



Weakly Interacting Dipolar Bose-Gases within Canonical Ensemble

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- 1. Motivation for Canonical Ensemble

R.M. Ziff, G.E. Uhlenbeck, and M. Kac, *The Ideal Bose-Einstein Gas, Revisited*, Phys. Reports **32**, 169 (1977)

- 2. Identical Noninteracting Particles

R.P. Feynman, *Statistical Mechanics* (Bejamin, Reading, 1972)

- 3. Canonical Approach to Interacting Systems

K. Glaum, H. Kleinert, and A. Pelster, *Bose-Einstein Condensation in Canonical Ensembles*, in preparation

- 4. Outlook

1. Grand-Canonical Ensemble Theory

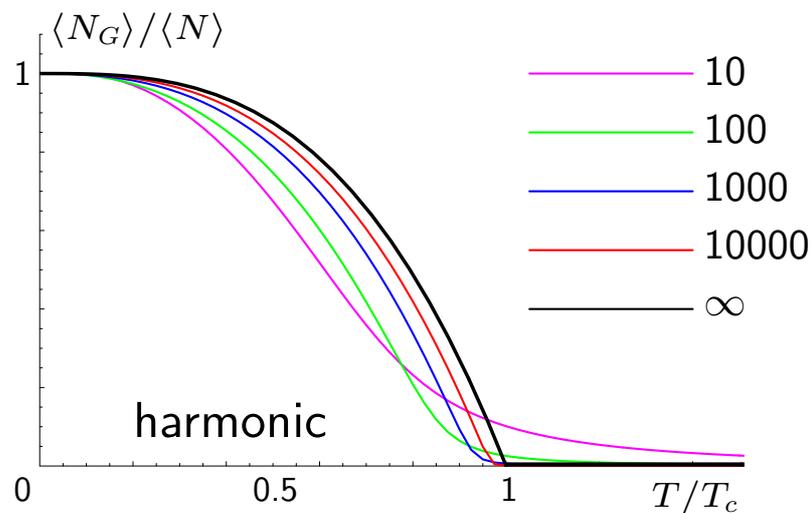
Grand-Canonical Potential:

$$\mathcal{F}_{GC}^B = \frac{1}{\beta} \sum_{\mathbf{k}} \ln \left\{ 1 - e^{-\beta(E_{\mathbf{k}} - \mu)} \right\}$$

Average Particle Number:

$$\langle N_{\mathbf{k}} \rangle = \frac{1}{e^{\beta(E_{\mathbf{k}} - \mu)} - 1}$$

Ground-State Fraction:



Ground-State Number Fluctuation:

$$\langle (\Delta N_G)^2 \rangle = \langle N_G \rangle \left[\langle N_G \rangle + 1 \right]$$

For $\beta \rightarrow \infty$ in Thermodynamic Limit: $\langle (\Delta N_G)^2 \rangle \rightarrow \langle N \rangle^2$

2.1. N -Particle Propagator

Definition:

$$\begin{aligned} & (\mathbf{x}_1, \dots, \mathbf{x}_N; \tau_b | \mathbf{x}'_1, \dots, \mathbf{x}'_N; \tau_a)^{(0)} \\ & \equiv \prod_{n=1}^N \left(\int_{\mathbf{x}_n(\tau_a)=\mathbf{x}'_n}^{\mathbf{x}_n(\tau_b)=\mathbf{x}_n} \mathcal{D}^D x_n(\tau) \right) \exp \left\{ -\frac{1}{\hbar} \mathcal{A}^{(0)}[\mathbf{x}_1, \dots, \mathbf{x}_N] \right\} \end{aligned}$$

Action:

$$\mathcal{A}^{(0)}[\mathbf{x}_1, \dots, \mathbf{x}_N] \equiv \sum_{n=1}^N \int_{\tau_a}^{\tau_b} d\tau' \left[\frac{M}{2} \dot{\mathbf{x}}_n^2(\tau') + V(\mathbf{x}_n(\tau')) \right]$$

Factorization:

$$\begin{aligned} & (\mathbf{x}_1, \dots, \mathbf{x}_N; \tau_b | \mathbf{x}'_1, \dots, \mathbf{x}'_N; \tau_a)^{(0)} \\ & = (\mathbf{x}_1; \tau_b | \mathbf{x}'_1; \tau_a)^{(0)} \dots (\mathbf{x}_N; \tau_b | \mathbf{x}'_N; \tau_a)^{(0)} \end{aligned}$$

Group Property:

$$\int d^D x'' (\mathbf{x}; \tau_b | \mathbf{x}''; \tau)^{(0)} (\mathbf{x}''; \tau | \mathbf{x}'; \tau_a)^{(0)} = (\mathbf{x}; \tau_b | \mathbf{x}'; \tau_a)^{(0)}$$

Time Translation Invariance:

$$(\mathbf{x}; \tau_b + \tau | \mathbf{x}'; \tau_a + \tau)^{(0)} = (\mathbf{x}; \tau_b | \mathbf{x}'; \tau_a)^{(0)}$$

2.2. N Identical Particles

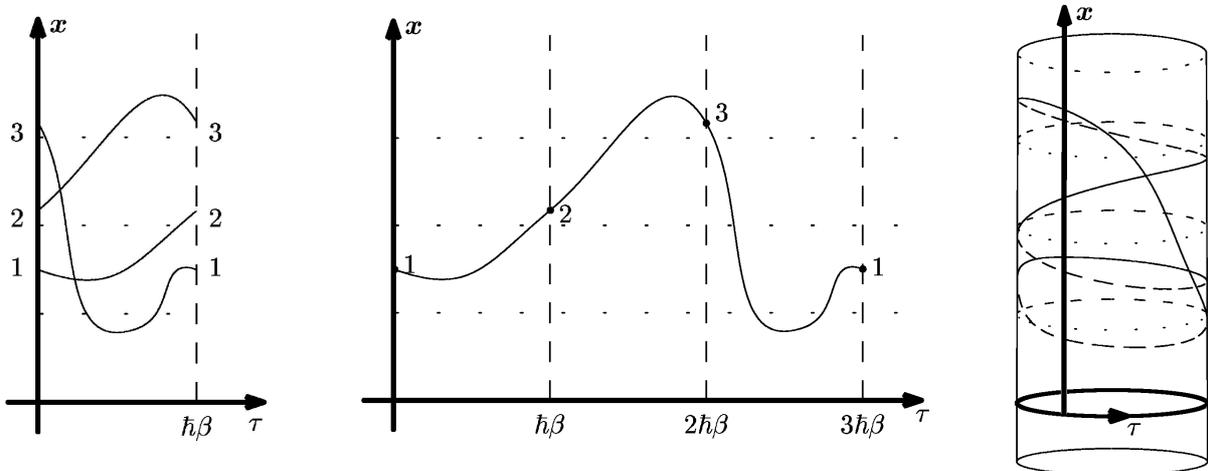
Propagator:

$$\begin{aligned}
 & (\mathbf{x}_1, \dots, \mathbf{x}_N; \tau_b | \mathbf{x}'_1, \dots, \mathbf{x}'_N; \tau_a)^{(0)B,F} \\
 &= \frac{1}{N!} \sum_P (\pm 1)^{p(P)} (\mathbf{x}_{P(1)}, \dots, \mathbf{x}_{P(N)}; \tau_b | \mathbf{x}'_1, \dots, \mathbf{x}'_N; \tau_a)^{(0)}
 \end{aligned}$$

Partition Function:

$$\begin{aligned}
 Z_N^{(0)B,F}(\beta) &\equiv \int d^D x_1 \dots d^D x_N (\mathbf{x}_1, \dots, \mathbf{x}_N; \hbar\beta | \mathbf{x}_1, \dots, \mathbf{x}_N; 0)^{(0)B,F} \\
 &= \frac{1}{N!} \sum_P (\pm 1)^{p(P)} \int d^D x_1 \dots d^D x_N \\
 &\quad \times (\mathbf{x}_{P(1)}; \hbar\beta | \mathbf{x}_1; 0)^{(0)} \dots (\mathbf{x}_{P(N)}; \hbar\beta | \mathbf{x}_N; 0)^{(0)}
 \end{aligned}$$

Closed Cycle:



2.3. Cyclic Representation

Contribution of a Closed Cycle:

$$h_n(\beta) \equiv \int d^D x_1 \dots d^D x_n (\mathbf{x}_1; \hbar\beta | \mathbf{x}_n; 0)^{(0)} \\ \times (\mathbf{x}_n; \hbar\beta | \mathbf{x}_{n-1}; 0)^{(0)} \dots (\mathbf{x}_2; \hbar\beta | \mathbf{x}_1; 0)^{(0)}$$

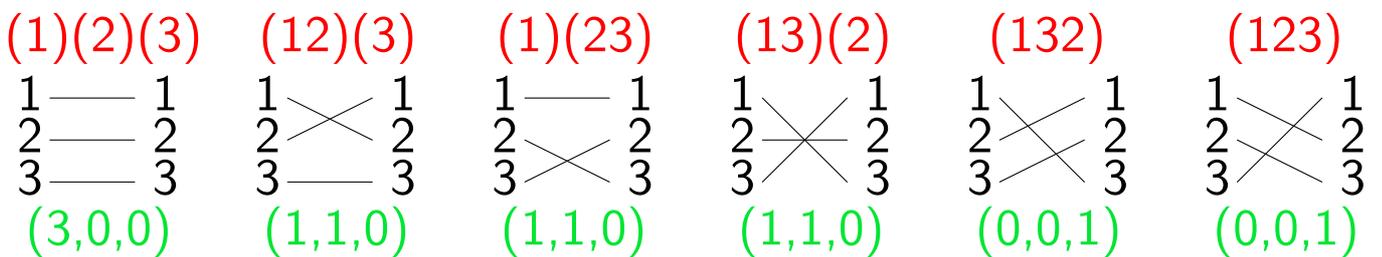
General Result:

$$h_n(\beta) = Z_1(n\beta)$$

Cycle Decomposition:

$$Z_N^{(0)B,F}(\beta) = \frac{1}{N!} \sum_P (\pm 1)^{p(P)} \prod_{n=1}^{(\sum n C_n = N)} [Z_1(n\beta)]^{C_n}$$

Permutation Group:



Cycle Length Representation:

$$Z_N^{(0)B,F}(\beta) = \sum_{C_1, \dots, C_N}^{(\sum n C_n = N)} \prod_{n=1}^N \frac{1}{C_n!} \left[\frac{(\pm 1)^{n+1}}{n} Z_1(n\beta) \right]^{C_n}$$

2.4. Recursion Relation

Generating Function:

$$Z_{GC}^{(0)B,F}(\beta, z) \equiv \sum_{N=0}^{\infty} Z_N^{(0)B,F}(\beta) z^N$$

Cyclic Representation:

$$Z_{GC}^{(0)B,F}(\beta, z) = \exp \left\{ \sum_{n=1}^{\infty} (\pm 1)^{n+1} \frac{Z_1(n\beta) z^n}{n} \right\}$$

N -Particle Part:

$$Z_N^{(0)B,F}(\beta) = \frac{1}{N!} \left. \frac{\partial^N Z_{GC}^{(0)B,F}(\beta, z)}{\partial z^N} \right|_{z=0}$$

Recursion for N -Particle Partition Function

$$Z_N^{(0)B,F}(\beta) = \frac{1}{N} \sum_{n=1}^N (\pm 1)^{n+1} Z_1(n\beta) Z_{N-n}^{(0)B,F}(\beta)$$

$$\text{with } Z_0^{(0)B,F}(\beta) = 1$$

Spectral Decomposition of a Cycle:

$$Z_1(n\beta) = \sum_{\mathbf{k}} e^{-n\beta E_{\mathbf{k}}}$$

2.5. Weight of Ground State

Separation of Ground State Partition:

$$Z_1(n\beta) = \gamma_n(\beta) + \xi_n(\beta)$$

$$\gamma_n(\beta) \equiv e^{-n\beta E_G} = \gamma_1^n(\beta) \quad , \quad \xi_n(\beta) \equiv \sum_{\mathbf{k}}' e^{-n\beta E_{\mathbf{k}}}$$

Partition Function:

$$Z_N^{(0)B} = \sum_{C_1, \dots, C_N}^{(\sum n C_n = N)} \sum_{m_1=0}^{C_1} \dots \sum_{m_N=0}^{C_N} \prod_{n=1}^N \frac{\gamma_1^{n m_n} \xi_n^{C_n - m_n}}{m_n! (C_n - m_n)! n^{C_n}}$$

Weight of Ground State:

$$w_N^{(0)B} = \frac{1}{N Z_N^{(0)B}} \sum_{C_1, \dots, C_N}^{(\sum n C_n = N)} \sum_{m_1=0}^{C_1} \dots \sum_{m_N=0}^{C_N} \left(\sum_{n=1}^N n m_n \right) \\ \times \gamma_1^{\left(\sum_{n=1}^N n m_n \right)} \prod_{n=1}^N \frac{\xi_n^{C_n - m_n}}{m_n! (C_n - m_n)! n^{C_n}}$$

Efficient Formula:

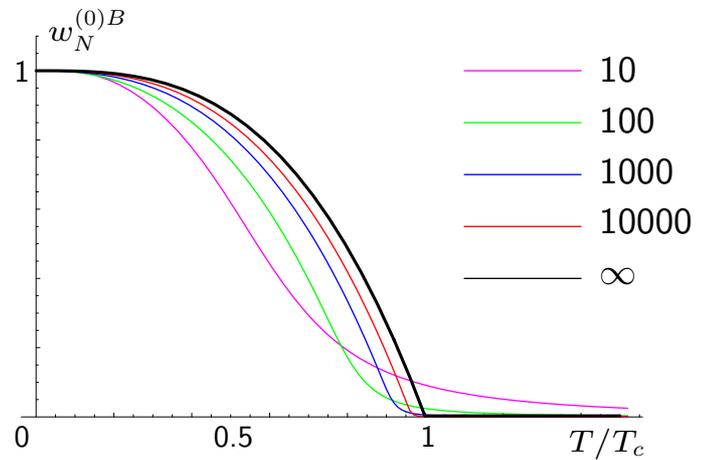
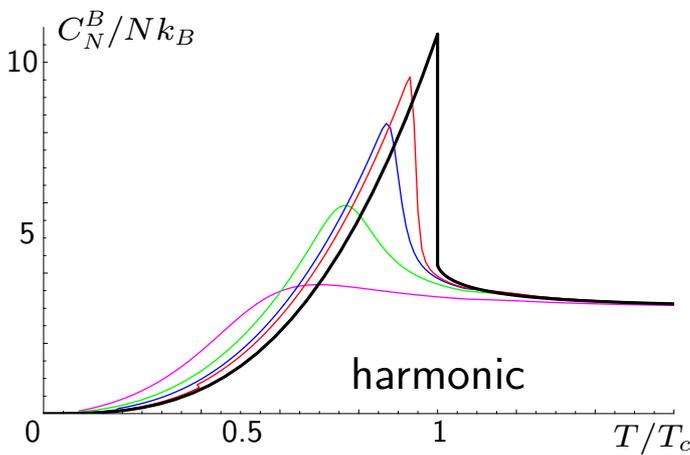
$$w_N^{(0)B}(\beta) = \frac{1}{N Z_N^{(0)B}(\beta)} \sum_{n=1}^N e^{-n\beta E_G} Z_{N-n}^{(0)B}(\beta)$$

2.6. N -Particle Results

Heat Capacity:

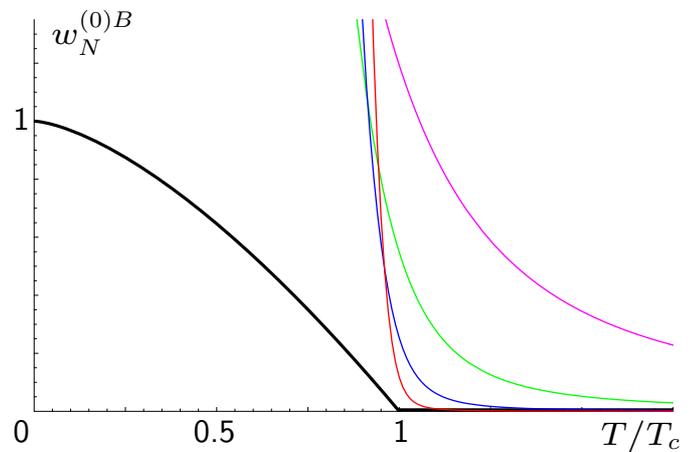
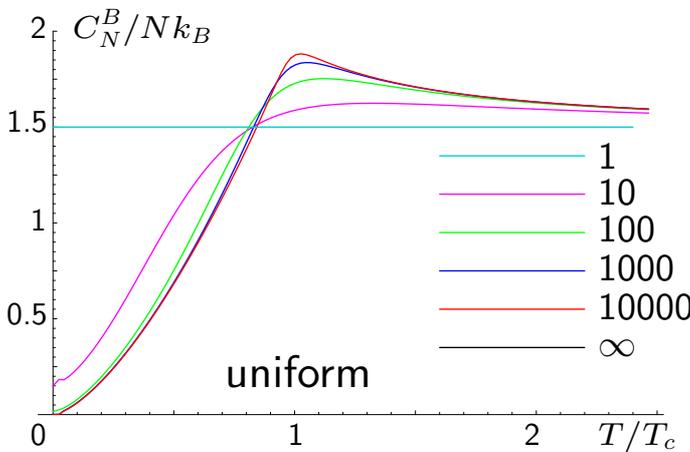
$$C_N^B(T) = k_B T \frac{\partial^2}{\partial T^2} \left\{ T \ln Z_N^{(0)B} (1/k_B T) \right\}$$

Heat Capacity and Ground-State Occupancy:



$$E_{\mathbf{k}} = \hbar\omega (k_1 + k_2 + k_3 + 3/2)$$

$$\sum_{\mathbf{k}} \mapsto \sum_{k_1, k_2, k_3=0}^{\infty}$$

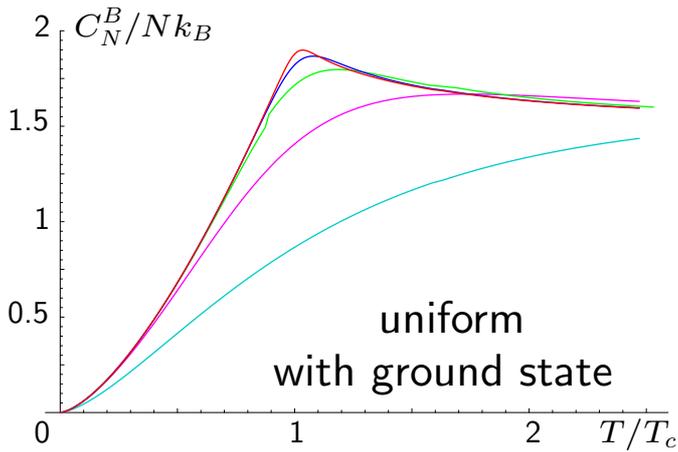


$$E_{\mathbf{k}} = \hbar^2 \mathbf{k}^2 / 2M$$

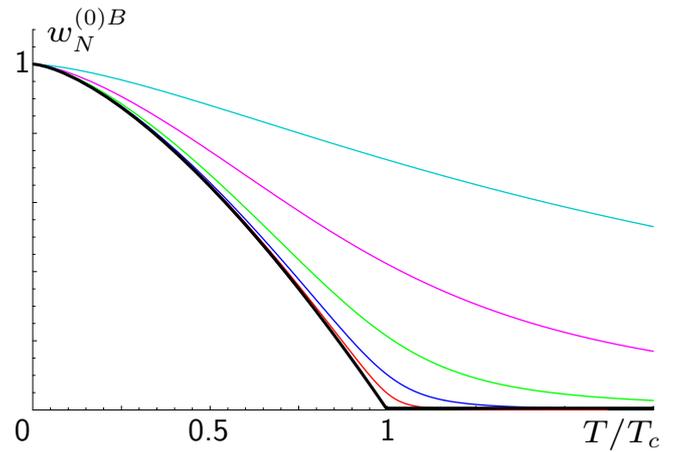
$$\sum_{\mathbf{k}} \mapsto V \int \frac{d^3 k}{(2\pi)^3}$$

2.6. N -Particle Results

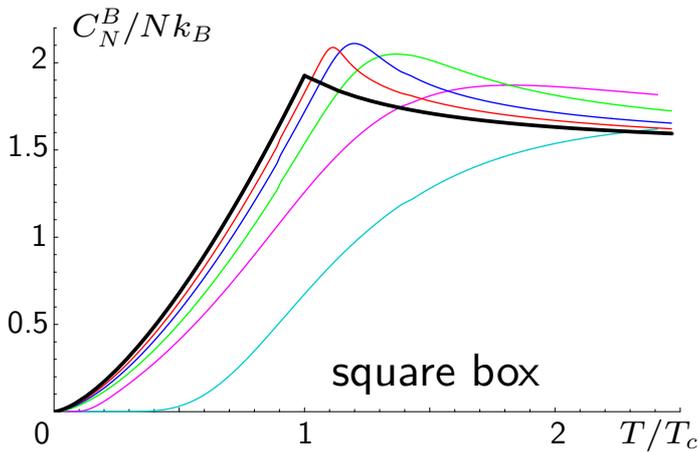
Heat Capacity and Ground-State Occupancy:



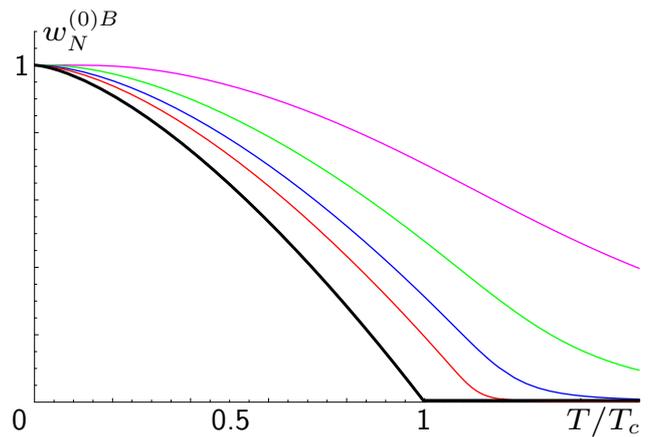
$$E_{\mathbf{k}} = \hbar^2 \mathbf{k}^2 / 2M$$



$$\sum_{\mathbf{k}} \mapsto \sum_{\mathbf{k}=0}^0 + V \int \frac{d^3 k}{(2\pi)^3}$$



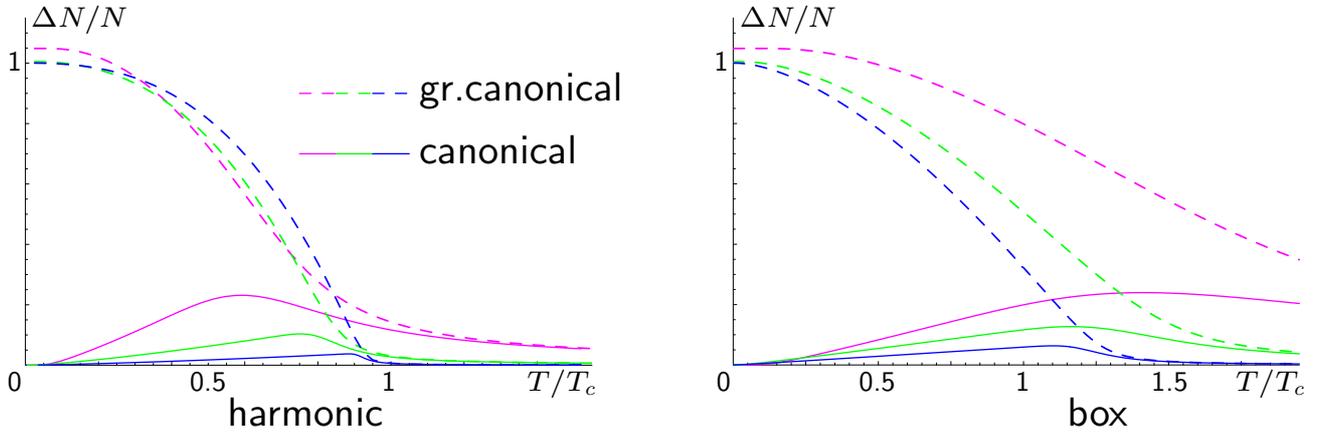
$$E_{\mathbf{k}} = \pi^2 \hbar^2 \mathbf{k}^2 / 2ML^2$$



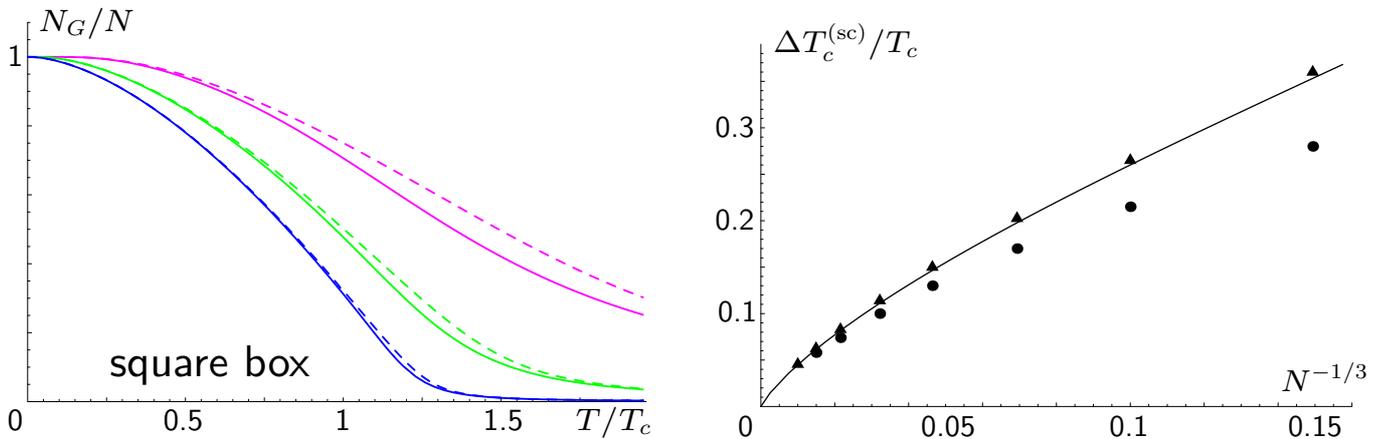
$$\sum_{\mathbf{k}} \mapsto \sum_{k_1, k_2, k_3=1}^{\infty}$$

2.7. Canonical Versus Grand-Canonical

Fluctuations of Ground-State:



Ground-State Occupancy and Finite-Size Effect:



Critical Temperature Shift in a Box:

$$\frac{\Delta T_c^{(sc)}}{T_c} = \frac{\ln C}{N^{1/3} \zeta^{2/3}(3/2)} + \frac{\ln^2 C + \ln C}{N^{2/3} \zeta^{4/3}(3/2)} - \frac{(\pi+1) \zeta(1/2)}{2N^{2/3} \zeta^{1/3}(3/2)} + \dots \quad \text{with} \quad C \equiv \frac{0.6649 N^{2/3}}{\zeta^{2/3}(3/2)}$$

K. Glaum, H. Kleinert, and A. Pelster, in preparation

3.1. Dipolar Interacting System

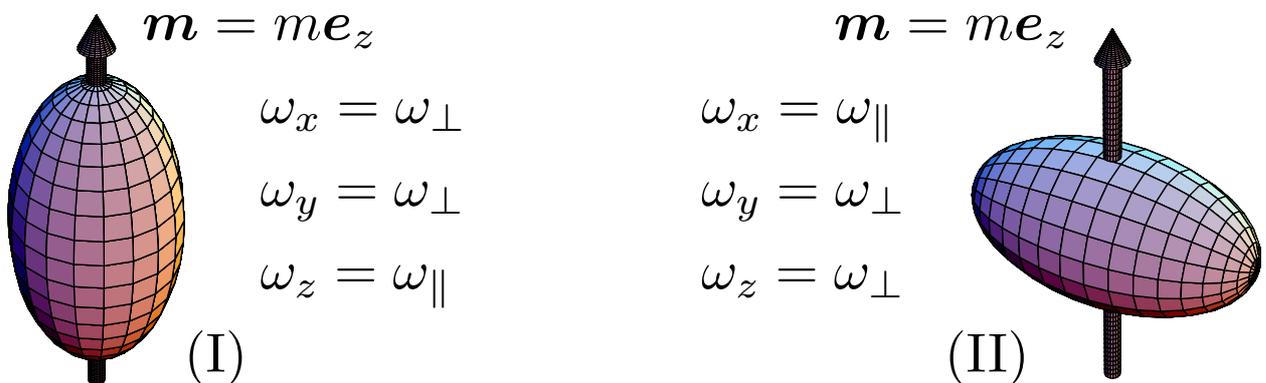
Trapping Potential:

$$V(\mathbf{x}) = \frac{M}{2} \left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2 \right)$$

Interaction Potential:

$$V^{\text{int}}(\mathbf{x}) = \frac{4\pi\hbar^2 a_s}{M} \delta(\mathbf{x}) + \frac{\mu_0 m^2}{4\pi} \left(\frac{1}{|\mathbf{x}|^3} - \frac{3z^2}{|\mathbf{x}|^5} \right)$$

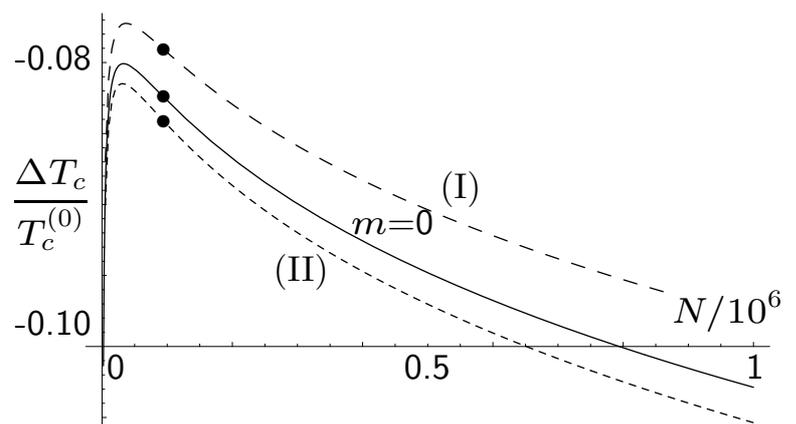
Configurations in ^{52}Cr -Experiment:



Shift of Critical Temperature:

K. Glaum, A. Pelster,
H. Kleinert, and T. Pfau,
PRL **98**, 080407 (2007)

K. Glaum and A. Pelster,
PRA **75** (in press)



3.2. Interacting Particles

N-Particle Propagator:

$$\begin{aligned}
 (\mathbf{x}_1, \dots, \mathbf{x}_N; \tau_b | \mathbf{x}'_1, \dots, \mathbf{x}'_N; \tau_a) &\equiv \prod_{n=1}^N \left(\int_{\mathbf{x}_n(\tau_a)=\mathbf{x}'_n}^{\mathbf{x}_n(\tau_b)=\mathbf{x}_n} \mathcal{D}^D x_n(\tau) \right) \\
 &\times \exp \left\{ -\frac{1}{\hbar} \left(\mathcal{A}^{(0)}[\mathbf{x}_1, \dots, \mathbf{x}_N] + \mathcal{A}^{(\text{int})}[\mathbf{x}_1, \dots, \mathbf{x}_N] \right) \right\}
 \end{aligned}$$

Action:

$$\begin{aligned}
 \mathcal{A}^{(0)}[\mathbf{x}_1, \dots, \mathbf{x}_N] &\equiv \sum_{n=1}^N \int_{\tau_a}^{\tau_b} d\tau \left[\frac{M}{2} \dot{\mathbf{x}}_n^2(\tau) + V(\mathbf{x}_n(\tau)) \right] \\
 \mathcal{A}^{(\text{int})}[\mathbf{x}_1, \dots, \mathbf{x}_N] &\equiv \frac{g}{2} \sum'_{n,m=1}^N \int_{\tau_a}^{\tau_b} d\tau V^{(\text{int})}(\mathbf{x}_n(\tau), \mathbf{x}_m(\tau))
 \end{aligned}$$

First-Order Contribution:

$$\begin{aligned}
 (\mathbf{x}_1, \dots, \mathbf{x}_N; \tau_b | \mathbf{x}'_1, \dots, \mathbf{x}'_N; \tau_a)^{(1)} &\equiv -\frac{g}{2\hbar} \sum'_{n,m=1}^N \int_{\tau_a}^{\tau_b} d\tau \times \\
 \prod_{n=1}^N \left(\int_{\mathbf{x}_n(\tau_a)=\mathbf{x}'_n}^{\mathbf{x}_n(\tau_b)=\mathbf{x}_n} \mathcal{D}^D x_n \right) &V^{(\text{int})}(\mathbf{x}_n(\tau), \mathbf{x}_m(\tau)) e^{-\mathcal{A}^{(0)}[\mathbf{x}_1, \dots, \mathbf{x}_N]/\hbar}
 \end{aligned}$$

3.3. First-Order Perturbation

Factorization:

$$\begin{aligned}
 (\mathbf{x}_1, \dots, \mathbf{x}_N; \tau_b | \mathbf{x}'_1, \dots, \mathbf{x}'_N; \tau_a)^{(1)} &\equiv -\frac{g}{2\hbar} \sum'_{n,m=1}^N \int_{\tau_a}^{\tau_b} d\tau \\
 &\times \int d^D x''_1 \dots d^D x''_N (\mathbf{x}_1, \dots, \mathbf{x}_N; \tau_b | \mathbf{x}''_1, \dots, \mathbf{x}''_N; \tau)^{(0)} \\
 &\times V^{(\text{int})}(\mathbf{x}''_n, \mathbf{x}''_m) (\mathbf{x}''_1, \dots, \mathbf{x}''_N; \tau | \mathbf{x}'_1, \dots, \mathbf{x}'_N; \tau_a)^{(0)}
 \end{aligned}$$

First-Order Partition Function:

$$\begin{aligned}
 Z_N^{(1)B}(\beta) &\equiv \frac{1}{N!} \int d^D x_1 \dots d^D x_N \\
 &\times (\mathbf{x}_{P(1)}, \dots, \mathbf{x}_{P(N)}; \hbar\beta | \mathbf{x}_1, \dots, \mathbf{x}_N; 0)^{(1)}
 \end{aligned}$$

Cyclic Decomposition:

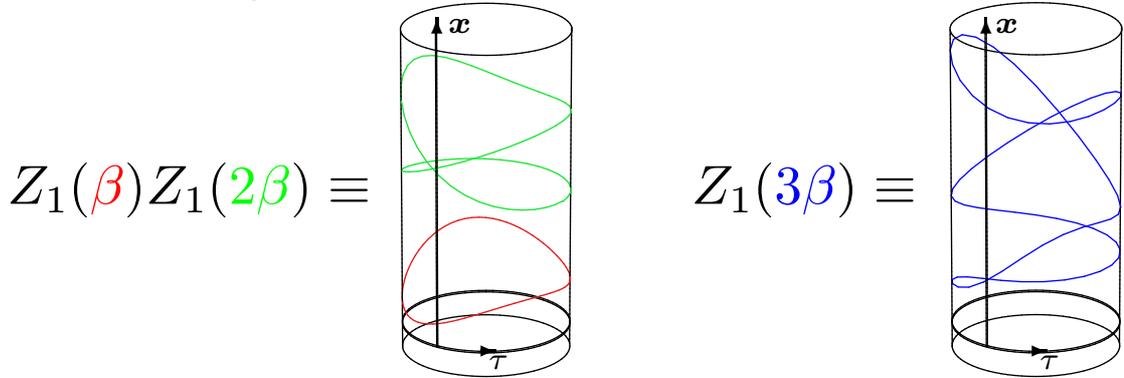
$$Z_N^{(1)B}(\beta) = -\frac{1}{2\hbar} \sum_{k=2}^N \sum_{l=1}^{k-1} \left\{ I_{l,k-l}^{(D)}(\beta) + I_{l,k-l}^{(E)}(\beta) \right\} Z_{N-k}^{(0)B}(\beta)$$

Recursion for Full Partition Function:

$$\begin{aligned}
 Z_N^B(\beta) &= \frac{1}{N} \sum_{n=1}^N \left\{ Z_1(n\beta) - \frac{n}{\hbar} \sum_{l=1}^{n-1} \left[I_{l,n-l}^{(D)}(\beta) \right. \right. \\
 &\quad \left. \left. + I_{l,n-l}^{(E)}(\beta) \right] + \dots \right\} Z_{N-n}^B(\beta)
 \end{aligned}$$

3.4. Interacting Cycles

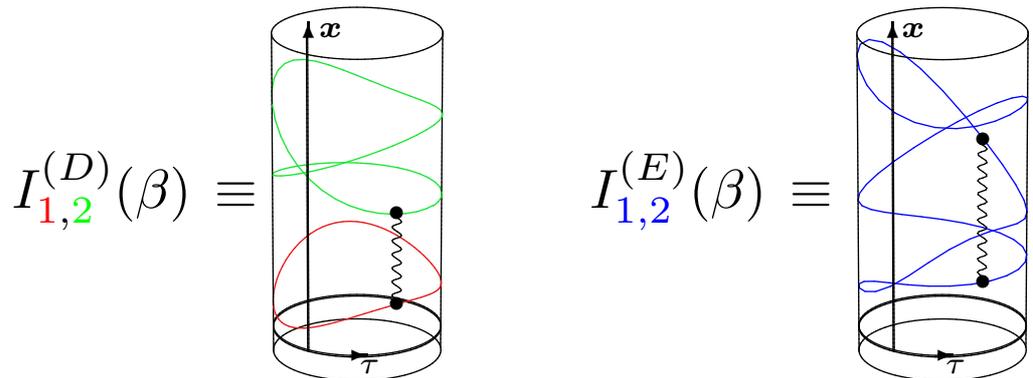
Interaction-Free Cycles:



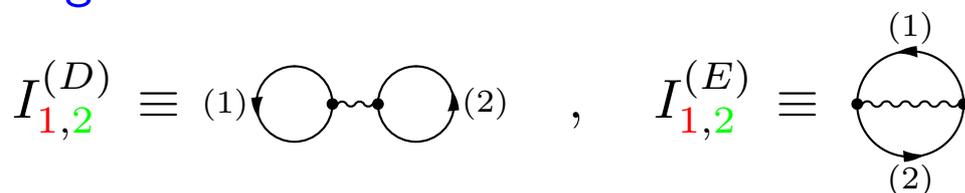
Direct and Exchange Cycles:

$$I_{n,m}^{(D)}(\beta) \equiv \hbar\beta \int d^D x_1 d^D x_2 (\mathbf{x}_1; n\hbar\beta | \mathbf{x}_1; 0)^{(0)} \times V^{(\text{int})}(\mathbf{x}_1, \mathbf{x}_2) (\mathbf{x}_2; m\hbar\beta | \mathbf{x}_2; 0)^{(0)}$$

$$I_{n,m}^{(E)}(\beta) \equiv \hbar\beta \int d^D x_1 d^D x_2 (\mathbf{x}_1; n\hbar\beta | \mathbf{x}_2; 0)^{(0)} \times V^{(\text{int})}(\mathbf{x}_1, \mathbf{x}_2) (\mathbf{x}_2; m\hbar\beta | \mathbf{x}_1; 0)^{(0)}$$



Feynman Diagrams:

$$I_{1,2}^{(D)} \equiv \text{(1)} \circlearrowleft \text{---} \text{(2)} \circlearrowright, \quad I_{1,2}^{(E)} \equiv \text{(1)} \circlearrowleft \text{---} \text{(2)} \circlearrowright$$


3.5. Perturbative Contributions

Interacting Cycles:

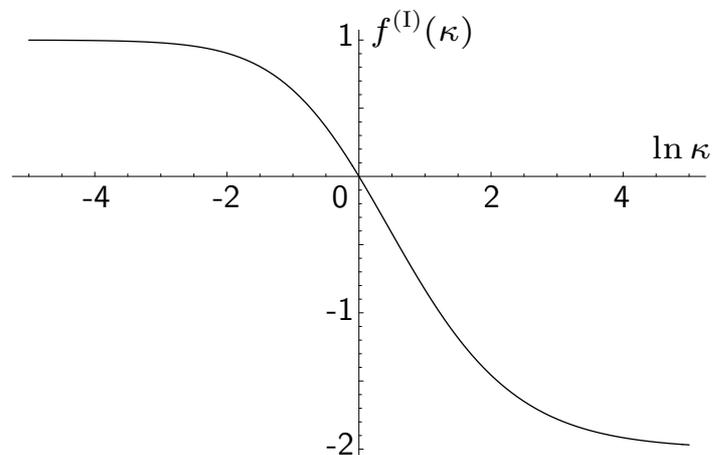
$$I_{l,n-l}^{(D,E)} = \hbar\beta \left(\frac{M\tilde{\omega}}{2\pi\hbar} \right)^{3/2} \left[Z_1(l\beta) Z_1([n-l]\beta) Z_1(n\beta) \right]^{1/2} \\ \times \left\{ \frac{4\pi\hbar^2 a}{M} - \frac{\mu_0 m^2}{3} f\left(\kappa_{l,n}^{(D,E)}[\omega_{\perp}, \omega_{\parallel}] \right) \right\}$$

Anisotropy Factor in Configuration (I):

$$f^{(I)}(\kappa) = \frac{2\kappa + 1}{1 - \kappa} - \frac{3\kappa}{(1 - \kappa)^{3/2}} \operatorname{Artanh}\sqrt{1 - \kappa}$$

Configuration (II):

$$f^{(II)}(\kappa) = -\frac{1}{2} f^{(I)}(\kappa)$$



Problem of Perturbation:

$$I_{l,k}^{(D,E)}(\beta) \propto \beta \implies \text{Further Resummation necessary}$$

3.6. Self Energy

Energy Level Shift:

$$\tilde{E}_n = E_n - \Sigma_l(\mathbf{n})/\hbar\beta$$

Self Energy:

$$\Sigma_l(\mathbf{x}, \tau; \mathbf{x}', \tau') = \Sigma_l^{(D)}(\mathbf{x}, \tau; \mathbf{x}', \tau') + \Sigma_l^{(E)}(\mathbf{x}, \tau; \mathbf{x}', \tau') + \dots$$

Perturbative Contributions:

$$\Sigma_l^{(D)}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \text{Diagram 1}, \quad \Sigma_l^{(E)}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \text{Diagram 2}$$

Energy Representation:

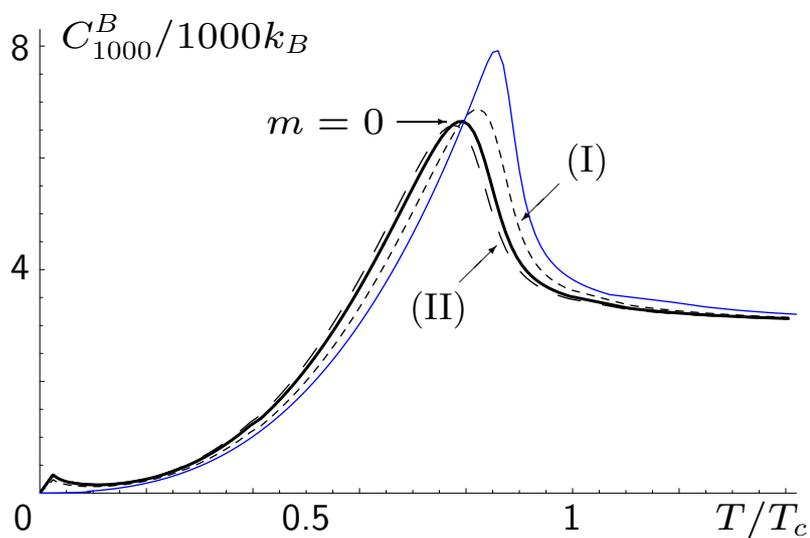
$$\Sigma_l(\mathbf{n}) = \int_0^{\hbar\beta} d\tau d\tau' \int d^3x d^3x' \psi_{\mathbf{n}}^*(\mathbf{x}, \tau) \Sigma_l(\mathbf{x}, \tau; \mathbf{x}', \tau') \psi_{\mathbf{n}}(\mathbf{x}', \tau')$$

Ground-State Self Energy:

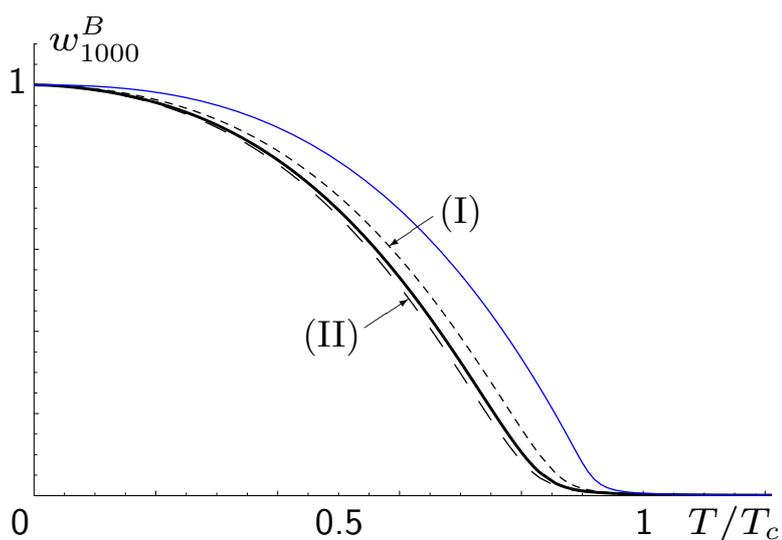
$$\Sigma_l^{(D,E)}(\mathbf{0}) = \hbar\beta \left(\frac{M\tilde{\omega}}{2\pi\hbar} \right)^{3/2} e^{-l\beta E_G} \left[Z_1(l\beta) \right]^{1/2} \times \left\{ \frac{4\pi\hbar^2 a}{M} - \frac{\mu_0 m^2}{3} f\left(\kappa_l^{(D,E)}[\omega_{\perp}, \omega_{\parallel}] \right) \right\}$$

3.7. Signature of Interaction

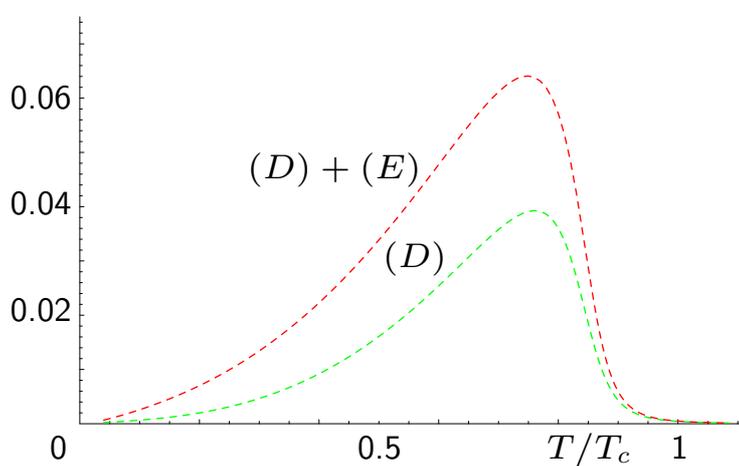
Heat Capacity:



Ground-State
Occupancy:

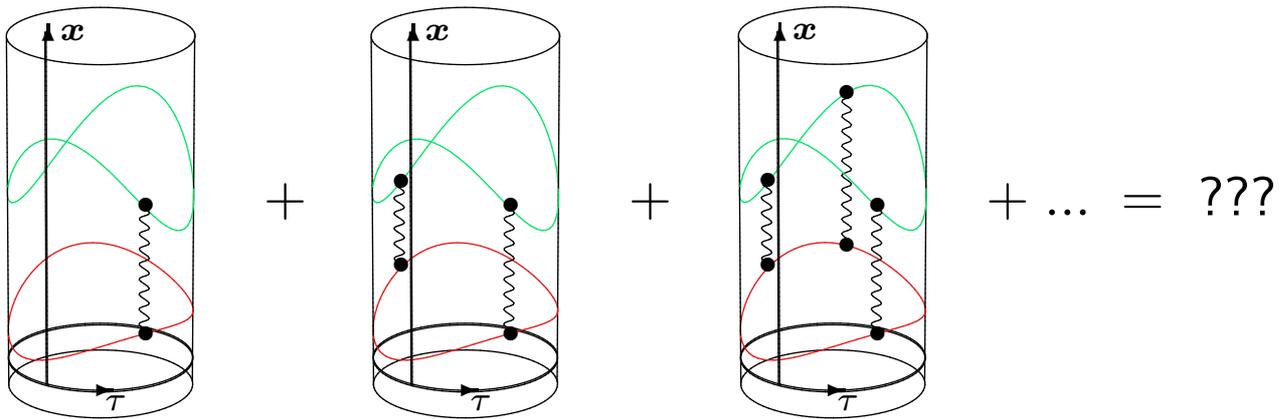


Special Role of
Exchange Terms:



4. Outlook

- 4.1. Determine Superfluid Density
- 4.2. Calculate T-Matrix for Multiple Interactions



- 4.3. Determine Depletion

Supported by Priority Program *Interaction in Ultracold Gases of Atoms and Molecules* (SPP 1116) of the German Research Foundation (DFG)