BEC-BCS-crossover

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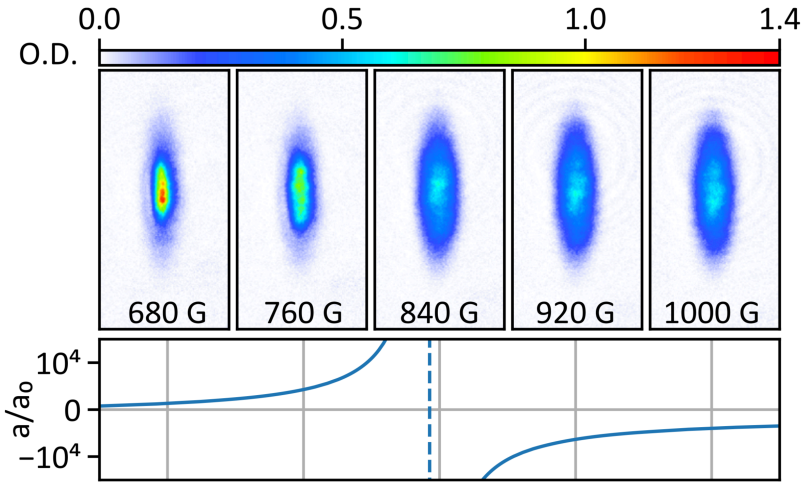

Fig.: Density distributions of ^{6}Li atoms along BEC-BCS crossover.(*)

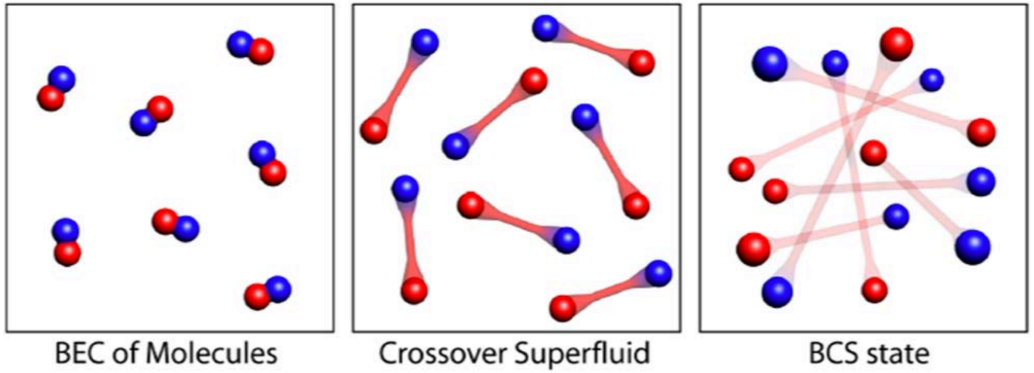

Fig.: Transition between BEC molecules and Cooper pairs.(**)

(*) Gänger, B., Phieler, J., Nagler, B., & Widera, A. (2018). *Rev. Sci. Instr.*
(**) Kidwani, N. M., & Dalton, B. J. (2020), *J. Phys. Comm.*

Introduction: History of Many-Body theory

- Functional integral with Grassmann fields
- Hubbard-Stratonovich transformation:
  Effective action of bosonic pairing field (*)
- Saddle point approximation: BCS-pairing below T_{pair}
- Gaussian fluctuation of pairing field around saddle point: BCS-BEC crossover at T_c
- Technical problems (N. Kaschewski):
  1. Above T_{pair}: ideal Fermi gas
  2. Gaussian fluctuation is analytically not accessible and numerically demanding

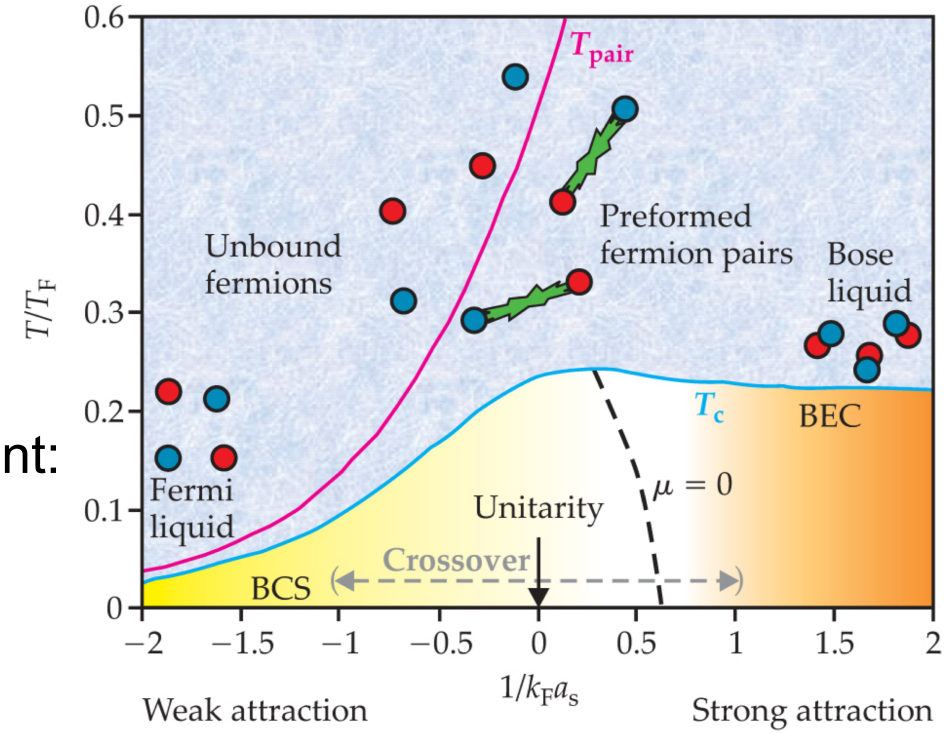

Fig.: BCS-BEC crossover phase diagram (**), originally published in (*).

$$k_F = \left(3\pi^2 n\right)^{1/3}$$

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(*) Sá de Melo, C. A. R., Randeria, M., & Engelbrecht, J. R. (1993), PRL.
(**) Sá de Melo, C. A. R. (2008), *Physics Today*.

Mean-field approach based on field operators

- Second quantised Hamiltonian
- Two-body contact interaction $g \propto a_s$
- Quartic interaction → quadratic operators with mean-field expectation values
- Classification of interaction channels:

  HFB-approximation

$$\hat{H} = \int d^3x \left\{ \sum_{\sigma=\uparrow,\downarrow} \hat{\psi}_\sigma^\dagger(\vec{x}) \left[-\frac{\hbar^2}{2M}\nabla^2 - \mu \right] \hat{\psi}_\sigma(\vec{x}) + g\hat{\psi}_\uparrow^\dagger(\vec{x})\hat{\psi}_\downarrow^\dagger(\vec{x})\hat{\psi}_\downarrow(\vec{x})\hat{\psi}_\uparrow(\vec{x}) \right\}$$

Mean-field HFB-approximation

$$\hat{H}_{\mathrm{MF}} = \int d^3x \left\{ \sum_{\sigma=\uparrow,\downarrow} \hat{\psi}_\sigma^\dagger(\vec{x}) \left[-\frac{\hbar^2}{2M}\nabla^2 - \mu \right] \hat{\psi}_\sigma(\vec{x}) \right.$$

$$\hat{\psi}_\uparrow^\dagger\hat{\psi}_\downarrow^\dagger\hat{\psi}_\downarrow\hat{\psi}_\uparrow \approx \underbrace{+\left\langle\hat{\psi}_\uparrow^\dagger\hat{\psi}_\uparrow\right\rangle\hat{\psi}_\downarrow^\dagger\hat{\psi}_\downarrow + \hat{\psi}_\uparrow^\dagger\hat{\psi}_\uparrow\left\langle\hat{\psi}_\downarrow^\dagger\hat{\psi}_\downarrow\right\rangle - \left\langle\hat{\psi}_\uparrow^\dagger\hat{\psi}_\uparrow\right\rangle\left\langle\hat{\psi}_\downarrow^\dagger\hat{\psi}_\downarrow\right\rangle}_{\text{Hartree channel}}$$

$$\underbrace{-\left\langle\hat{\psi}_\uparrow^\dagger\hat{\psi}_\downarrow\right\rangle\hat{\psi}_\downarrow^\dagger\hat{\psi}_\uparrow - \hat{\psi}_\uparrow^\dagger\hat{\psi}_\downarrow\left\langle\hat{\psi}_\downarrow^\dagger\hat{\psi}_\uparrow\right\rangle + \left\langle\hat{\psi}_\uparrow^\dagger\hat{\psi}_\downarrow\right\rangle\left\langle\hat{\psi}_\downarrow^\dagger\hat{\psi}_\uparrow\right\rangle}_{\text{Fock channel}}$$

$$\underbrace{+\left\langle\hat{\psi}_\uparrow^\dagger\hat{\psi}_\downarrow^\dagger\right\rangle\hat{\psi}_\downarrow\hat{\psi}_\uparrow + \hat{\psi}_\uparrow^\dagger\hat{\psi}_\downarrow^\dagger\left\langle\hat{\psi}_\downarrow\hat{\psi}_\uparrow\right\rangle - \left\langle\hat{\psi}_\uparrow^\dagger\hat{\psi}_\downarrow^\dagger\right\rangle\left\langle\hat{\psi}_\downarrow\hat{\psi}_\uparrow\right\rangle}_{\text{Bogoliubov channel}}$$

BCS-mean-field theory (*) →

(*) →

$$+\Gamma_\downarrow^{\mathrm{H}}\hat{\psi}_\uparrow^\dagger(\vec{x})\hat{\psi}_\uparrow(\vec{x}) + \Gamma_\uparrow^{\mathrm{H}}\hat{\psi}_\downarrow^\dagger(\vec{x})\hat{\psi}_\downarrow(\vec{x}) - \frac{\Gamma_\uparrow^{\mathrm{H}}\Gamma_\downarrow^{\mathrm{H}}}{g}$$

$$-\Gamma_{\uparrow\downarrow}^{\mathrm{F}}\hat{\psi}_\downarrow^\dagger(\vec{x})\hat{\psi}_\uparrow(\vec{x}) - \Gamma_{\downarrow\uparrow}^{\mathrm{F}}\hat{\psi}_\uparrow^\dagger(\vec{x})\hat{\psi}_\downarrow(\vec{x}) + \frac{\Gamma_{\uparrow\downarrow}^{\mathrm{F}}\Gamma_{\downarrow\uparrow}^{\mathrm{F}}}{g}$$

$$\left. +\Delta^*\hat{\psi}_\downarrow(\vec{x})\hat{\psi}_\uparrow(\vec{x}) + \Delta\hat{\psi}_\uparrow^\dagger(\vec{x})\hat{\psi}_\downarrow^\dagger(\vec{x}) - \frac{\Delta^*\Delta}{g} \right\}$$

$$\Gamma_\uparrow^{\mathrm{H}} := g\left\langle\hat{\psi}_\uparrow^\dagger\hat{\psi}_\uparrow\right\rangle; \Gamma_\downarrow^{\mathrm{H}} := g\left\langle\hat{\psi}_\downarrow^\dagger\hat{\psi}_\downarrow\right\rangle \quad \text{(Hartree channel)}$$

$$\Gamma_{\uparrow\downarrow}^{\mathrm{F}} := g\left\langle\hat{\psi}_\uparrow^\dagger\hat{\psi}_\downarrow\right\rangle; \Gamma_{\downarrow\uparrow}^{\mathrm{F}} := g\left\langle\hat{\psi}_\downarrow^\dagger\hat{\psi}_\uparrow\right\rangle \quad \text{(Fock channel)}$$

$$\Delta := g\left\langle\hat{\psi}_\downarrow\hat{\psi}_\uparrow\right\rangle; \Delta^* := g\left\langle\hat{\psi}_\uparrow^\dagger\hat{\psi}_\downarrow^\dagger\right\rangle \quad \text{(Bogoliubov channel)}$$

(*) Becker. A. (2021), Master thesis, Technical University of Kaiserslautern.

Mean-field approach: Different models

- Fourier transformation for diagonalisation
- Choice of interaction channels leads to different models
- **BCS-Bogoliubov model** (*):

  Condensation below T_{pair}
- **Hartree-model**:

  Normal fluid with Hartree-interaction
- **Hartree-Bogoliubov model**:

  Condensation + Hartree-interaction

$$\hat{H}_{\mathrm{MF}} = \sum_{\vec{k}} \Bigg\{ \left[\frac{\hbar^2 \vec{k}^2}{2M} - \mu + \Gamma_{\downarrow}^{\mathrm{H}} \right] \hat{a}_{\vec{k},\uparrow}^{\dagger} \hat{a}_{\vec{k},\uparrow} + \left[\frac{\hbar^2 \vec{k}^2}{2M} - \mu + \Gamma_{\uparrow}^{\mathrm{H}} \right] \hat{a}_{\vec{k},\downarrow}^{\dagger} \hat{a}_{\vec{k},\downarrow} - \Gamma_{\uparrow\downarrow}^{\mathrm{F}} \hat{a}_{\vec{k},\downarrow}^{\dagger} \hat{a}_{\vec{k},\uparrow} - \Gamma_{\downarrow\uparrow}^{\mathrm{F}} \hat{a}_{\vec{k},\uparrow}^{\dagger} \hat{a}_{\vec{k},\downarrow} + \Delta^* \hat{a}_{-\vec{k},\downarrow} \hat{a}_{\vec{k},\uparrow} + \Delta \hat{a}_{\vec{k},\uparrow}^{\dagger} \hat{a}^{\dagger}_{-\vec{k},\downarrow} \Bigg\} - V \frac{\Gamma_{\uparrow}^{\mathrm{H}} \Gamma_{\downarrow}^{\mathrm{H}}}{g} + V \frac{\Gamma_{\uparrow\downarrow}^{\mathrm{F}} \Gamma_{\downarrow\uparrow}^{\mathrm{F}}}{g} - V \frac{\Delta^* \Delta}{g}$$

$$\Gamma_{\uparrow}^{\mathrm{H}} := g \left\langle \hat{\psi}_{\uparrow}^{\dagger} \hat{\psi}_{\uparrow} \right\rangle ; \Gamma_{\downarrow}^{\mathrm{H}} := g \left\langle \hat{\psi}_{\downarrow}^{\dagger} \hat{\psi}_{\downarrow} \right\rangle \quad \text{(Hartree channel)}$$

$$\Gamma_{\uparrow\downarrow}^{\mathrm{F}} := g \left\langle \hat{\psi}_{\uparrow}^{\dagger} \hat{\psi}_{\downarrow} \right\rangle ; \Gamma_{\downarrow\uparrow}^{\mathrm{F}} := g \left\langle \hat{\psi}_{\downarrow}^{\dagger} \hat{\psi}_{\uparrow} \right\rangle \quad \text{(Fock channel)}$$

$$\Delta := g \left\langle \hat{\psi}_{\downarrow} \hat{\psi}_{\uparrow} \right\rangle ; \Delta^* := g \left\langle \hat{\psi}_{\uparrow}^{\dagger} \hat{\psi}_{\downarrow}^{\dagger} \right\rangle \quad \text{(Bogoliubov channel)}$$

(*) Becker. A. (2021), Master thesis, Technical University of Kaiserslautern.

Mean-field approach: BCS-Bogoliubov model

$$\hat{H}_{\mathrm{B}} = \sum_{\vec{k}} \epsilon_{\mathrm{B}}(\vec{k}) \left(\hat{\alpha}^{\dagger}_{\vec{k}} \hat{\alpha}_{\vec{k}} + \hat{\beta}^{\dagger}_{\vec{k}} \hat{\beta}_{\vec{k}} \right) - V \frac{|\Delta|^2}{g} - \sum_{\vec{k}} \left[\epsilon_{\mathrm{B}}(\vec{k}) - \left(\frac{\hbar^2 \vec{k}^2}{2M} - \mu \right) \right]$$

- Bogoliubov channel for condensation
- Diagonalisation: Bogoliubov transformation

$$\hat{\alpha}_{\vec{k}} = u_{\vec{k}} \hat{a}_{\vec{k},\uparrow} - v_{\vec{k}} \hat{a}^{\dagger}_{-\vec{k},\downarrow},$$

$$\hat{\beta}_{\vec{k}} = u_{\vec{k}} \hat{a}_{-\vec{k},\downarrow} + v_{\vec{k}} \hat{a}^{\dagger}_{\vec{k},\uparrow},$$

- Thermodynamic potential $\mathcal{F} = -\beta^{-1} \log \mathrm{Tr} e^{-\beta \hat{H}}$

  $\rightarrow$Order parameter equation: $\partial_{\Delta^*} \mathcal{F} = 0$

  $\rightarrow$Particle number equation: $-\partial_{\mu} \mathcal{F} = N$

- Equivalent to saddle point approximation of functional integral formulation

BCS-Bogoliubov-order parameter equation

$$\frac{\Delta}{g} = \frac{1}{2} \frac{1}{V} \sum_{\vec{k}} \frac{-\Delta}{\epsilon_{\mathrm{B}}\left(\vec{k}\right)} \tanh\left(\frac{\beta \epsilon_{\mathrm{B}}\left(\vec{k}\right)}{2} \right)$$

BCS-Bogoliubov-density equation

$$n = \frac{1}{V} \sum_{\vec{k}} \left\{ 1 - \frac{\frac{\hbar^2 \vec{k}^2}{2M} - \mu}{\epsilon_{\mathrm{B}}\left(\vec{k}\right)} \tanh\left(\frac{\beta \epsilon_{\mathrm{B}}\left(\vec{k}\right)}{2} \right) \right\}$$

$$\epsilon_{\mathrm{B}}\left(\vec{k}\right) := \sqrt{\left(\frac{\hbar^2 \vec{k}^2}{2M} - \mu \right)^2 + \Delta^2}$$

Mean-field approach: Hartree-model

$$\hat{H}_{\mathrm{H}} = \sum_{\vec{k}} \left\{ \left[\frac{\hbar^2 \vec{k}^2}{2M} - \mu + \Gamma_{\downarrow}^{\mathrm{H}} \right] \hat{a}_{\vec{k},\uparrow}^{\dagger} \hat{a}_{\vec{k},\uparrow} + \left[\frac{\hbar^2 \vec{k}^2}{2M} - \mu + \Gamma_{\uparrow}^{\mathrm{H}} \right] \hat{a}_{\vec{k},\downarrow}^{\dagger} \hat{a}_{\vec{k},\downarrow} \right\} - V \frac{\Gamma_{\downarrow}^{\mathrm{H}} \Gamma_{\uparrow}^{\mathrm{H}}}{g}$$

- Hartree-interaction between fermions
- Thermodynamic potential $\mathcal{F} = -\beta^{-1} \log \mathrm{Tr} e^{-\beta \hat{H}}$

  →Particle number equation $-\partial_{\mu} \mathcal{F} = N$

  →Hartree equations:

Coincidence with result from effective single-body approximation approach of Hartree-Fock theory (*)

$$\frac{\partial \mathcal{F}}{\partial \Gamma_{\downarrow}^{\mathrm{H}}} = 0 \Rightarrow \frac{\Gamma_{\uparrow}^{\mathrm{H}}}{g} = \frac{1}{V} \sum_{\vec{k}} \frac{1}{e^{-\beta\left(\frac{\hbar^2 \vec{k}^2}{2M} - \mu + \Gamma_{\downarrow}^{\mathrm{H}}\right)} + 1}$$

$$\frac{\partial \mathcal{F}}{\partial \Gamma_{\uparrow}^{\mathrm{H}}} = 0 \Rightarrow \frac{\Gamma_{\downarrow}^{\mathrm{H}}}{g} = \frac{1}{V} \sum_{\vec{k}} \frac{1}{e^{-\beta\left(\frac{\hbar^2 \vec{k}^2}{2M} - \mu + \Gamma_{\uparrow}^{\mathrm{H}}\right)} + 1}$$

$$\Gamma_{\downarrow}^{\mathrm{H}} = \Gamma_{\uparrow}^{\mathrm{H}} = \frac{1}{2} g n$$

Hartree-density equation

$$n = -\frac{2}{\lambda^3} \mathrm{Li}_{3/2}\left(-e^{\beta\left(\mu - \frac{1}{2} g n\right)}\right)$$

$$\lambda = \sqrt{\frac{2\pi\hbar^2}{M k_{\mathrm{B}} T}} \qquad \mathrm{Li}_s(x) = \sum_{n=1}^{\infty} \frac{x^n}{n^s}$$

(*) Czycholl, G. (2016). *Theoretische Festkörperphysik Band 1* (4 ed.).

Mean-field approach: Trapped Fermi gas with LDA

- Harmonic trapping potential:

$$V(\vec{x}) = \frac{M}{2}\sum_{i=1}^{3}\omega_i^2 x_i^2$$

- Local Density Approximation (LDA)

$$\mu \to \mu - V(\vec{x}) \Rightarrow n \to n(\vec{x})$$

- Experimental parameters and measured quantities:
  $1/(k_F a_s)$, $(\omega_1, \omega_2, \omega_3)$, N
- Free fitting parameters:

$$k_F = \sqrt{\frac{M}{\hbar}}\left(\omega_1\omega_2\omega_3 N\right)^{1/6}$$

T, μ: Choose T and fit μ for $N = \int d^3x n(\vec{x})$

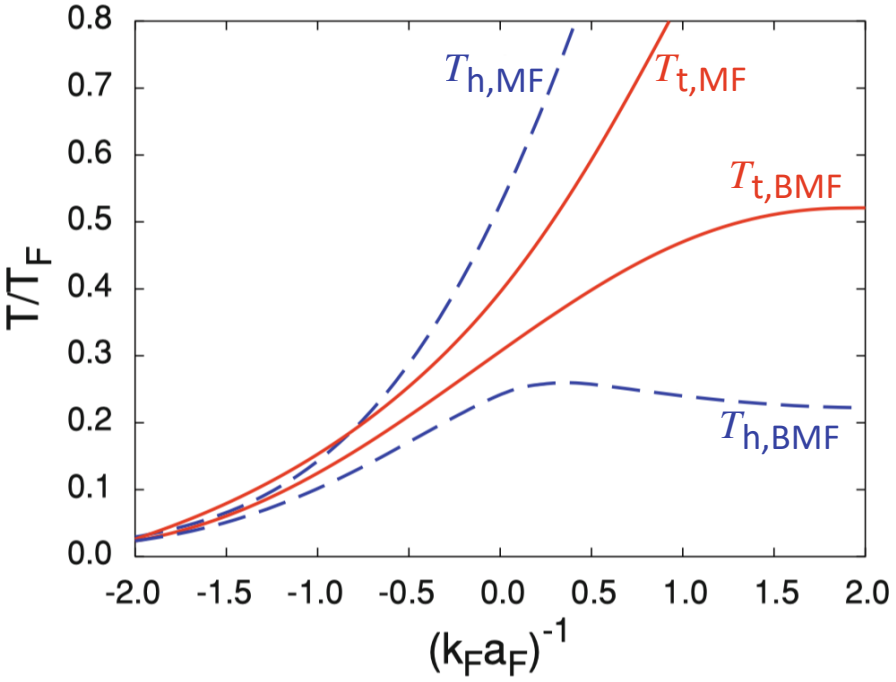


Fig.: Critical temperatures of homogenous(h)(*)- and trapped(t)(**) gas.

(*) Sá de Melo, C. A. R., Randeria, M., & Engelbrecht, J. R. (1993), PRL.
(**) Perali, A., Pieri, P., Pisani, L., & Strinati, G. C. (2004). PRL.

Mean-field approach: Density profile in normal fluid phase

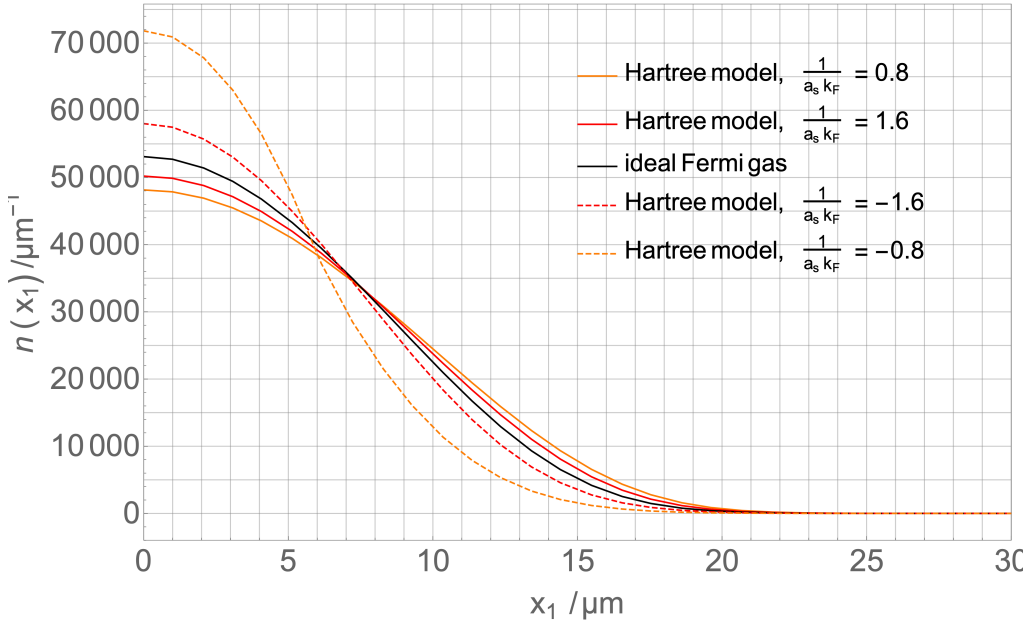
Parameter values inspired by experimental data from AG Widera

$N = 982998,\ (\omega_1, \omega_2, \omega_3) = 2\pi \cdot (498,\ 25,\ 340)$ Hz

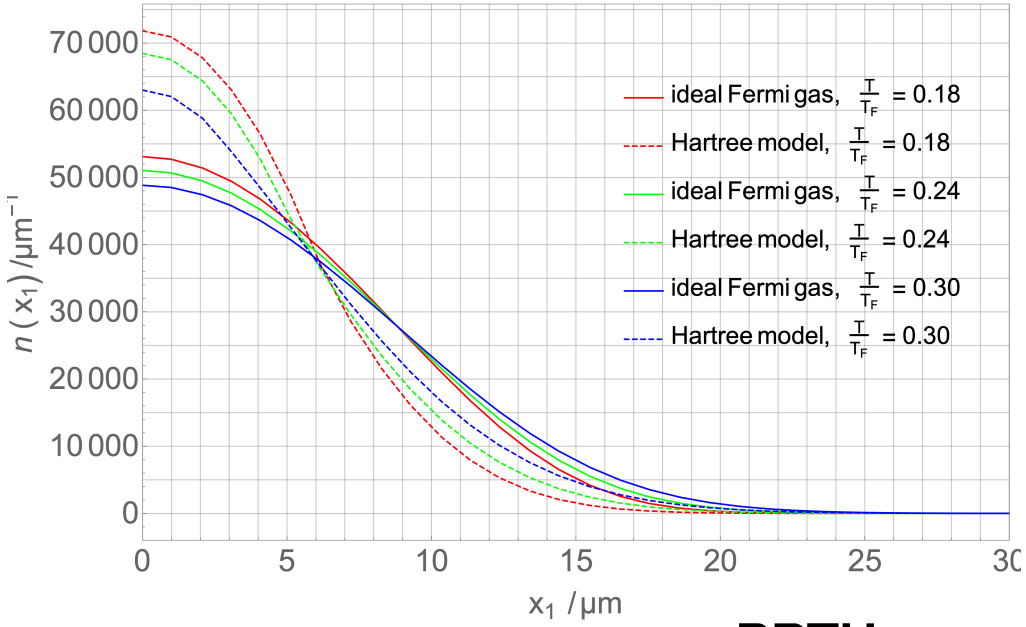
Hartree-density equation with LDA

$$n(\vec{x}) = -\frac{2}{\lambda^3}\mathrm{Li}_{3/2}\left(-e^{\beta\left(\mu - V(\vec{x}) - \frac{1}{2}gn(\vec{x})\right)}\right)$$

Interaction dependency at $T = 0.18T_F$



Temperature dependency at $1/(k_F a_s) = -0.8$



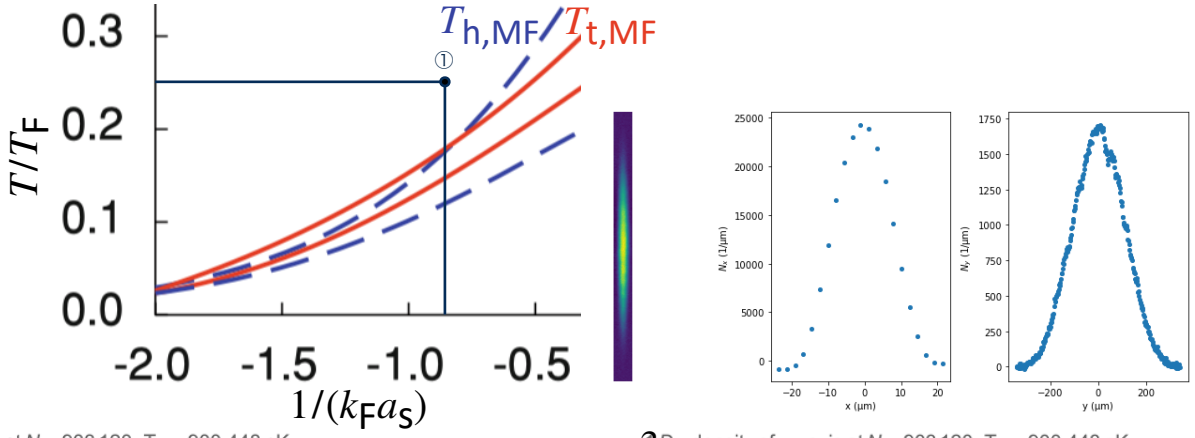
Experiments: Hartree model fitting for temperature 1

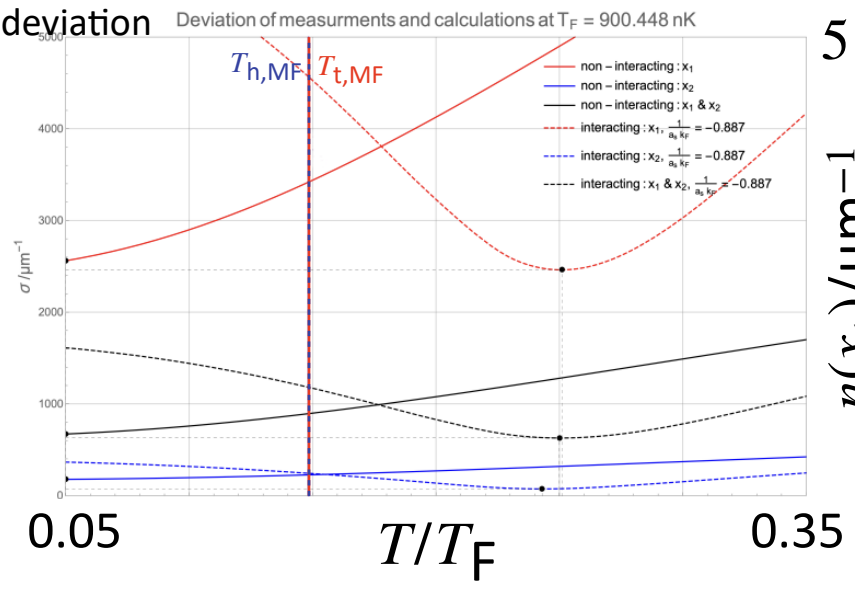
$$\frac{1}{k_F a_s} = -0.887 \rightarrow \frac{T}{T_F} = 0.250$$

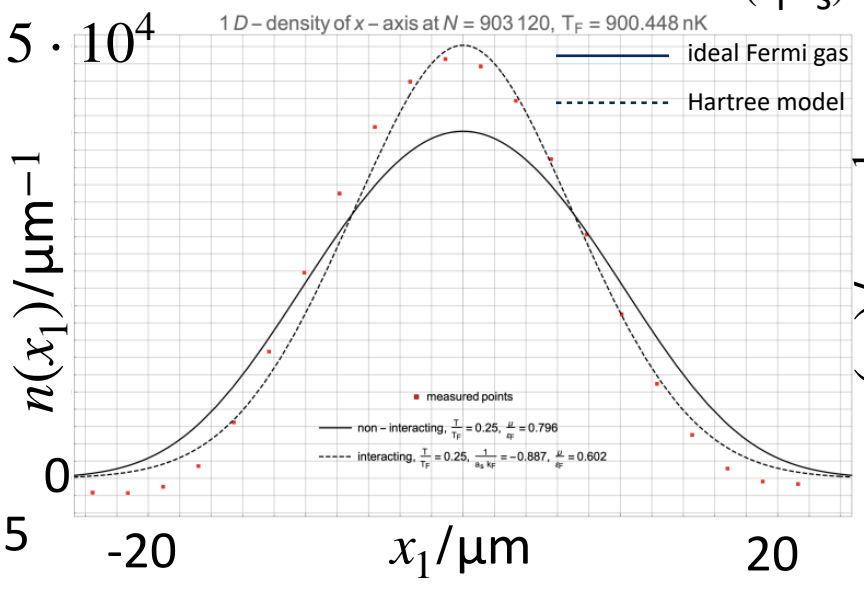
ideal Fermi gas, x_1 — Hartree model, x_1

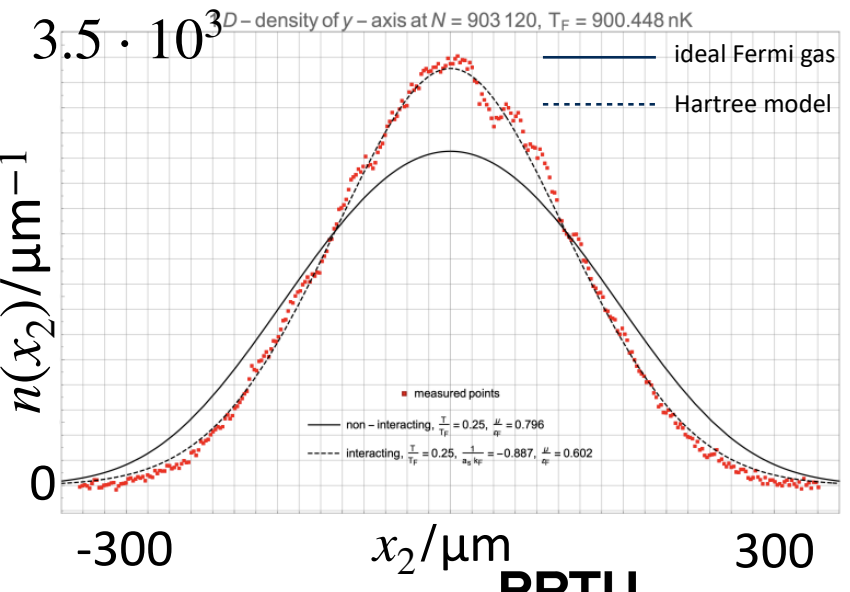
ideal Fermi gas, x_2 — Hartree model, x_2

ideal Fermi gas, x_1 & x_2 — Hartree model, x_1 & x_2









Experimental data due to AG Widera

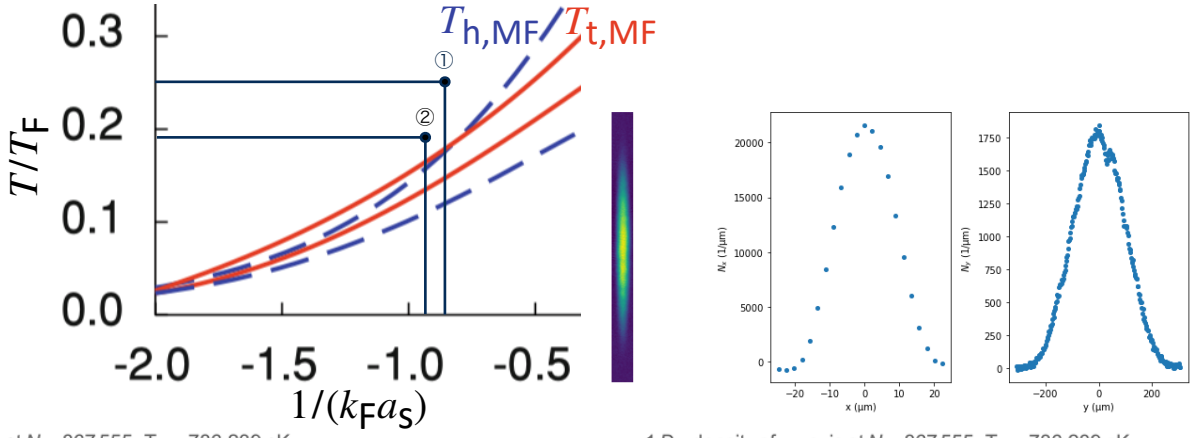
Experiments: Hartree model fitting for temperature 2

$$\frac{1}{k_F a_s} = -0.949 \rightarrow \frac{T}{T_F} = 0.194$$

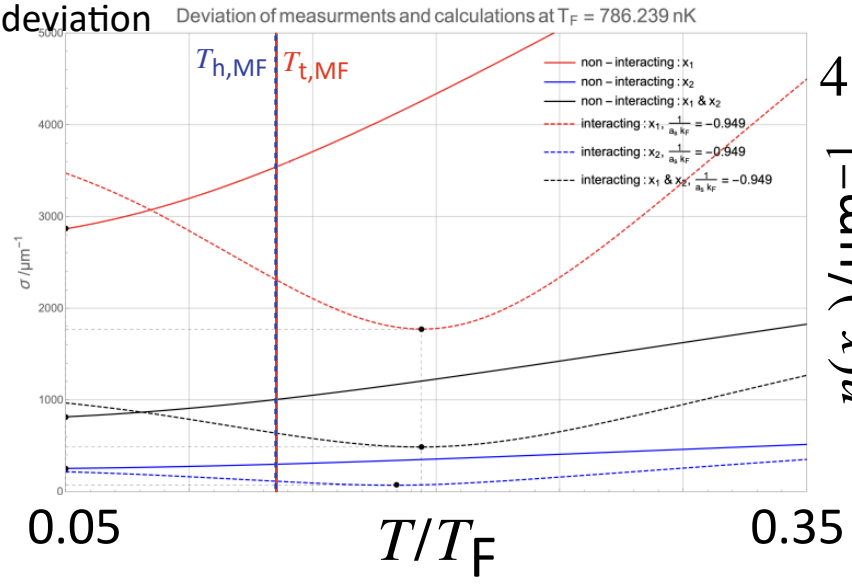
ideal Fermi gas, x_1 — Hartree model, x_1

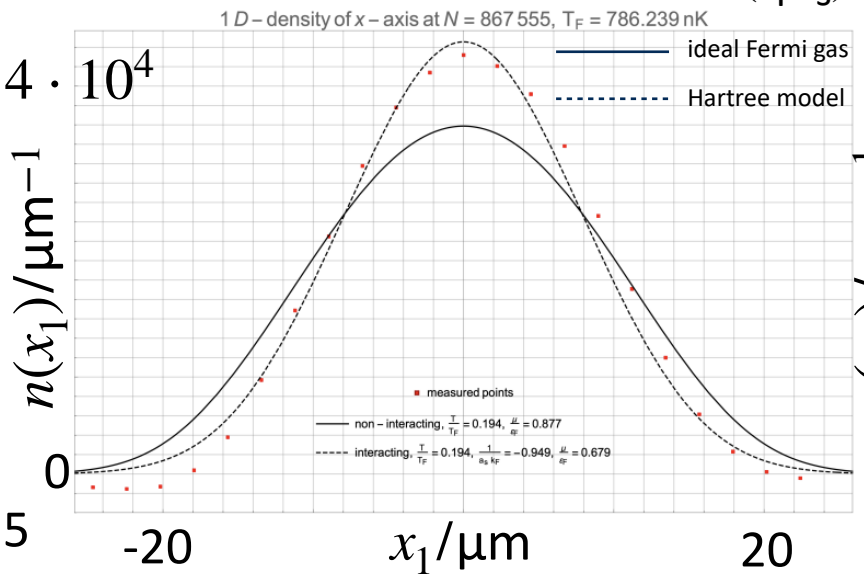
ideal Fermi gas, x_2 — Hartree model, x_2

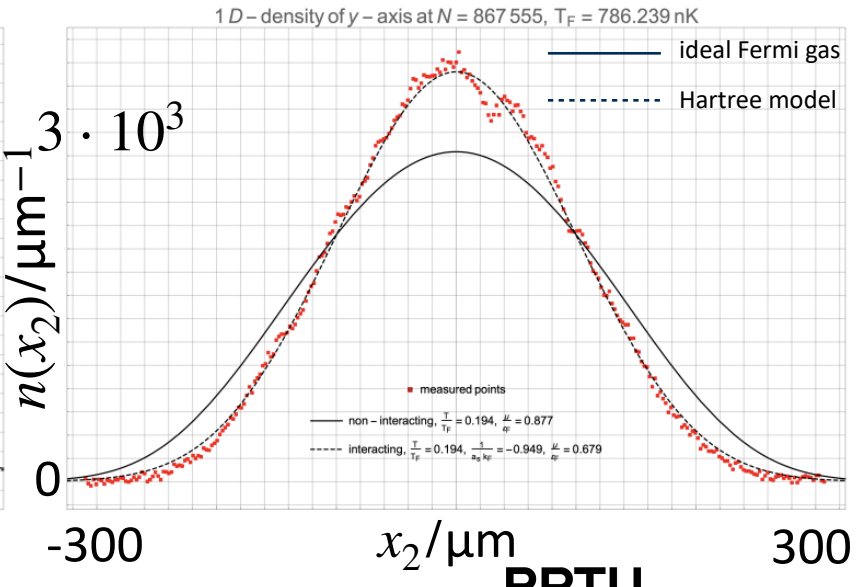
ideal Fermi gas, x_1 & x_2 — Hartree model, x_1 & x_2



deviation







Experimental data due to AG Widera

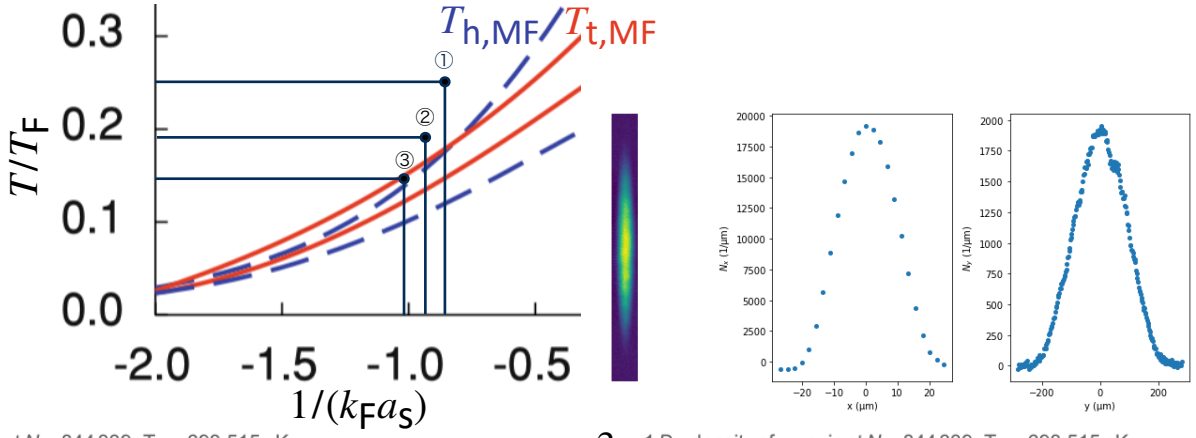
Experiments: Hartree model fitting for temperature 3

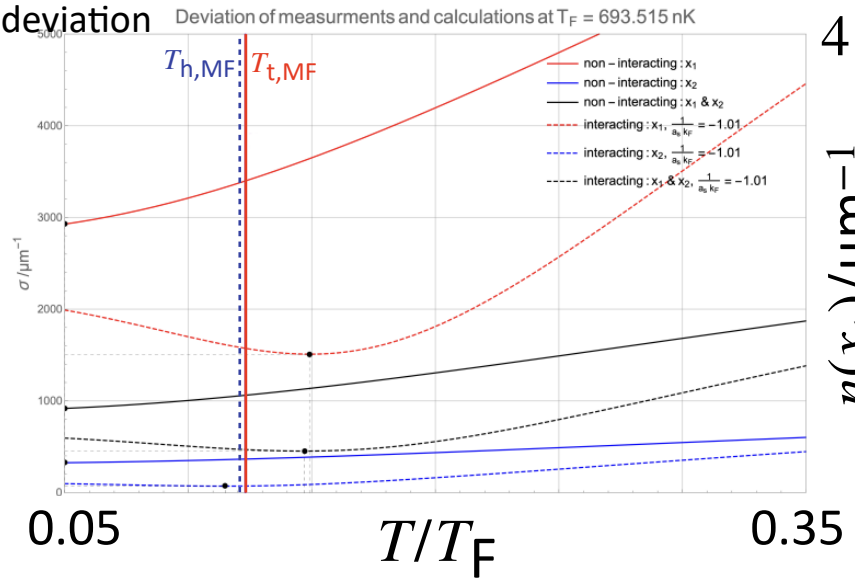
$$\frac{1}{k_F a_s} = -1.010 \rightarrow \frac{T}{T_F} = 0.147$$

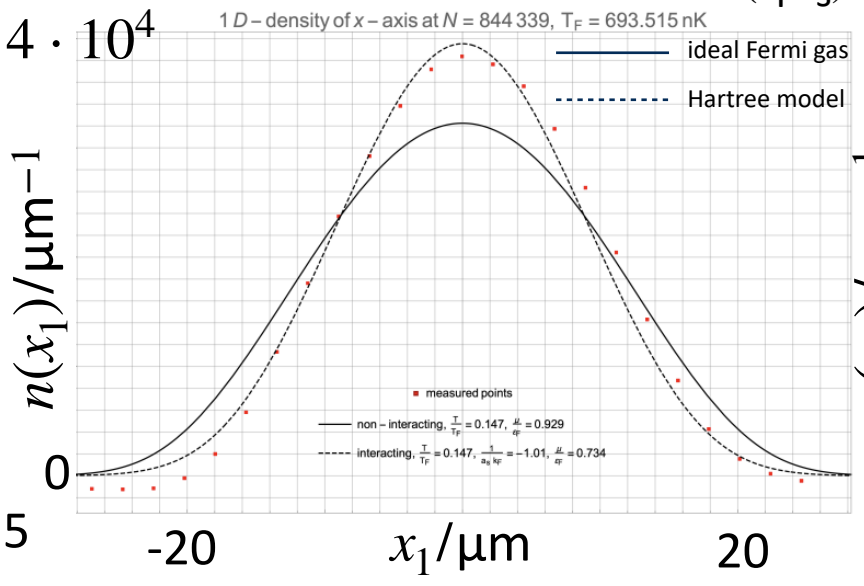
ideal Fermi gas, x_1 — Hartree model, x_1

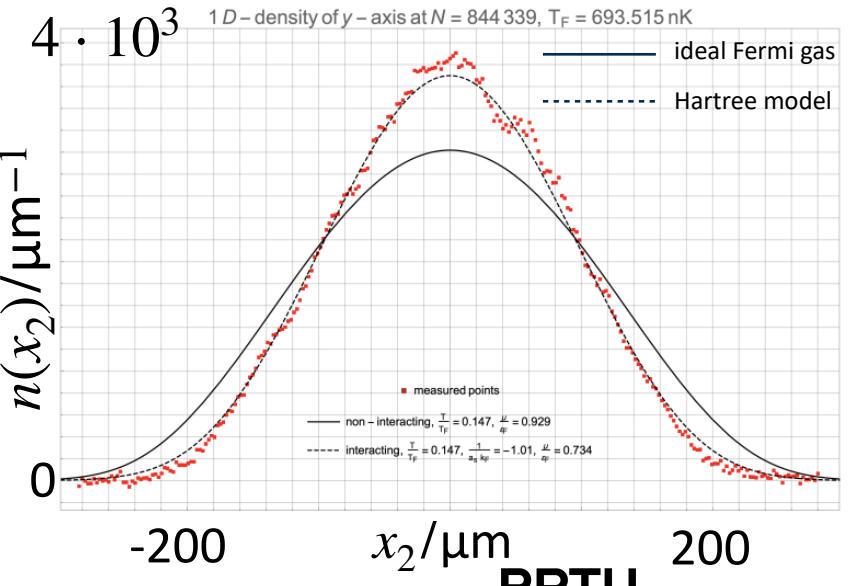
ideal Fermi gas, x_2 — Hartree model, x_2

ideal Fermi gas, x_1 & x_2 — Hartree model, x_1 & x_2









Experimental data due to AG Widera

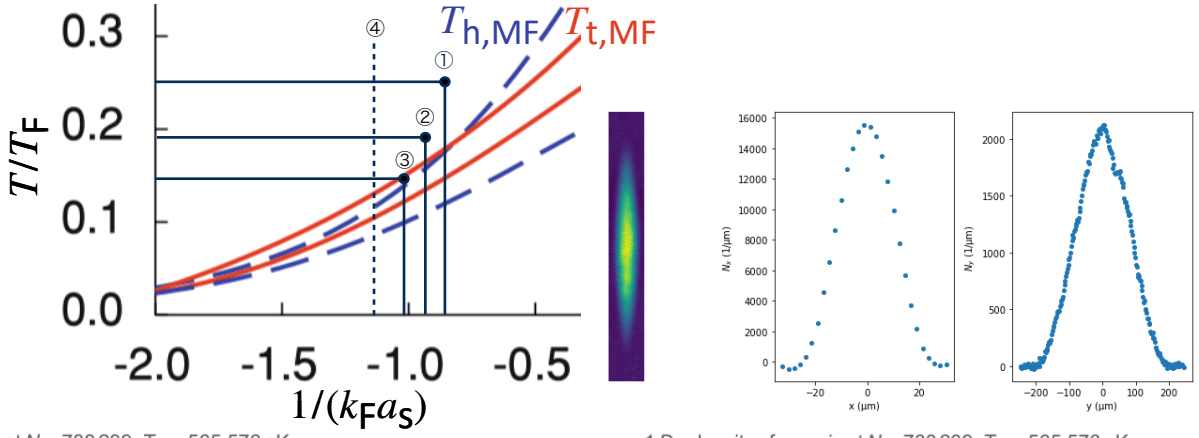
Experiments: Hartree model fitting for temperature 4

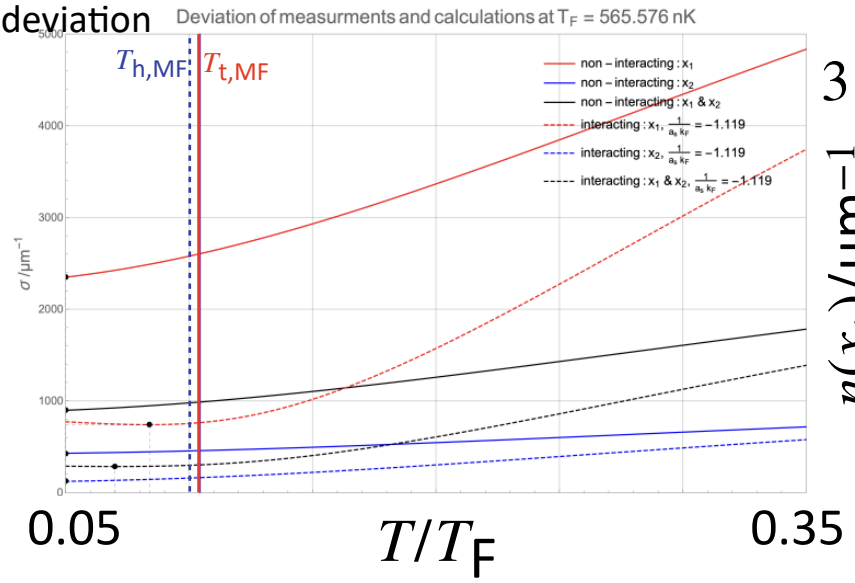
$$\frac{1}{k_F a_s} = -1.119 \rightarrow \text{(dev. minimum not found)}$$

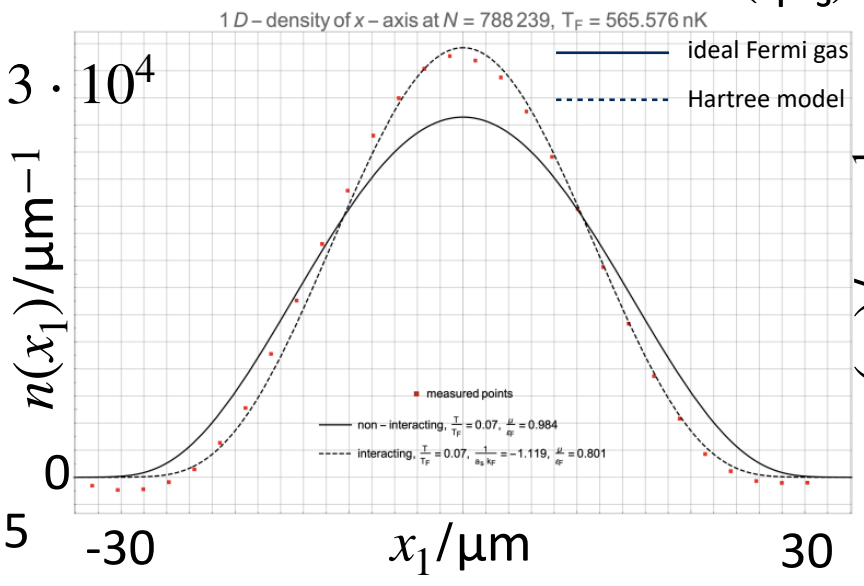
ideal Fermi gas, x_1 — Hartree model, x_1

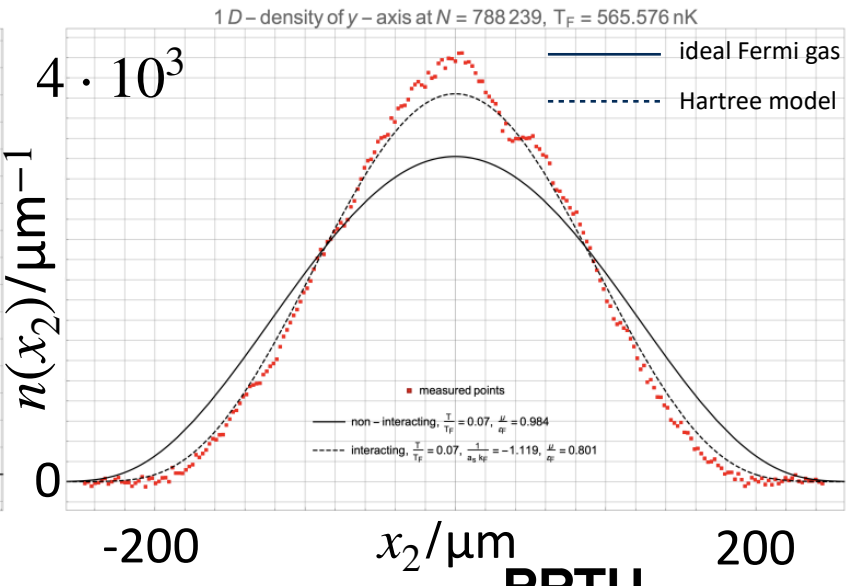
ideal Fermi gas, x_2 — Hartree model, x_2

ideal Fermi gas, x_1 & x_2 — Hartree model, x_1 & x_2









Experimental data due to AG Widera

Outlook: Hartree-Bogoliubov model

- Taking Hartree-and Bogoliubov channels:
  Interaction and condensation
- Extremalisation of thermodynamic potential:
  $\partial_{\Delta^*}\mathcal{F} = 0$: Order parameter equation
  $\partial_{\Gamma^{\mathrm{H}}}\mathcal{F} = 0$: Hartree equation
- Expectations:
  - $T^{(B)}_{\mathrm{t,MF}} \neq T^{(HB)}_{\mathrm{t,MF}}$
  - Improved thermometry

Equivalent to saddle point of pairing field and interaction field of functional integral approach? (N. Kaschewski)

HB-order parameter equation with LDA

$$\frac{\Delta(\vec{x})}{g} = \frac{1}{2}\frac{1}{V}\sum_{\vec{k}} \frac{-\Delta(\vec{x})}{\epsilon_{\mathrm{HB}}\left(\vec{k},\vec{x}\right)} \tanh\left(\frac{\beta\epsilon_{\mathrm{HB}}\left(\vec{k},\vec{x}\right)}{2}\right)$$

HB-density equation with LDA

$$n(\vec{x}) = \frac{1}{V}\sum_{\vec{k}} \left\{1 - \frac{\frac{\hbar^2\vec{k}^2}{2M} - \mu + V(\vec{x}) + \frac{1}{2}gn(\vec{x})}{\epsilon_{\mathrm{HB}}\left(\vec{k},\vec{x}\right)} \tanh\left(\frac{\beta\epsilon_{\mathrm{HB}}\left(\vec{k},\vec{x}\right)}{2}\right)\right\}$$

$$\epsilon_{\mathrm{HB}}\left(\vec{k},\vec{x}\right) := \sqrt{\left(\frac{\hbar^2\vec{k}^2}{2M} - \mu + V(\vec{x}) + \frac{1}{2}gn(\vec{x})\right)^2 + \Delta^2(\vec{x})}$$

Outlook: Preliminary result from Hartree-Bogoliubov model

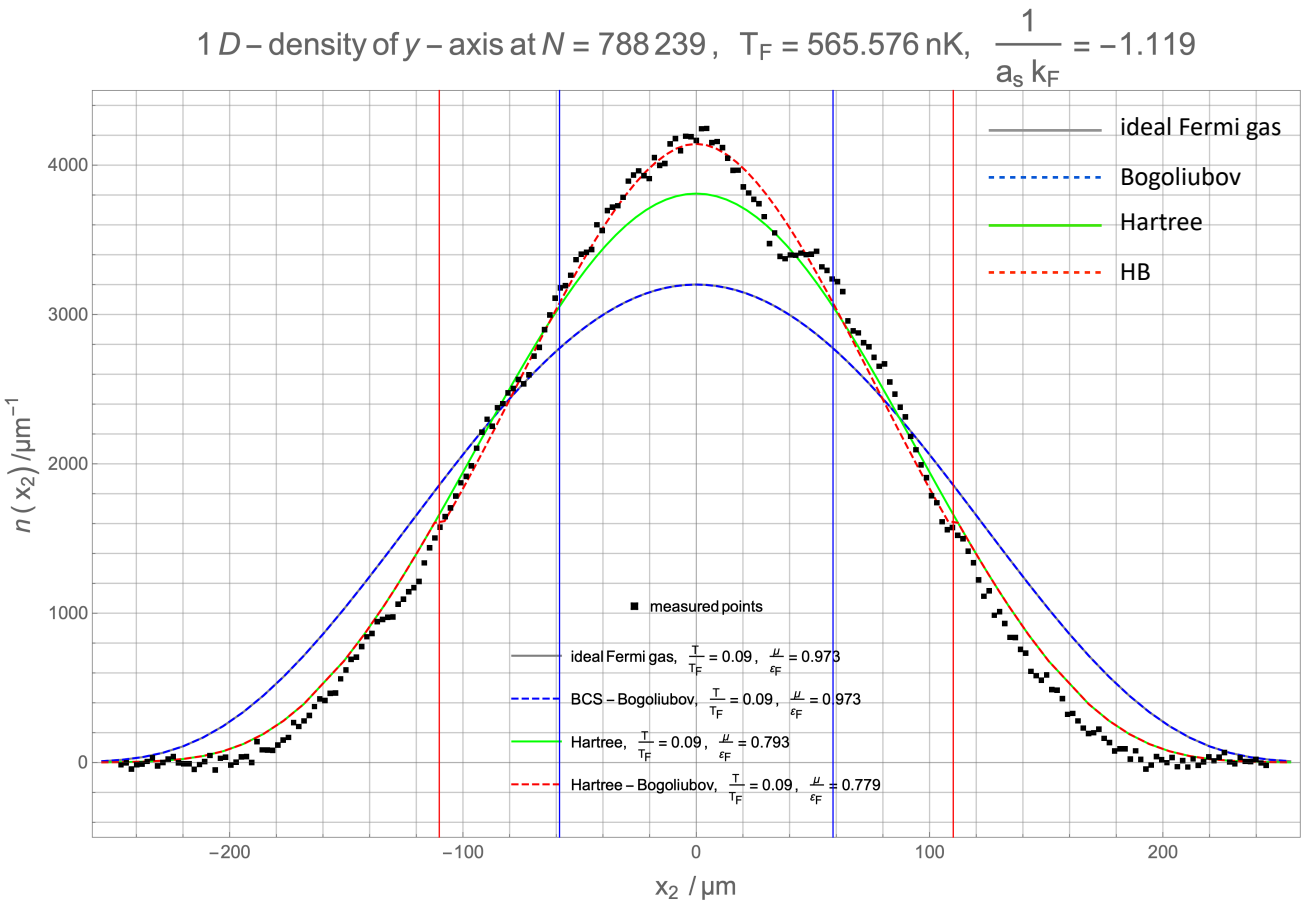


Fig.: 1D-density of y-axis with arbitrary choice of $T/T_F = 0.09$.

Experimental data due to AG Widera

Outlook: Thermometry for Fermi gas

- Thermometry of Fermi gas is challenging
- Indirect thermometry by adiabatic sweeping:

  Isentropic sweep of a_s to BEC limit to measure T with thermometry of Bose gas
- HB model as thermometry for Fermi gas

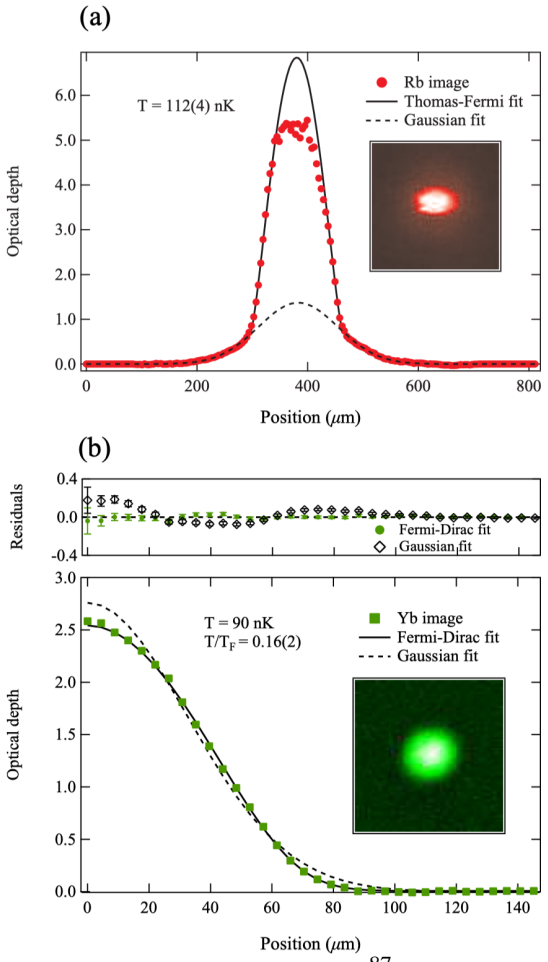


Fig.: Thermometry of bosonic ^{87}Rb (a) and fermionic ^{171}Yb (b) from same mixture.(*)

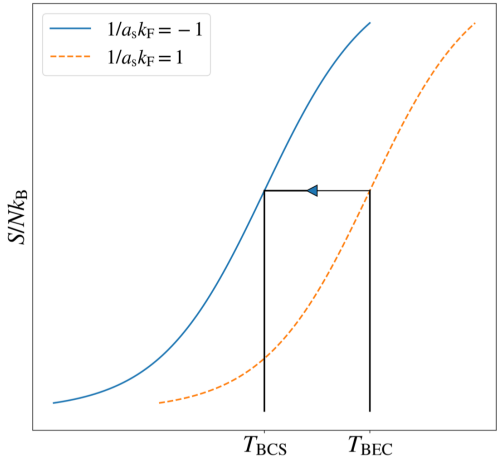


Fig.: Adiabatic sweep for temperature measurement of Fermi gas.(**)

(*) Vaidya, V. D., Tiamsuphat, J., Rolston, S. L., & Porto, J. V. (2015). Physical Review A.
(**) Becker. A. (2021), Master thesis, Technical University of Kaiserslautern.

Outlook: Theoretical support for OSCAR project B5

- Controlled temporally- and spatially random potential for ^{6}Li along BEC-BCS crossover
- Perturbation theory:

  HB model as unperturbed system
- Bosonic limit (**):

  Condensate deformation due to switching on of random potential consists of reversible and irreversible contribution

  → BEC-BCS crossover?

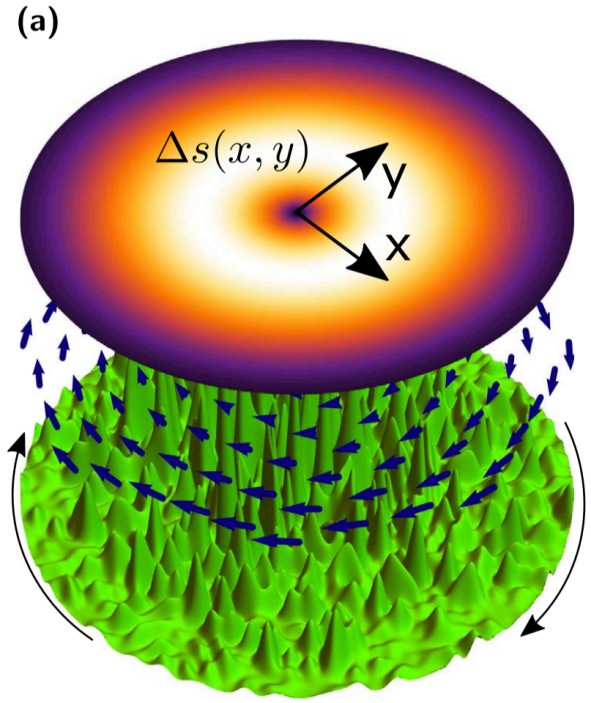


Fig.: Temporally random potential produced by rotating disk.(*)

(*) Nagler, B., Radonjić, M., Barbosa, S., Koch, J., Pelster, A., & Widera, A. (2020). *New J. Phys*.
(**) Radonjic, M., & Pelster, A. (2021). *SciPost Phys.*

Outlook: Training data for machine learning

- Estimation of condensate fraction by neural network algorithm
- Supervised machine learning based on labelled data of condensation

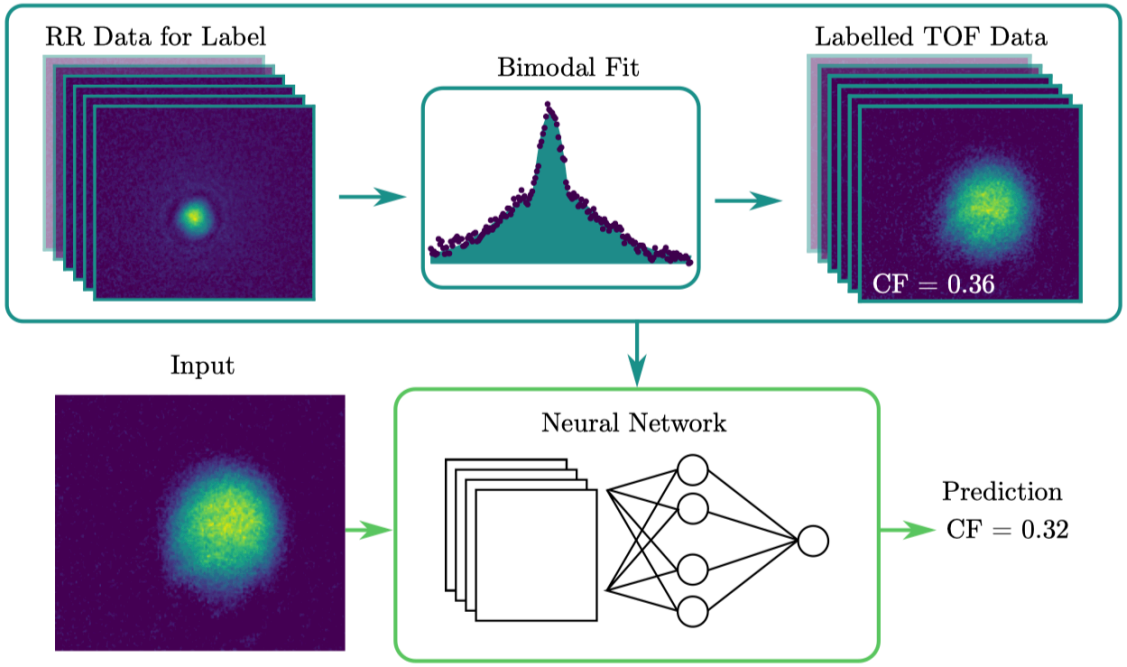


Fig.: Neural network assisted detection of condensate fraction.(*)

(*) Link, M. (2021). PhD. thesis, University of Bonn.