



RISE

Deutscher Akademischer Austauschdienst
German Academic Exchange Service

BCS-Bose Crossover in 2D

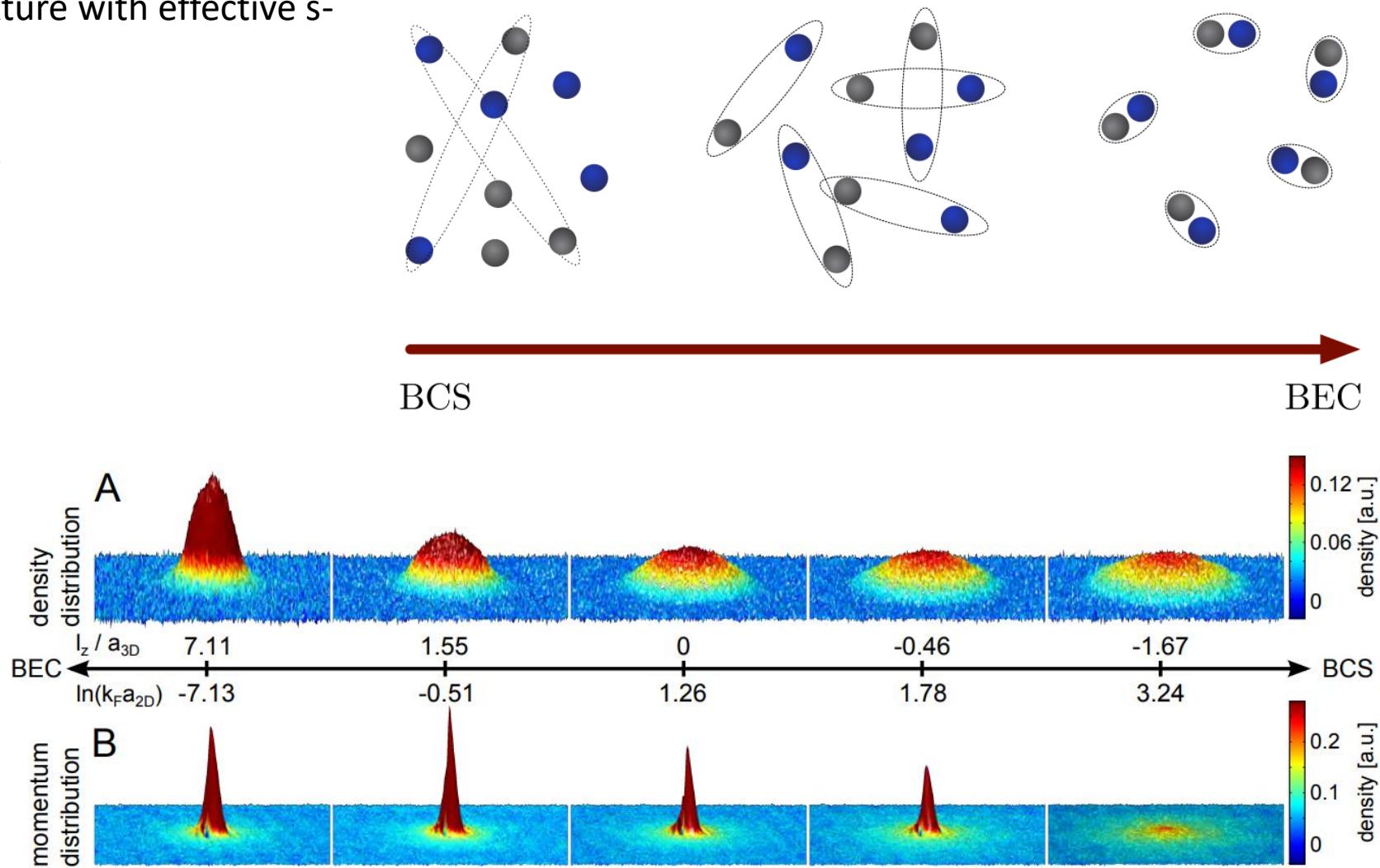
Harry Donegan

An overview

- BEC-BCS Crossover
 - I. An overview
- Berezinskii–Kosterlitz–Thouless Transition
 - I. Mermin-Wagner Theorem
 - II. BKT Transition
 - III. 2D Superfluidity
- Mean-Field Analysis of Homogenous Fermi Mixture
 - I. 2D Scattering
 - II. Zero Temperature Description
 - III. Finite Temperature Description
- Putting it all in a trap
 - I. LDA and failure of mean-field

Ultracold two-component Fermi gas mixture with effective s-wave scattering

- First realised in 3D in 2004 onwards
- Investigate lower dimensionality effects
- High T_c superconductors



Mermin-Wagner-Hohenberg Theorem: homogenous systems in 1D and 2D cannot have spontaneous broken continuous symmetries at finite temperature

$$\langle \{\hat{A}, \hat{A}^\dagger\} \rangle \langle [\hat{B}^\dagger, [\hat{H}, \hat{B}]] \rangle \geq 2k_B T |\langle [\hat{A}, \hat{B}] \rangle|^2$$

Bogoliubov Inequality

$$\hat{H} = \sum_{\mathbf{p}} \epsilon_{\mathbf{p}} \hat{b}_{\mathbf{p}}^\dagger \hat{b}_{\mathbf{p}} + \frac{1}{2} \sum_{\mathbf{k}, \mathbf{p}, \mathbf{q}} V_{\mathbf{k}} \hat{b}_{\mathbf{p}-\mathbf{k}}^\dagger \hat{b}_{\mathbf{q}+\mathbf{k}}^\dagger \hat{b}_{\mathbf{p}} \hat{b}_{\mathbf{q}}$$

$$\hat{A} = \hat{b}_{\mathbf{p}}^\dagger \quad \hat{B} = \sum_{\mathbf{k}} \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}+\mathbf{p}}$$

$$\langle \{\hat{A}, \hat{A}^\dagger\} \rangle = 2n_{\mathbf{p}} + 1$$

$$[\hat{H}, \hat{B}] = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{p}}) \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}+\mathbf{p}} \longrightarrow [\hat{B}^\dagger, [\hat{H}, \hat{B}]] = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}+\mathbf{p}} - 2\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{k}-\mathbf{p}}) \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} = \frac{\hbar^2 \mathbf{p}^2}{m} \hat{N}$$

$$[\hat{A}, \hat{B}] = -\hat{b}_0^\dagger$$

$$\therefore n_{\mathbf{p}} \geq \frac{k_B T m |\langle b_0 \rangle|^2}{N \hbar^2 \mathbf{p}^2} - \frac{1}{2}$$

We thus conclude $\langle b_0 \rangle \neq 0$ and $T \neq 0$ cannot be held simultaneously

$$N = \sum_{\mathbf{p}} n_{\mathbf{p}}$$

$$\sum_{\mathbf{p}} \frac{k_B T m |\langle b_0 \rangle|^2}{N \hbar^2 \mathbf{p}^2} - \frac{1}{2} \rightarrow \infty \quad (d = 1, 2)$$

Mermin, N.D., and Wagner, H. Phys Rev Lett **17**, 1133 (1966)
Hohenberg, P.C. Phys Rev Lett **158**, 383 (1967)

Ising model for continuous symmetries: XY Model

$$\hat{H} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) \approx \frac{J}{2} \int d^2 \mathbf{r}^2 |\nabla \theta|^2$$

$$z(\beta) = \int D[\theta](\mathbf{r}) \exp[-\beta \frac{J}{2} \int d^2 \mathbf{r}^2 |\nabla \theta|^2]$$

$$\langle S_x \rangle = \frac{1}{z(\beta)} \int D[\theta(\mathbf{r})] \cos(\theta(\mathbf{r})) e^{-\beta H} \rightarrow 0 \quad (d = 1, 2)$$

$$C(\mathbf{r}, \mathbf{r}') = \left(\frac{|\mathbf{r}-\mathbf{r}'|}{l} \right)^{-\frac{T}{2\pi J}}$$

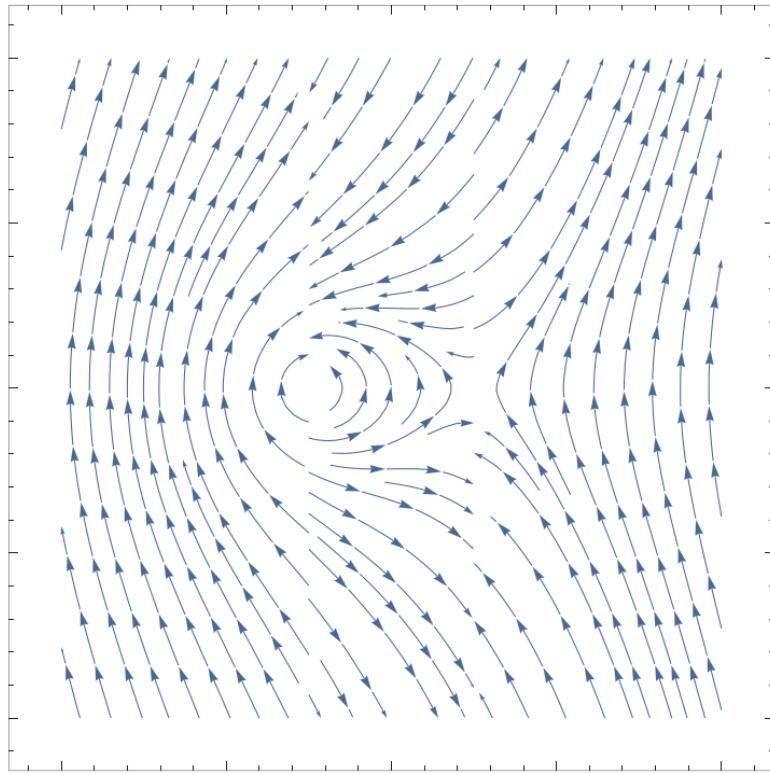
Superfluids:

$$H = \frac{1}{2} m n_s \int d^2 \mathbf{r} \mathbf{v}_s^2 \\ = \frac{\hbar^2 n_s}{2m} \int d^2 \mathbf{r} (\nabla \theta)^2$$

XY Hamiltonian exhibits quasi-long range order:

$$\lim_{|\mathbf{r}-\mathbf{r}'| \rightarrow \infty} C(\mathbf{r}, \mathbf{r}') \propto \begin{cases} \text{const} & \text{Long-range order} \\ e^{-|\mathbf{r}-\mathbf{r}'|/l} & \text{Disordered} \end{cases}$$

What has been avoided?



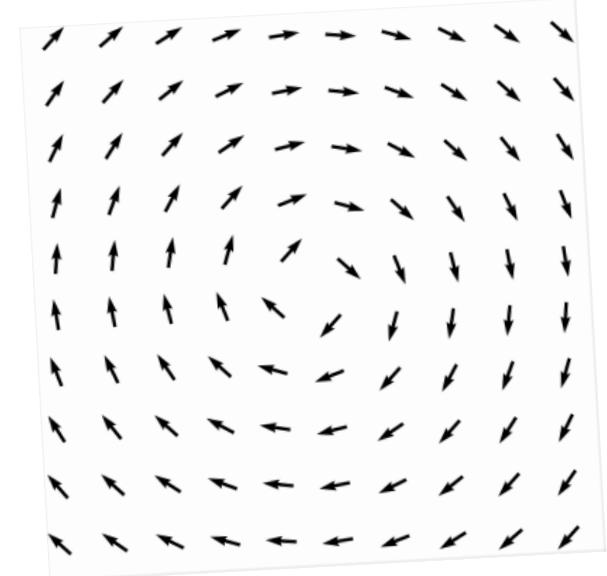
Vortex-anti-vortex pair

$$C(\mathbf{r}, \mathbf{r}') \propto |\mathbf{r} - \mathbf{r}'|^{-\eta}$$

High temperature, system
should become disordered

$$C(\mathbf{r}, \mathbf{r}') \propto e^{-|\mathbf{r}-\mathbf{r}'|/l}$$

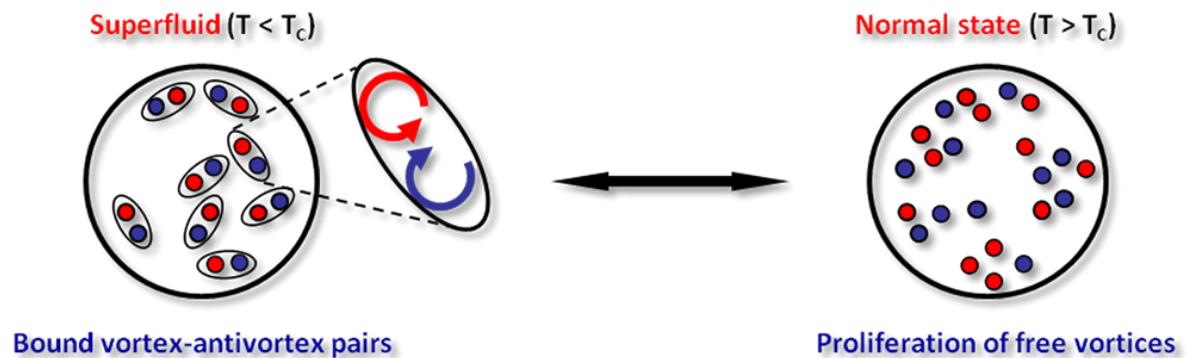
Single vortex



Simple thermodynamic argument

$$\begin{aligned}\Delta F &= \Delta U - T\Delta S \\ \downarrow &\quad \searrow \\ \Delta U &= \pi J \ln\left(\frac{L}{A}\right) \longrightarrow \Delta F = \left(\pi J - 2k_B T\right) \ln\left(\frac{L}{A}\right) \\ &\quad \downarrow\end{aligned}$$

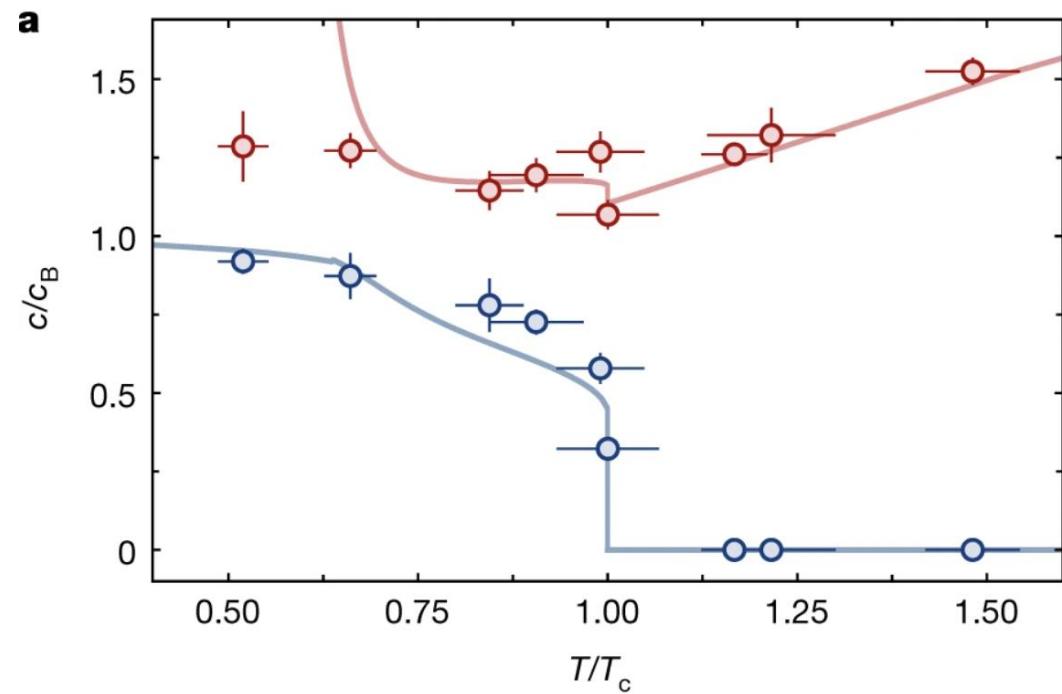
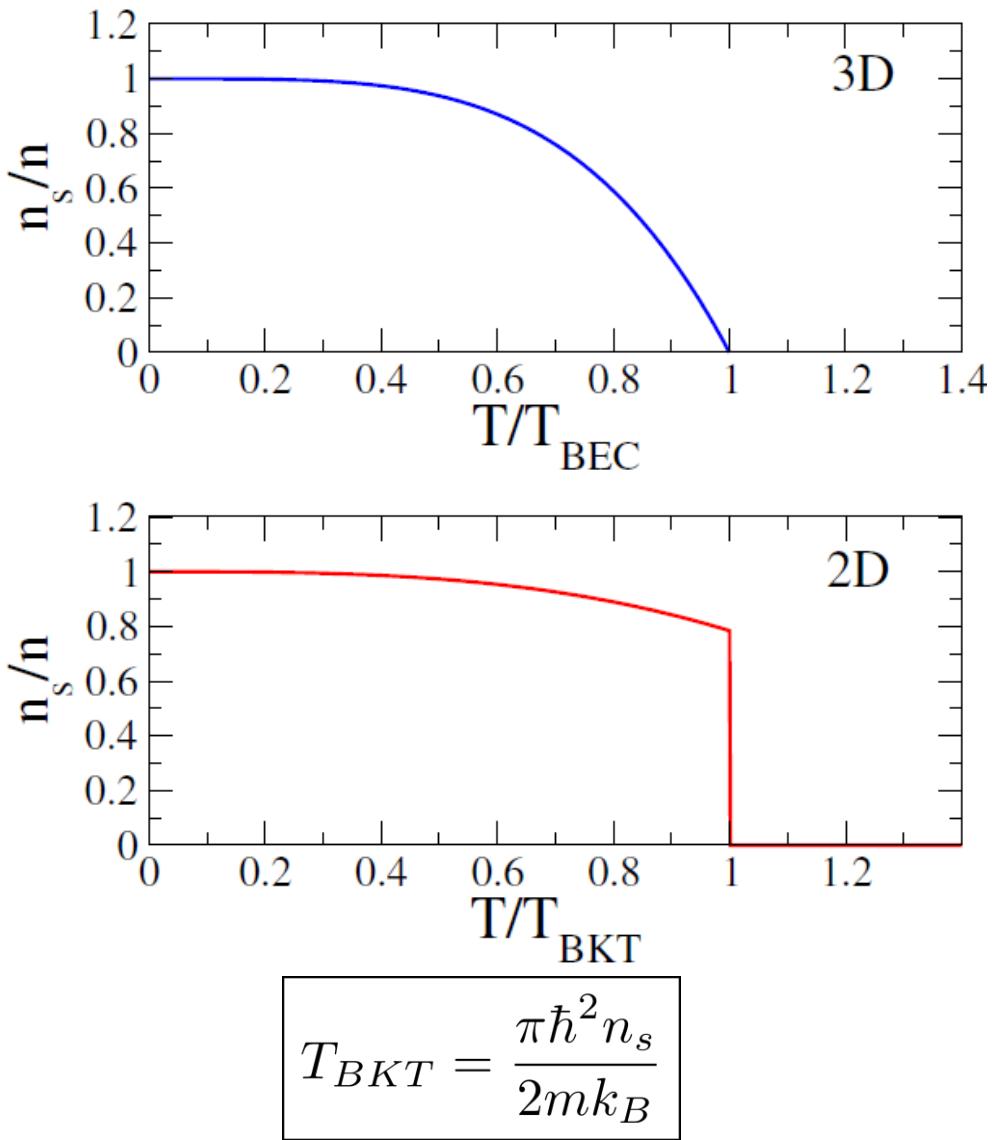
$$\boxed{T_C = \frac{\pi J}{2k_B}} \quad \begin{aligned}T < T_C : \Delta F &> 0 \\ T > T_C : \Delta F &< 0\end{aligned}$$



Berezinskii, V.L., Sov Phys JETP **32**, 493 (1971)

Berezinskii, V.L., Sov Phys JETP **34**, 610 (1972)

Kosterlitz, J.M. and Thouless J.D., Journal of Physics C: Solid State Physics **6**, 1181 (1973)



Christodoulou, P. et al., Nature 594, 191 (2021)

2D Scattering Theory

$$-\frac{\hbar^2}{2m_r} \frac{1}{r} \frac{d}{dr} \left(r \frac{dR}{dr} \right) + \frac{\hbar^2 l^2}{2m_r r^2} R(r) + V(r) = ER(r)$$

2D:

$$\cot(\delta_s(k)) = \frac{2}{\pi} \ln(ka)$$

$$\therefore a_{2D} > 0$$

3D:

$$\cot(\delta_s(k)) = -\frac{1}{ka}$$

$$\psi(r, \theta) \rightarrow e^{ikx} - \sqrt{\frac{i}{8\pi k}} f_k(\theta) \frac{e^{ikr}}{\sqrt{r}}$$

$$f_k(\theta) = \sum_{l=0}^{\infty} (2 - \delta_{0,l}) \cos(l\theta) f_l(k)$$

$$f_l(k) = \frac{-4}{\cot(\delta_{l(k)}) - i}$$

$$\frac{\hbar^2}{2m_r} (\nabla^2 - k^2) \psi = V \psi \longrightarrow \psi_{\mathbf{k}}(\mathbf{q}) = -\frac{2m_r}{\hbar^2} \frac{1}{q^2+k^2} \int \frac{d^n q'}{(2\pi)^n} V(\mathbf{q} - \mathbf{q}') \psi_{\mathbf{k}}(\mathbf{q}')$$

Short range potential: $|\mathbf{q}| < R, V(q) \approx V_0$

$$-\frac{1}{V_0} = \frac{1}{\Omega} \int_{\epsilon < E_R} d\epsilon \frac{\rho_n(\epsilon)}{2\epsilon + |E|}$$

D.O.S.

Bound state energy

Solution for small V_0 if RHS is diverging as $|\epsilon| \rightarrow 0$

Model

Generic two-body interaction Hamiltonian, here we consider a two-spin Fermi gas

$$H_\Omega = \int d^2\mathbf{r} \sum_{\sigma} \psi_{\sigma}^{\dagger}(\mathbf{r}) \left[\frac{\hbar^2 \nabla^2}{2m} - \mu \right] \psi_{\sigma}(\mathbf{r}) + \int d^2\mathbf{r} d^2\mathbf{r}' \psi_{\uparrow}^{\dagger}(\mathbf{r}) \psi_{\downarrow}^{\dagger}(\mathbf{r}') U(\mathbf{r} - \mathbf{r}') \psi_{\downarrow}(\mathbf{r}') \psi_{\uparrow}(\mathbf{r})$$

with contact interactions:

$$U(\mathbf{r} - \mathbf{r}') = g\delta^2(\mathbf{r} - \mathbf{r}')$$



$$H = \int d^2\mathbf{r} \left\{ \sum_{\sigma} \psi_{\sigma}^{\dagger}(\mathbf{r}) \left[\frac{\hbar^2 \nabla^2}{2m} - \mu \right] \psi_{\sigma}(\mathbf{r}) + g \psi_{\uparrow}^{\dagger}(\mathbf{r}) \psi_{\downarrow}^{\dagger}(\mathbf{r}) \psi_{\downarrow}(\mathbf{r}) \psi_{\uparrow}(\mathbf{r}) \right\}$$

Mean-field approach

$$\langle \psi_{\downarrow}^{\dagger} \psi_{\downarrow} \rangle \psi_{\uparrow}^{\dagger} \psi_{\uparrow} + \langle \psi_{\uparrow}^{\dagger} \psi_{\uparrow} \rangle \psi_{\downarrow}^{\dagger} \psi_{\downarrow} - \langle \psi_{\downarrow}^{\dagger} \psi_{\downarrow} \rangle \langle \psi_{\uparrow}^{\dagger} \psi_{\uparrow} \rangle \quad \text{Hartree Channel – Direct energy}$$

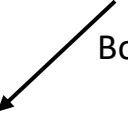
$$\psi_{\uparrow}^{\dagger} \psi_{\downarrow}^{\dagger} \psi_{\downarrow} \psi_{\uparrow} \simeq - \langle \psi_{\uparrow}^{\dagger} \psi_{\downarrow} \rangle \psi_{\downarrow}^{\dagger} \psi_{\uparrow} - \langle \psi_{\downarrow}^{\dagger} \psi_{\uparrow} \rangle \psi_{\uparrow}^{\dagger} \psi_{\downarrow} + \langle \psi_{\uparrow}^{\dagger} \psi_{\downarrow} \rangle \langle \psi_{\downarrow}^{\dagger} \psi_{\uparrow} \rangle \quad \text{Fock Channel – Exchange energy}$$

$$\langle \psi_{\uparrow}^{\dagger} \psi_{\downarrow}^{\dagger} \rangle \psi_{\downarrow} \psi_{\uparrow} + \langle \psi_{\downarrow} \psi_{\uparrow} \rangle \psi_{\uparrow}^{\dagger} \psi_{\downarrow}^{\dagger} - \langle \psi_{\uparrow}^{\dagger} \psi_{\downarrow}^{\dagger} \rangle \langle \psi_{\downarrow} \psi_{\uparrow} \rangle \quad \text{Bogoliubov Channel – Pairing energy}$$

We focus on the Bogoliubov channel and write in momentum space:

$$H = \sum_{\mathbf{k}} \left\{ \left(\frac{\hbar^2 k^2}{2m} - \mu \right) \hat{a}_{\sigma, \mathbf{k}}^{\dagger} \hat{a}_{\sigma, \mathbf{k}} - \Delta_0^* \hat{a}_{\downarrow, -\mathbf{k}} \hat{a}_{\uparrow, \mathbf{k}} - \Delta_0 \hat{a}_{\uparrow, \mathbf{k}}^{\dagger} \hat{a}_{\downarrow, -\mathbf{k}}^{\dagger} \right\} - V \frac{|\Delta_0|^2}{g}$$

Bogoliubov transformation



$$H = \sum_{\mathbf{k}} E(\mathbf{k}) [\hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}} + \hat{\beta}_{\mathbf{k}}^{\dagger} \hat{\beta}_{\mathbf{k}}] - V \frac{|\Delta_0|^2}{g} + \sum_{\mathbf{k}} (\epsilon(\mathbf{k}) - E(\mathbf{k}))$$

Bogoliubov dispersion relation:
 $E(\mathbf{k}) = \sqrt{\epsilon^2(\mathbf{k}) + \Delta^2}$

$$\Omega = -V \frac{|\Delta_0|^2}{g} + \sum_{\mathbf{k}} (\epsilon(\mathbf{k}) - E(\mathbf{k})) - \frac{2}{\beta} \sum_{\mathbf{k}} \ln[1 + e^{-\beta E(\mathbf{k})}]$$

$$\partial_\Delta \Omega = 0$$

$$n = -\frac{1}{V} \partial_\mu \Omega$$

$$n = \frac{1}{V} \sum_{\mathbf{k}} \left(1 - \frac{\epsilon(\mathbf{k})}{E(\mathbf{k})} \tanh \left(\frac{\beta E(\mathbf{k})}{2} \right) \right)$$

$$\frac{1}{g} = -\frac{1}{2A} \sum_{\mathbf{k}} \frac{1}{\frac{\hbar^2 k^2}{2m} + \frac{1}{2}\epsilon_b}$$

$$\frac{1}{g} = \frac{-1}{2V} \sum_{\mathbf{k}} \frac{1}{E(\mathbf{k})} \tanh \left(\frac{\beta E(\mathbf{k})}{2} \right)$$

$$0 = \Delta \int_0^\infty d\epsilon \left(\frac{1}{\sqrt{(\epsilon - \mu)^2 + \Delta^2}} \tanh \left(\frac{\beta}{2} \sqrt{(\epsilon - \mu)^2 + \Delta^2} \right) - \frac{1}{\epsilon + \frac{1}{2}\epsilon_b} \right)$$

$$n = \frac{m}{2\pi\hbar^2} \int_0^\infty d\epsilon \left(1 - \frac{\epsilon - \mu}{\sqrt{(\epsilon - \mu)^2 + \Delta^2}} \tanh \left(\frac{\beta}{2} \sqrt{(\epsilon - \mu)^2 + \Delta^2} \right) \right)$$

Zero Temperature

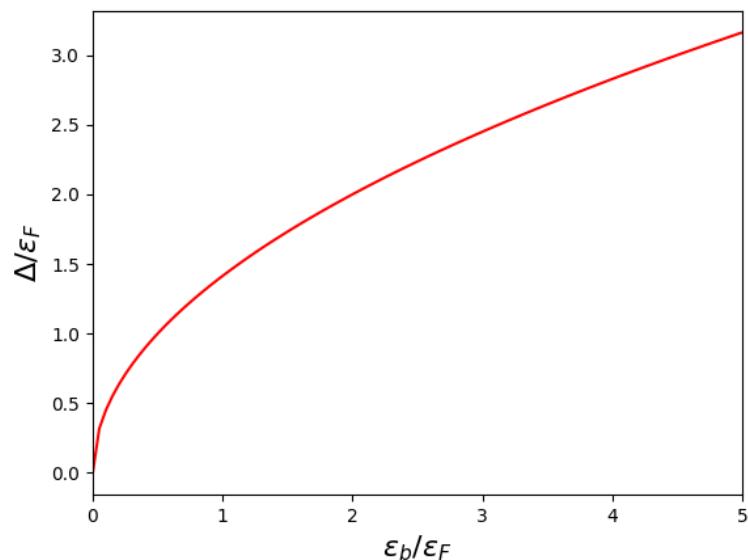
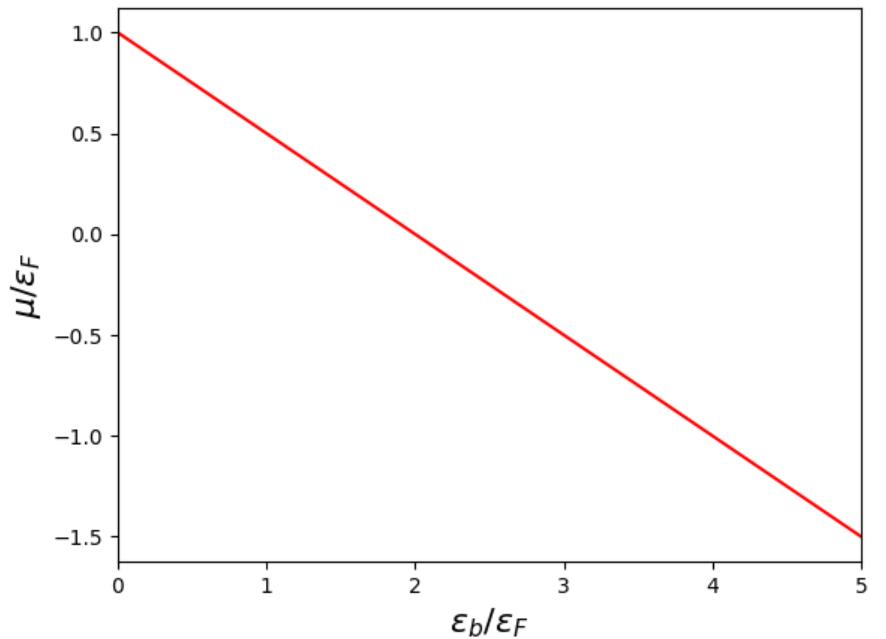
$$2 = \int_0^\infty d\tilde{\epsilon} \left(1 - \frac{\tilde{\epsilon} - \tilde{\mu}}{\sqrt{(\tilde{\epsilon} - \tilde{\mu})^2 + \tilde{\Delta}^2}} \right)$$

$$0 = \int_0^\infty d\tilde{\epsilon} \left(\frac{1}{\sqrt{(\tilde{\epsilon} - \tilde{\mu})^2 + \tilde{\Delta}^2}} - \frac{1}{\tilde{\epsilon} + \frac{1}{2}\tilde{\epsilon}_b} \right)$$

Scaled by the Fermi energy:

$$\epsilon_F = \frac{\pi \hbar^2 n}{m}$$

$$\tilde{\mu} = 1 - \frac{1}{2}\tilde{\epsilon}_b$$



$$\tilde{\Delta} = \sqrt{2\tilde{\epsilon}_b}$$

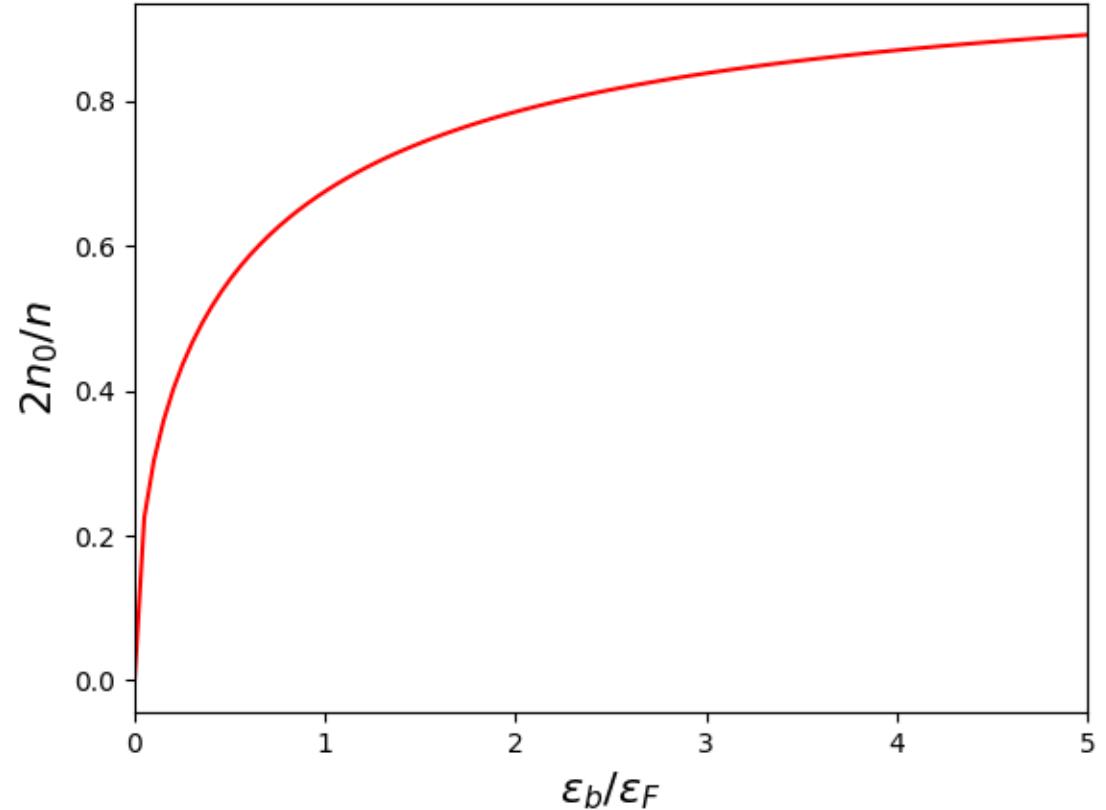
$$\lim_{|\mathbf{r}-\mathbf{r}'| \rightarrow \infty} \rho_2(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}'_1, \mathbf{r}'_2) = \langle \Psi^\dagger(\mathbf{r}_1) \Psi^\dagger(\mathbf{r}_2) \rangle \langle \Psi(\mathbf{r}_2) \Psi(\mathbf{r}_1) \rangle$$

Bose systems:

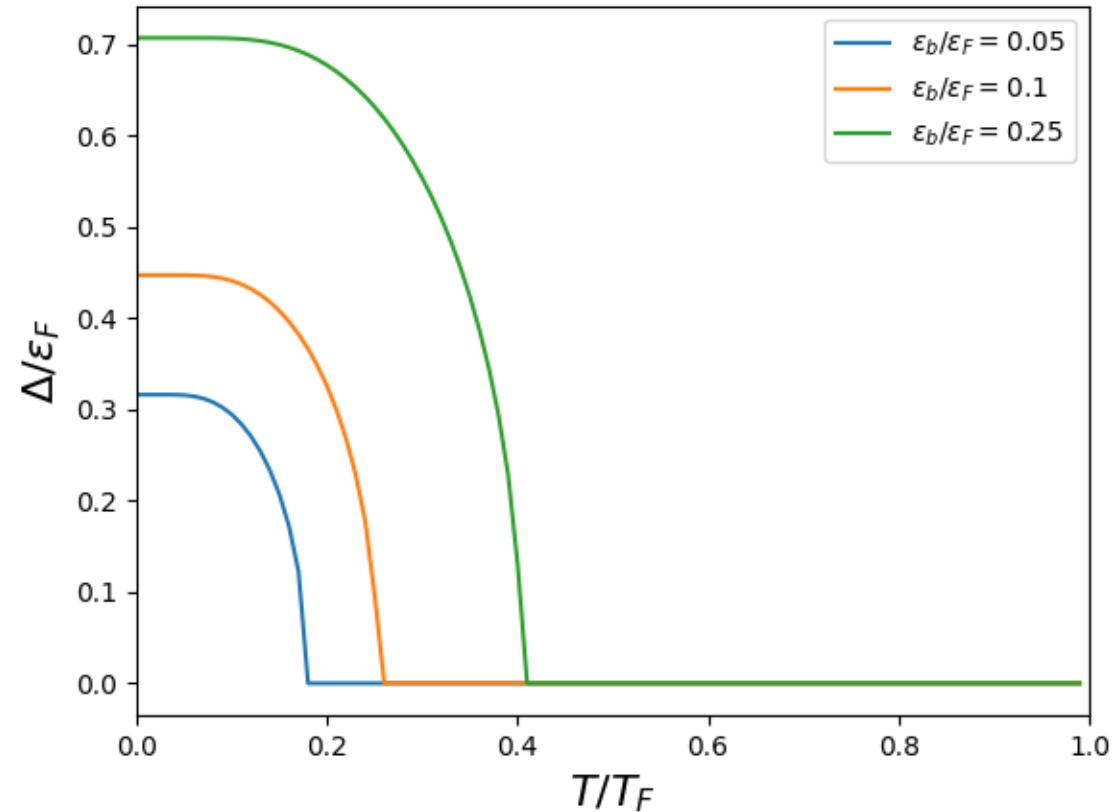
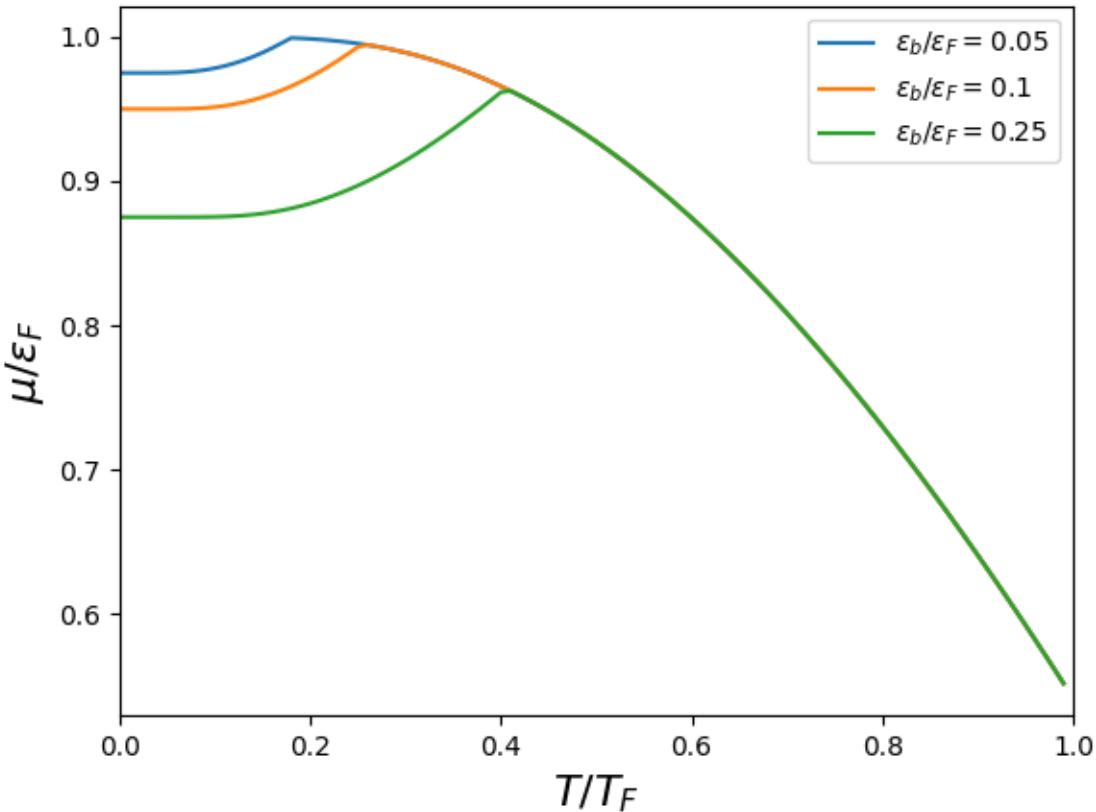
$$n_0 = |\psi_B|^2$$

$$n_0 = \frac{1}{V} \sum_{\mathbf{k}} u_{\mathbf{k}}^2 v_{\mathbf{k}}^2 = \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{4} \frac{\Delta^2}{(\epsilon^2(\mathbf{k}) + \Delta^2)}$$

$$\boxed{\frac{2n_0}{n} = \frac{\sqrt{2\tilde{\epsilon}_b}}{4} \left(\frac{\pi}{2} + \arctan \left(\frac{1 - \frac{1}{2}\tilde{\epsilon}_b}{\sqrt{2\tilde{\epsilon}_b}} \right) \right)}$$

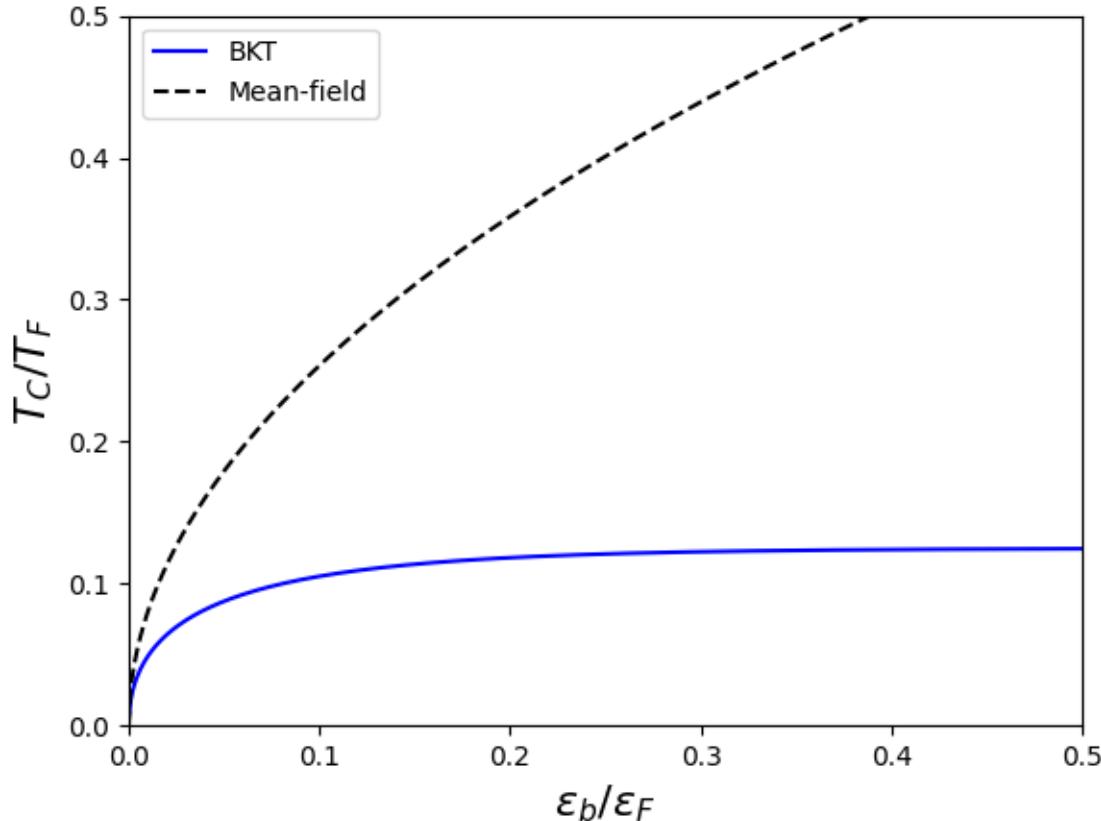


Finite Temperature



Mean-field:

$$\frac{T_{BCS}}{T_F} = \frac{\sqrt{2}e^\gamma}{\pi} \sqrt{\frac{\epsilon_b}{\epsilon_F}}$$



BKT:

$$T_{BKT} = \frac{\pi \hbar^2 n_s}{2m k_B} \quad n_s = n - n_n$$

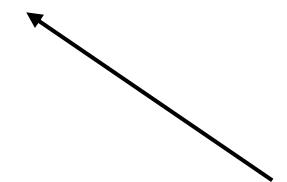
where we approximate with mean-field density

$$\mathbf{P}^{B,F} = \sum_{\mathbf{k}} \hbar \mathbf{k} f_{B,F}(\epsilon - \hbar \mathbf{k} \cdot \mathbf{v}) \approx \frac{1}{2} \mathbf{v} \sum_k \hbar^2 k^2 \left(-\frac{\partial f_{B,F}}{\partial \epsilon} \right)$$

Two types of excitations:

- Fermionic quasi-particles – related to breaking of cooper pairs
- Bosonic – excitations of cooper pairs

$$n_n = \frac{1}{V} \sum_k \epsilon(k) \left(-\frac{\partial f_F}{\partial \epsilon} \right) = \frac{1}{V} \sum_k \beta \epsilon(k) \frac{1}{\cosh^2 \left(\frac{\beta E(k)}{2} \right)}$$



Neglects vortex contributions, requires RG methods

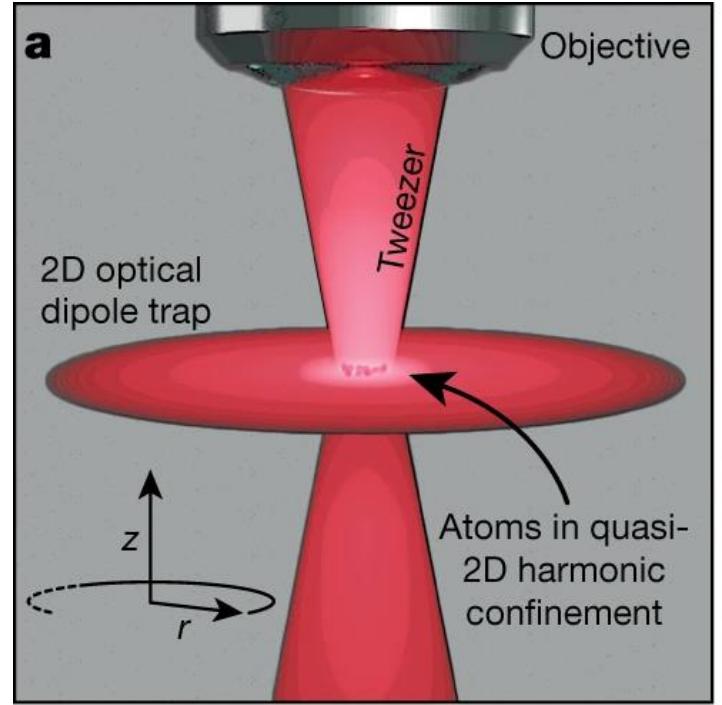
Trapping

Harmonic trapping potential:

$$V(\mathbf{r}) = \frac{m}{2} \sum_i \omega_i^2 r_i^2$$

In an inhomogeneous system, relevant system parameters gain spatial dependence

$$n \rightarrow n(\mathbf{r}) \quad \mu \rightarrow \mu(\mathbf{r}) \quad \Delta \rightarrow \Delta(\mathbf{r})$$



Holten, M., Bayha, L., Subramanian, K. et al. *Nature* **606**, 287–291 (2022).

Apply semi-classical approach:

$$\mu(\mathbf{r}) = \mu - V(\mathbf{r})$$

Fixed by normalisation condition:

$$N = \int d^2\mathbf{r} n(\mathbf{r})$$

Mean-Field Result:

$$n(r) = \frac{2N}{\pi r_{TF}^2} \left(1 - \frac{r^2}{r_{TF}^2}\right)$$

Identical to ideal case

Zero-temp QMC Result:

$$\mu(\mathbf{r}) = \mu - V(\mathbf{r}) = \frac{\epsilon_b}{2} + \frac{\pi\hbar^2}{m} f_\mu [\ln \sqrt{2\pi n(\mathbf{r})} a_f]$$

where in the BCS limit:

$$\frac{n(r)}{n_0} = \left(1 + \frac{1}{2 \ln(k_F a_f)}\right) - \left(1 + \frac{1}{2 \ln(k_F a_f)}\right)^2 \frac{r^2}{r_{TF}^2}$$

