum_{m=0}^{M} b_m \; g^{-2m/q}$$

Example:

	p	q	p/q	$2/q$
anharmonic oscillator	1	3	1/3	2/3

2.2. Quantum Mechanical Example

Anharmonic Oscillator:

$$V(x) = \frac{1}{2}\,\omega^2 x^2 + g\,x^4$$

Weak-Coupling Series of Ground-State Energy:

$$E_0 = \frac{\omega}{2} + g\,\frac{3}{4\omega^2} - g^2\,\frac{21}{8\omega^5} + g^3\,\frac{333}{16\omega^8} + \ldots$$

Identity:

$$V(x) = \underbrace{\frac{1}{2}\,\Omega^2 x^2}_{\text{effective harmonic oscillator}} + \underbrace{g\,x^4 + \frac{1}{2}\left(\omega^2 - \Omega^2\right) x^2}_{\text{perturbation}}$$

Ω: variational parameter

Substitution:

$$V(x) = \frac{1}{2}\left(\Omega\sqrt{1 + g\,\frac{\omega^2 - \Omega^2}{g\Omega^2}}\right)^2 x^2 + g\,x^4$$

$$\omega \quad \Rightarrow \quad \Omega\sqrt{1 + gr}\,, \qquad r = \frac{\omega^2 - \Omega^2}{g\Omega^2}$$

First Order:

$$E_0^{(1)} = \frac{\omega}{2} + g\,\frac{3}{4\omega^2}$$

$$E_0^{(1)}(\Omega) = \frac{\Omega}{4} + \frac{\omega^2}{4\Omega} + g\,\frac{3}{4\Omega^2}$$

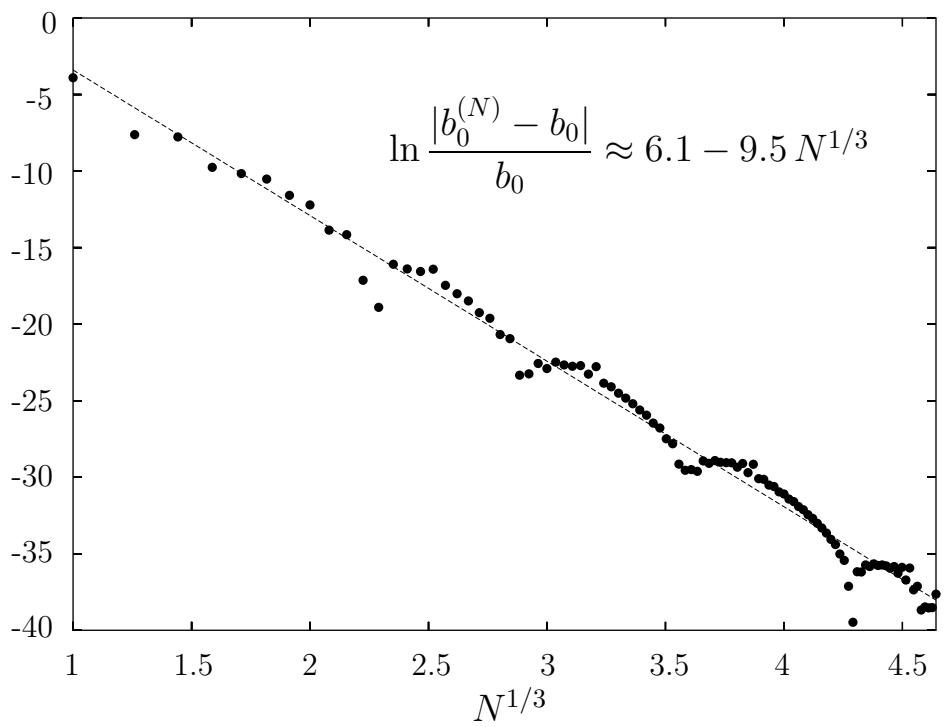
Principle of Minimal Sensitivity:

$$\frac{\partial E_0^{(1)}(\Omega)}{\partial \Omega} = 0 \quad \Rightarrow \quad \Omega^{(1)} \quad \Rightarrow \quad E_0^{(1)} \approx E_0^{(1)}(\Omega^{(1)})$$

Strong-Coupling Limit $g \to \infty$:

$$E_0^{(1)} = g^{1/3}\left(b_0^{(1)} + b_1^{(1)}\,g^{-2/3} + b_2^{(1)}\,g^{-4/3} + \ldots\right)$$

Exponential Convergence:



3. High-Temperature Perturbation Theory

Leading Critical Temperature Shift:

no interaction: $$T_c^{(0)} = \frac{2\pi\hbar^2}{M k_B} \left[\frac{n}{\zeta(3/2)}\right]^{2/3}$$

interaction: $$T^{(\mathrm{int})} = \frac{4\pi\hbar^2 a_s}{M} \frac{n}{k_B}$$

limit $a_s \longrightarrow 0$: $$T^{(\mathrm{int})} \ll T_c^{(0)}$$

High-Temperature Approximation:

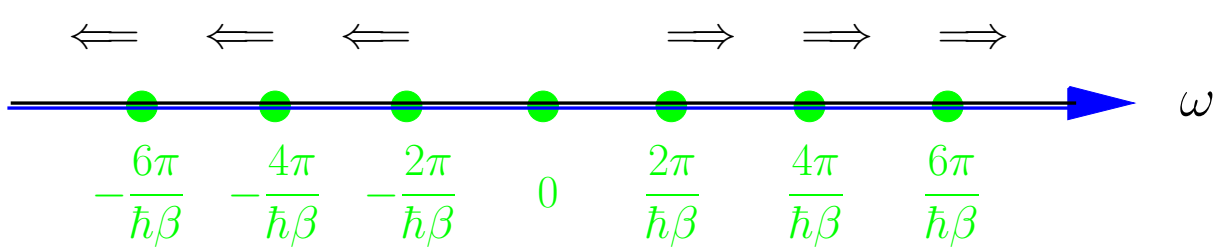
Bose fields require periodicity:

$$\psi(\mathbf{x}, 0) = \psi(\mathbf{x}, \hbar\beta)$$

Matsubara decomposition:

$$\psi(\mathbf{x}, \tau) = \sum_{m=-\infty}^{+\infty} \psi_m(\mathbf{x})\, e^{-i\omega_m \tau}\,, \qquad \omega_m = \frac{2\pi}{\hbar\beta}\, m$$

Limit $\beta \longrightarrow 0$: survival of zero mode



Lagrangian:

$$\mathcal{L}^{(3+1)} = \psi^* \left(\hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2}{2M} \boldsymbol{\Delta} - \mu \right) \psi + \frac{g}{2} |\psi|^4$$

$$\Downarrow \qquad \text{limit } \beta \to 0$$

$$\mathcal{L}^{(3)} = \frac{1}{2} |\boldsymbol{\nabla} \psi_0|^2 + \frac{1}{2} m^2 |\psi_0|^2 + \frac{u}{4!} |\psi_0|^4$$

ψ_0	...	Matsubara zero mode
$m^2 \propto -\mu$	...	mass term
$u \propto a_s$	...	interaction term

Leading Critical Temperature Shift:

- Baym, Blaizot, Holzmann, Laloë, Vautherin (1999):

$$\frac{\Delta T_c}{T_c^{(0)}} \approx -\frac{2}{3} \frac{\Delta n}{n} \approx c_1 \, a_s \, n^{1/3} \,, \qquad \Delta n \propto \Delta \langle \psi_0^2 \rangle$$

- high-order perturbative calculation:

$$c_1^{(N)} = \sum_{k=1}^{N} a_k \left(\frac{u}{m_r} \right)^k$$

- c_1: nonperturbative result

critical limit $m_r \to 0 \quad \Longleftrightarrow \quad$ strong-coupling problem

VPT Results for c_1:

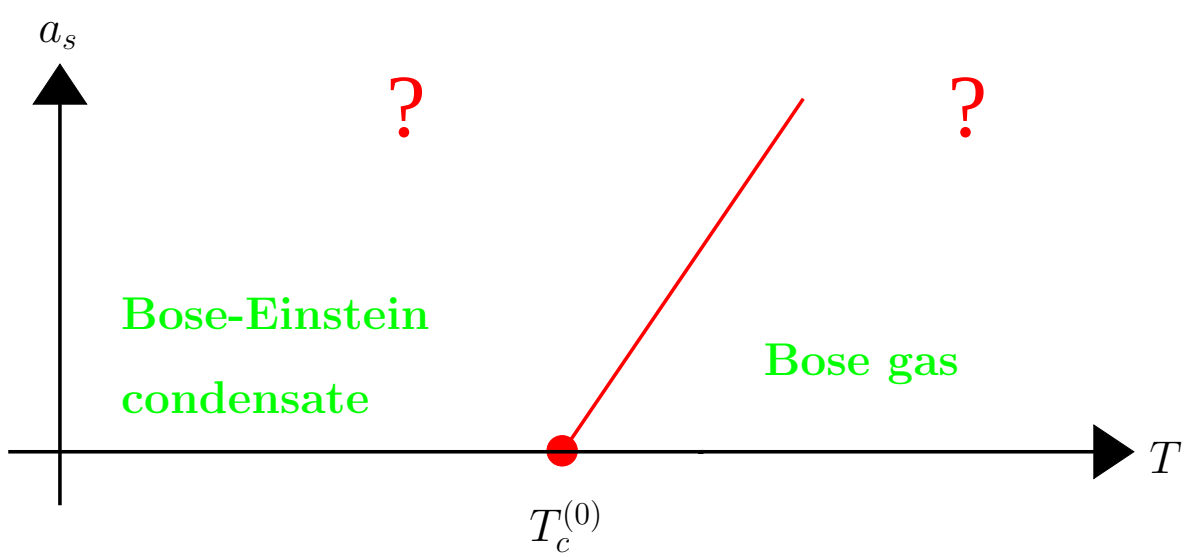
Kleinert, 5 loops	cond-mat/0210162	1.23 ± 0.17
Kastening, 6 loops	cond-mat/0303486	1.25 ± 0.13
Kastening, 7 loops	cond-mat/0309060	1.27 ± 0.11

renormalized chemical potential as variational parameter

Monte Carlo Results for c_1:

Arnold, Moore	PRL **87**, 120401 (2001)	1.32 ± 0.02
Svistunov et al.	PRL **87**, 120402 (2001)	1.29 ± 0.05

Phase Diagram:



$\Longrightarrow$ global structure?

4. Finite-Temperature Perturbation Theory

Lagrangian:

$$\mathcal{L} = \psi^* \left(\hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2}{2M} \boldsymbol{\Delta} - \mu \right) \psi + \frac{2\pi\hbar^2 a_s}{M} |\psi|^4$$

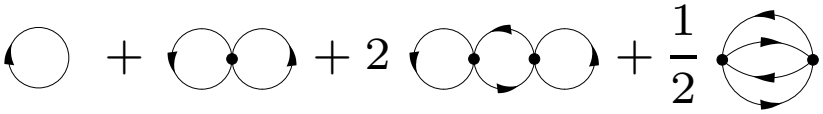
Feynman Rules:

$$\equiv \int \frac{d^3p}{(2\pi\hbar)^3} \frac{e^{i\mathbf{p}(\mathbf{x}_1-\mathbf{x}_2)/\hbar}}{2\sinh\frac{\beta}{2}\left(\frac{\mathbf{p}^2}{2M}-\mu\right)}$$

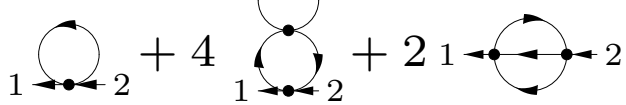
$$\times \left[\Theta(\tau_1-\tau_2)\, e^{-\frac{1}{\hbar}\left(\frac{\mathbf{p}^2}{2M}-\mu\right)\left(\tau_1-\tau_2-\frac{\hbar\beta}{2}\right)} + (1 \Longleftrightarrow 2) \right]$$

$$\equiv -\frac{4\pi\hbar a_s}{M} \int d^3x \int_0^{\hbar\beta} d\tau$$

Grand-Canonical Potential:

$F =$  $+ \ldots$

Self-Energy:

$\Sigma(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_2) =$ 2  $+ \ldots$

Technical Procedure:

- particle density: $$n(\mu) = -\frac{1}{V}\frac{\partial F}{\partial \mu} = n^{(0)} + n^{(1)} + \ldots$$
- renormalized chemical potential:

$$\mu_r(\mu) = \mu + \hbar\Sigma\left(\mathbf{p} = \mathbf{0}, \omega_m = 0\right) = \mu_r^{(0)} + \mu_r^{(1)} + \ldots$$

- renormalization: $$n(\mu_r) = n\left(\mu\left(\mu_r\right)\right)$$

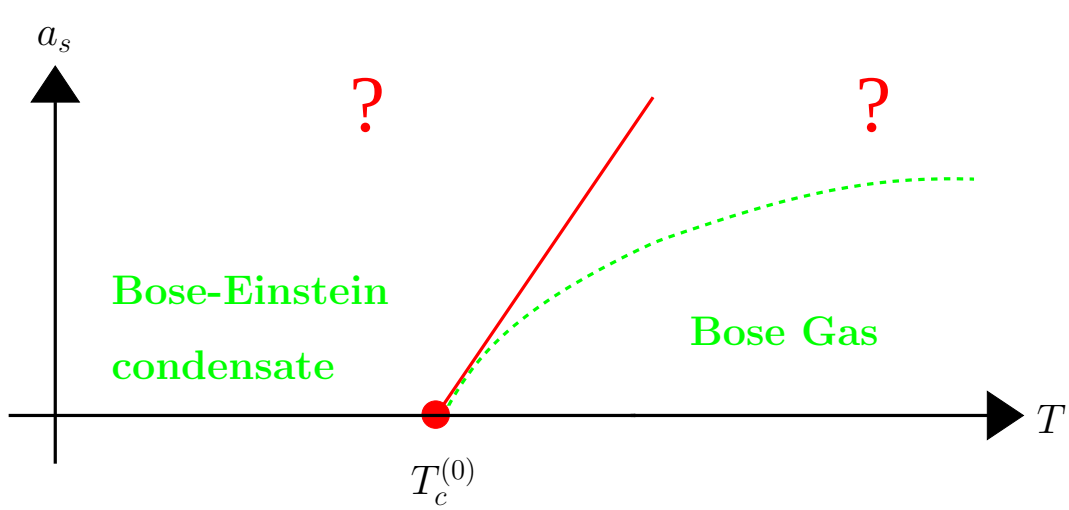
Problems:

- UV divergencies: $D = 3 - 2\epsilon$
- IR divergencies: Robinson formula

Critical Temperature Shift:

Arnold, Moore, Tomášik (2002): $c_2 \approx 19.75, \quad c_2' \approx 75.7$

$$\frac{\Delta T_c}{T_c^{(0)}} = c_1 a_s n^{1/3} + a_s^2 n^{2/3}\left(c_2 \ln a_s n^{1/3} + c_2'\right)$$



5. Loop Expansion

Lagrangian:

$$\mathcal{L} = \psi^* \left[\hbar \frac{\partial}{\partial \tau} + \epsilon \left(-i\hbar \boldsymbol{\nabla} \right) - \mu \right] \psi + \frac{g}{2} |\psi|^4$$

$\epsilon(\mathbf{k})$ . . . one-particle energies

1-Loop Result: Effective Potential

$$\begin{aligned} \mathcal{F}(\Psi, \Psi^*) &= V \left(-\mu |\Psi|^2 + \frac{g}{2} |\Psi|^4 \right) \\ &\quad + \eta \sum_{\mathbf{k}} \left\{ \frac{E(\mathbf{k})}{2} + k_B T \, \ln \left[1 - e^{-E(\mathbf{k})/k_B T} \right] \right\} \\ E(\mathbf{k}) &= \sqrt{[\epsilon(\mathbf{k}) - \mu + 2g|\Psi|^2]^2 - g^2 |\Psi|^4} \end{aligned}$$

η . . . loop counter

Extremization in Ψ, Ψ^*:

$$\begin{aligned} \text{condensate density:} \quad n_0(\mu, T) &= \Psi^* \Psi \\ \text{grand-canonical potential:} \quad F(\mu, T) &= \underset{\Psi^*, \Psi}{\text{Ext}} \; \mathcal{F}(\Psi^*, \Psi) \\ \text{particle density:} \quad n(\mu, T) &= -\frac{1}{V} \frac{\partial F(\mu, T)}{\partial \mu} \end{aligned}$$

Elimination of μ:

$$n - n_0 = \frac{\eta}{V} \sum_{\mathbf{k}} \frac{\epsilon(\mathbf{k}) + g n_0}{\sqrt{\epsilon(\mathbf{k})^2 + 2 g n_0 \epsilon(\mathbf{k})}} \times \left(\frac{1}{2} + \frac{1}{e^{\sqrt{\epsilon(\mathbf{k})^2 + 2 g n_0 \epsilon(\mathbf{k})}/k_B T} - 1} \right)$$

$\Longrightarrow$ Popov approximation

VPT Resummation:

chemical potential as variational parameter:

$$\mu = M\,(1 + r\,\eta)\ , \qquad r = \frac{\mu - M}{\eta M}$$

VPT Result:

$$n - n_0 = \frac{\eta}{V} \sum_{\mathbf{k}} \frac{\epsilon(\mathbf{k}) + g n}{\sqrt{\epsilon(\mathbf{k})^2 + 2 g n \epsilon(\mathbf{k})}} \times \left(\frac{1}{2} + \frac{1}{e^{\sqrt{\epsilon(\mathbf{k})^2 + 2 g n \epsilon(\mathbf{k})}/k_B T} - 1} \right)$$

$\Longrightarrow$ self-consistent Popov approximation

$\Longrightarrow$ quantum phase transition: $\quad n_0 \equiv 0\ , \quad \eta = 1$

6. Homogeneous BEC

Dispersion:

$$\epsilon(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2}{2M}\,, \qquad \sum_{\mathbf{k}} = V \int \frac{d^3k}{(2\pi)^3}$$

Quantum Phase Transition:

$$\begin{aligned}
\left(\frac{9\pi}{64}\right)^{1/3} &= a_s^c\, n^{1/3} \left[1 + \frac{3\alpha}{16} I(\alpha)\right]^{2/3} \\
I(\alpha) &= \int_0^\infty dx\, \frac{x\alpha + 8}{2\sqrt{x\alpha + 16}\;\left(e^{\sqrt{x + x^2\alpha/16}} - 1\right)} \\
\alpha &= \left(\frac{T}{a_s^c\, n^{1/3} \zeta^{2/3}(3/2)\, T_c^{(0)}}\right)^2
\end{aligned}$$

Expansion For $T \geq 0$:

$$a_s^c\, n^{1/3} = \sum_{k=0}^{N} a_k \alpha^k + \mathcal{O}(\alpha^{N+1})$$

$$a_0 = \left(\frac{9\pi}{64}\right)^{1/3} \approx 0.762\,, \quad a_1 \approx -0.313\,, \quad a_2 \approx 0.200$$

Expansion For $T \approx T_c^{(0)}$:

$$\frac{\Delta T}{T_c^{(0)}} = \frac{4\sqrt{2\pi}}{3\zeta^{2/3}(3/2)} \sqrt{a_s^c n^{1/3}} + \mathcal{O}(a_s^c n^{1/3})$$

VPT Resummation:

$$a_s^c\, n^{1/3} = a_0 + a_1\alpha + a_2\alpha^2 + \ldots \quad ; \quad \alpha \propto \left(\frac{T}{a_s^c}\right)^2$$

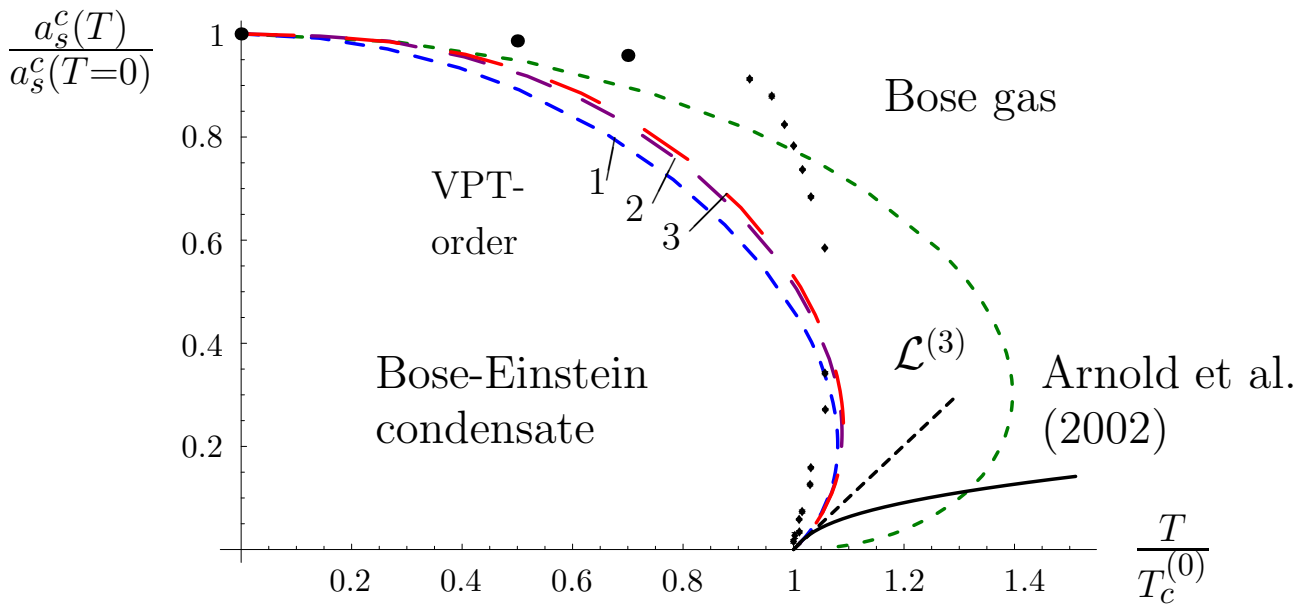
$$\Downarrow \qquad \text{limit } a_s^c \to 0 \iff \alpha \to \infty$$

$$\frac{\Delta T}{T_c^{(0)}} = c_1\, a_s^c\, n^{1/3} + \ldots$$

H. Kleinert, S. Schmidt, A. Pelster:

`cond-mat/0307412` , `cond-mat/0308561`

Calculated Phase Diagram:

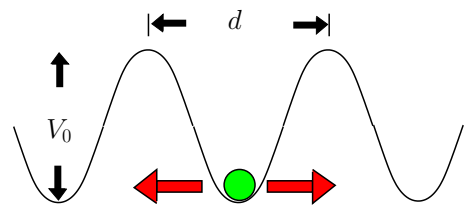


- ♦ Grüter, Ceperley, Laloë (1997)
- • Pollock, Runge (1992)

7. Optical Bose Lattice

BEC in Optical Lattice:

$$V(\mathbf{x}) = V_0 \sum_{i=1}^{3} \sin^2\left(\frac{\pi x_i}{d}\right)$$



Dispersion:

$$\epsilon(\mathbf{k}) = 2J \sum_{i=1}^{3} (1 - \cos k_i d)\,, \qquad \sum_{\mathbf{k}} = V \prod_{i=1}^{3} \int_{-\pi/d}^{\pi/d} \frac{dk_i}{2\pi}$$

Quantum Phase Transition:

- remaining integral:

$$n = \prod_{i=1}^{3} \int_{-\pi/d}^{\pi/d} \frac{dk_i}{2\pi}\, f\left(\epsilon(\mathbf{k})\right)$$

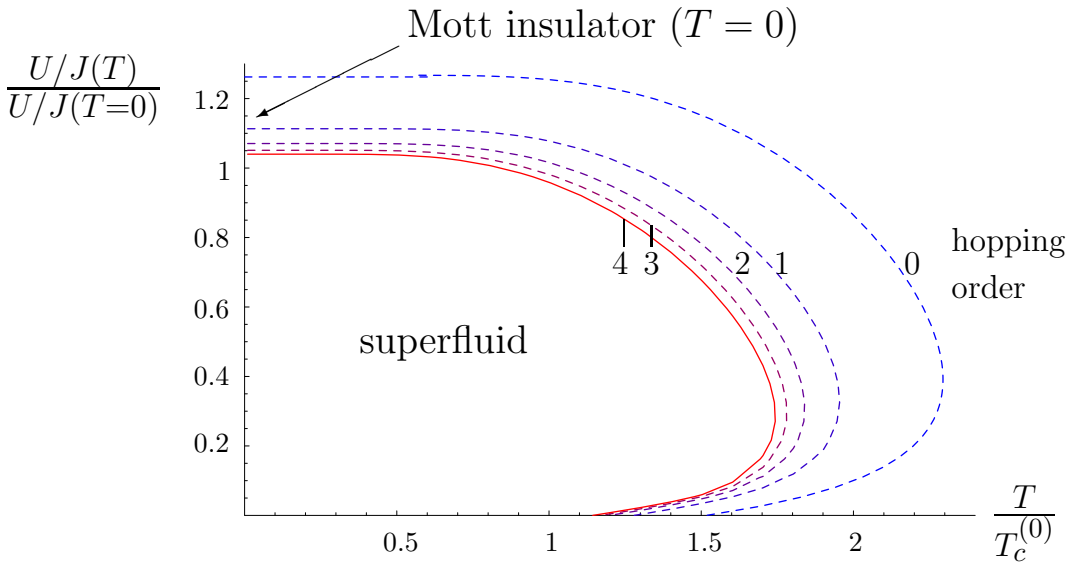
- expansion with respect to hopping parameter κ:

$$\epsilon(\mathbf{k}) = 2J \sum_{i=1}^{3} (1 - \kappa \cos k_i d)\,,$$

- transition line:

$$F\left(\frac{k_B T}{J}, \frac{U}{J}\right) \quad = \quad 0\,, \qquad U = g\,n$$

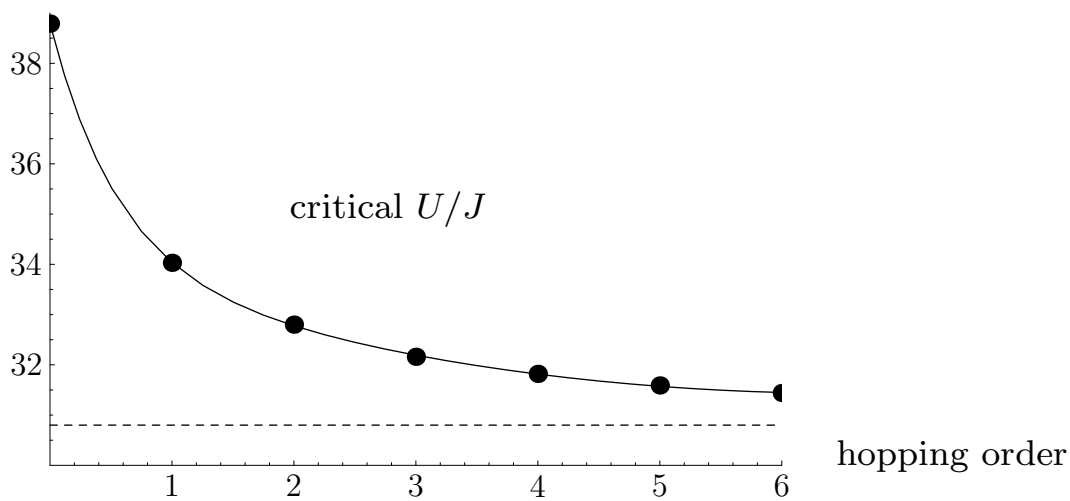
Calculated Phase Diagram:



H. Kleinert, S. Schmidt, A. Pelster: `cond-mat/0307412`

Critical $U/J|_{T=0}$:

Convergence of hopping expansion:



hopping expansion: $U/J(T = 0) \approx 31$

Greiner et al. (2002): $U/J(T = 0) \approx 33 - 36$

8.1. Arbitrary 2-Particle Interaction

Model:

$$\mathcal{A}[\psi^*,\psi] = \int_0^{\hbar\beta} d\tau \int d^3x\, \psi^*(\mathbf{x},\tau) \left(\hbar \frac{\partial}{\partial\tau} - \frac{\hbar^2}{2M} \mathbf{\Delta} - \mu \right) \psi(\mathbf{x},\tau)$$

$$+ \frac{1}{2} \int_0^{\hbar\beta} d\tau \int d^3x \int d^3x'\, V^{(\mathrm{int})}(\mathbf{x}-\mathbf{x}')\, \psi^*(\mathbf{x},\tau)\psi^*(\mathbf{x}',\tau)\psi(\mathbf{x}',\tau)\psi(\mathbf{x},\tau)$$

Particle Number:

$$n = \frac{1}{\lambda^3}\, \zeta_{3/2}\left(e^{\beta\mu_r}\right) + \frac{\beta}{\lambda^6}\, \zeta_{1/2}\left(e^{\beta\mu_r}\right) \sum_{k=1}^{\infty} \frac{e^{\beta\mu_r k}}{k^{3/2}} \int d^3x\, V^{(\mathrm{int})}(\mathbf{x})\, \exp\left(-\frac{\pi}{\lambda^2 k}\, \mathbf{x}^2\right)$$

$$-\frac{\beta}{\lambda^6} \sum_{k=1}^{\infty}\sum_{l=1}^{\infty} \frac{e^{\beta\mu_r(k+l)}}{k^{1/2} l^{3/2}} \int d^3x\, V^{(\mathrm{int})}(\mathbf{x})\, \exp\left[-\frac{\pi(k+l)}{\lambda^2 kl}\, \mathbf{x}^2\right] + \ldots$$

Long-Range Magnetic Dipole-Dipole Interaction:

S. Giovanazzi, A. Görlitz, and T. Pfau,
Phys. Rev. Lett. **89**, 130401 (2002)

$$V^{(\mathrm{int})}(r,\vartheta,\varphi) = -\frac{\mu_0 m^2}{4\pi}\, \frac{3\cos^2\vartheta - 1}{r^3}$$

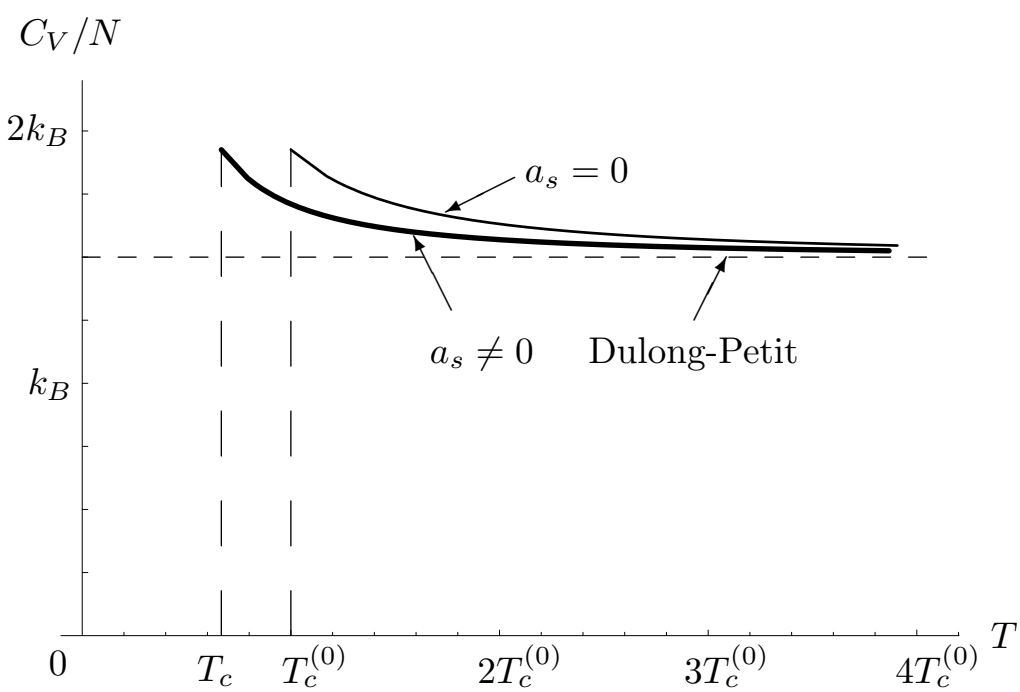
m . . . magnetic dipole moment

Short-Range Interaction:

$$\frac{\Delta T_c}{T_c^{(0)}} = \frac{M n^{1/3}}{3\pi\hbar^2 \zeta^{4/3}(3/2)} \sum_{k=1}^{\infty} \left[\frac{-\pi n^{2/3}}{\zeta^{2/3}(3/2)} \right]^k$$
$$\times \int d^3x\, V^{(\mathrm{int})}(\mathbf{x}) (\mathbf{x}^2)^k \sum_{l=1}^{k} \frac{\zeta(l+1/2)\zeta(3/2+k-l)}{l!(k-l)!}$$

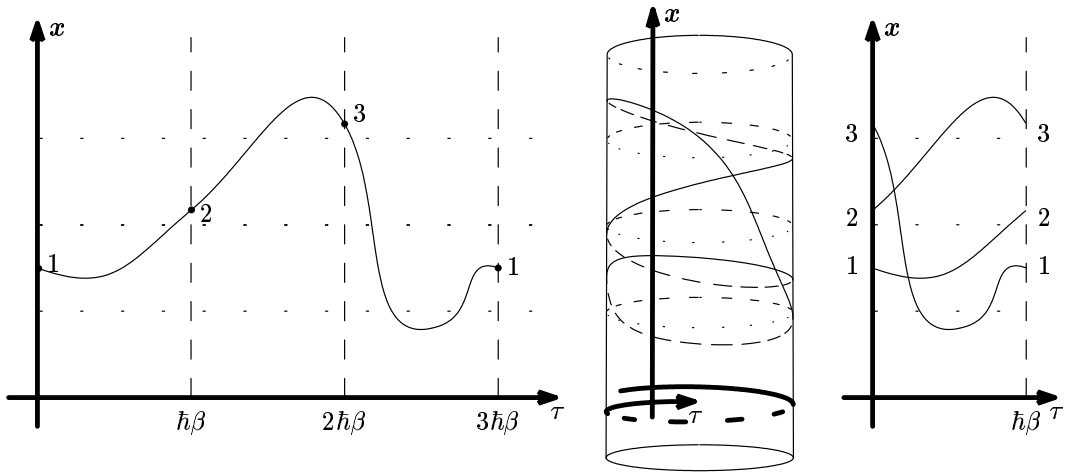
Example:

$$V^{(\mathrm{int})}(\mathbf{x}) = \frac{4\pi\hbar^2 a_s}{M} \left(1 + \frac{r^2}{6} \boldsymbol{\Delta} \right) \delta(\mathbf{x})$$
$$\frac{\Delta T_c}{T_c^{(0)}} = -\frac{4\pi}{3} a_s r^2 n$$



8.2. Canonical Ensemble Without Interaction

Cycles:



$$Z_N^{(0)}(\beta) \quad = \quad \sum_{C_1,\ldots,C_N}^{(\sum nC_n=N)} \prod_{n=1}^{N} \frac{1}{C_n!} \left[\frac{Z_1^{(0)}(n\beta)}{n} \right]^{C_n}$$

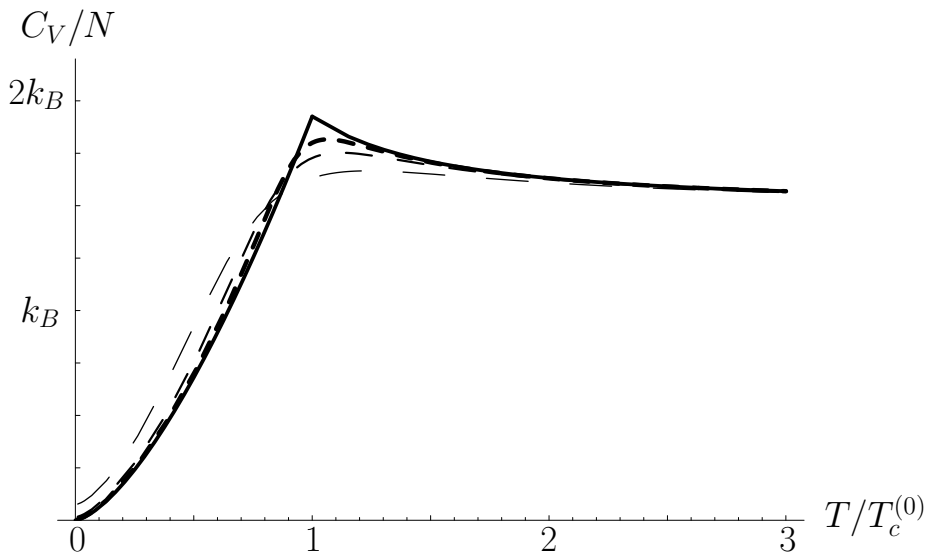
n . . . length of a cycle $\qquad$ C_n ... number of cycles

Rekursion:

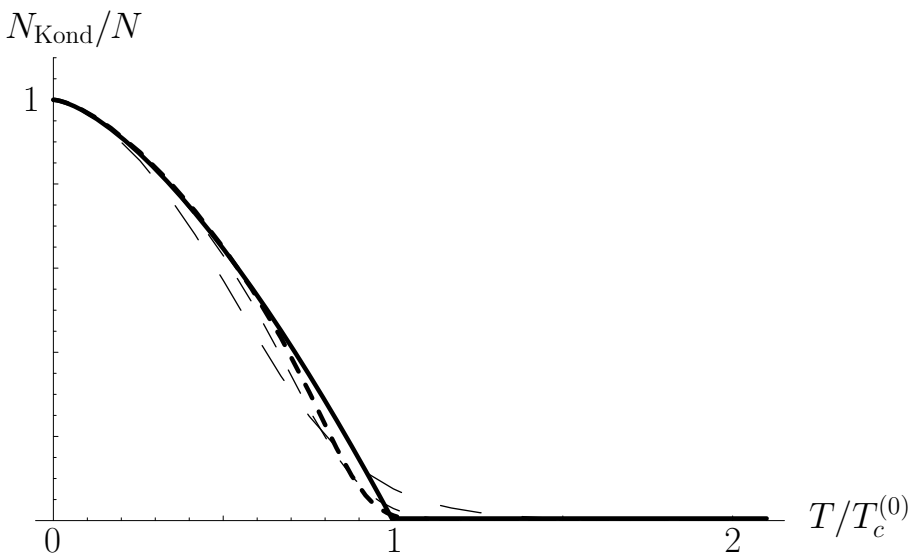
$$Z_N^{(0)}(\beta) \quad = \quad \frac{V}{\lambda^3 N} \sum_{n=1}^{N} \frac{1}{n^{3/2}} Z_{N-n}^{(0)}(\beta)$$

$$Z_0^{(0)}(\beta) \quad = \quad 1$$

Heat Capacity:



Condensate:



canonical ensemble: N=20 (— —), N=100 (- - -), N=500 (- - - -)

grand-canonical ensemble: ——