

Functional theory for Bose-Einstein condensates

Julia Liebert

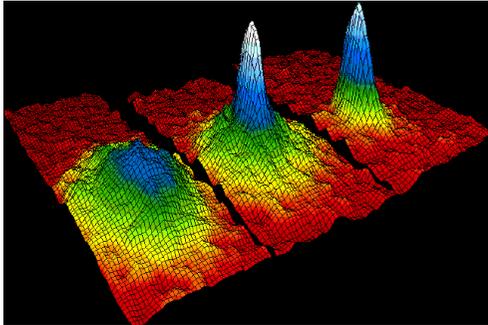
07.10.2022

In collaboration with:

Christian Schilling



Criterion for Bose-Einstein Condensation



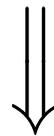
Nobel prize 2001: C.E. Wieman,
E.A. Cornell, W. Ketterle

$$\lambda_{\max} = \max_{\alpha} \langle \alpha | \gamma | \alpha \rangle \propto N$$

[O. Penrose, L. Onsager,
Phys. Rev. **104**, 576 (1956)]

One-particle reduced
density operator (1RDM)

⇒ Need to involve full 1RDM rather than particle density



↓
Density functional theory
(DFT)

**One-particle reduced density matrix functional theory
(1-RDMFT)**

Outline

I) Homogeneous Bose gas

II) Derivation of the universal functional

III) Novel concept: BEC force

IV) Applications and illustrations

I) Homogeneous Bose gases

- No external potential: $h = t \equiv \sum_{\mathbf{p}} \varepsilon(\mathbf{p}) \hat{n}_{\mathbf{p}}$

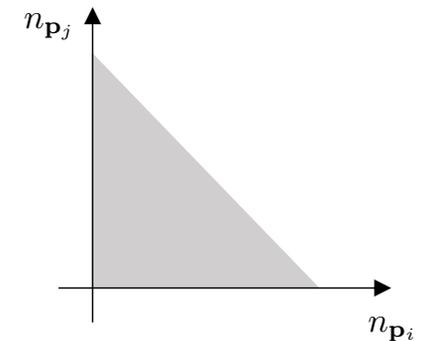
- Translational invariance:

$$\mathcal{F}(\mathbf{n}) = \min_{|\Phi\rangle \rightarrow \mathbf{n}} \langle \Phi | \hat{W} | \Phi \rangle, \quad \mathbf{n} = (n_{\mathbf{p}})_{\mathbf{p}}$$

- Domain of \mathcal{F} :

$$\Delta = \left\{ \mathbf{n} \equiv (n_{\mathbf{p}})_{\mathbf{p} \neq \mathbf{0}} \mid n_{\mathbf{p}} \geq 0, \sum_{\mathbf{p} \neq \mathbf{0}} n_{\mathbf{p}} \leq N \right\}$$

$$n_{\mathbf{0}} = N - \sum_{\mathbf{p} \neq \mathbf{0}} n_{\mathbf{p}}$$



II) Derivation of the universal functional

Particle number conserving Bogoliubov theory:

Pair interaction:

$$W_P = \frac{N(N-1)W_0}{2V} + \frac{1}{2V} \sum_{\mathbf{p} \neq 0} W_{\mathbf{p}} \left[2\hat{n}_0 \hat{n}_{\mathbf{p}} + a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger a_0^2 + (a_0^\dagger)^2 a_{\mathbf{p}} a_{-\mathbf{p}} \right]$$
$$+ \frac{1}{2V} \sum_{\substack{\mathbf{p}, \mathbf{p}' \neq 0 \\ \mathbf{p} \neq \mathbf{p}'}} W_{\mathbf{p}} a_{\mathbf{p}'}^\dagger a_{-\mathbf{p}'}^\dagger a_{\mathbf{p}'-\mathbf{p}} a_{\mathbf{p}-\mathbf{p}'} + \frac{1}{2V} \sum_{\substack{\mathbf{p}' \neq 0 \\ \mathbf{p} \neq \mathbf{p}', \mathbf{p} \neq 2\mathbf{p}'}} W_{\mathbf{p}} \hat{n}_{\mathbf{p}'-\mathbf{p}} \hat{n}_{\mathbf{p}'}$$

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Bogoliubov

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Trial states: $|\Psi\rangle \equiv U_G|N\rangle, \quad |N\rangle = \frac{1}{\sqrt{N!}}(a_0^\dagger)^N|0\rangle$

$$U_G = \exp \left\{ \frac{1}{2} \sum_{\mathbf{p} \neq \mathbf{0}} \theta_{\mathbf{p}} \left[(a_0^\dagger)^2 a_{\mathbf{p}} a_{-\mathbf{p}} - a_0^2 a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger \right] \right\}$$

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Quasiparticle operators:

$$U_G^\dagger a_{\mathbf{p}} U_G \approx \frac{1}{\sqrt{1 - \phi_{\mathbf{p}}^2}} \left(a_{\mathbf{p}} - \phi_{\mathbf{p}} a_0^2 a_{-\mathbf{p}}^\dagger \right), \quad \phi_{\mathbf{p}} = \tanh(\theta_{\mathbf{p}})$$

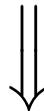
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Average particle numbers: $n_{\mathbf{p}} \equiv \langle \Psi | a_{\mathbf{p}}^\dagger a_{\mathbf{p}} | \Psi \rangle \approx \frac{\phi_{\mathbf{p}}^2}{1 - \phi_{\mathbf{p}}^2}$



$$\phi_{\mathbf{p}} = \sigma_{\mathbf{p}} \sqrt{\frac{n_{\mathbf{p}}}{1 + n_{\mathbf{p}}}}, \quad \sigma_{\mathbf{p}} = \sigma_{-\mathbf{p}} = \pm 1$$

Calculation of \mathcal{F} :

Recall: $\mathcal{F} = \min_{|\Phi\rangle \rightarrow \mathbf{n}} \langle \Phi | W | \Phi \rangle$

- $W \rightarrow W_P$
- $|\Phi\rangle \rightarrow |\Psi\rangle \equiv U_G |N\rangle$

$$\left. \vphantom{\begin{matrix} \bullet \\ \bullet \end{matrix}} \right\} \Rightarrow \mathcal{F}_G = \min_{|\Psi\rangle \rightarrow \mathbf{n}} \langle \Psi | W_P | \Psi \rangle$$

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$$\Rightarrow \mathcal{F}_G = \min_{|\Psi\rangle \rightarrow \mathbf{n}} \langle \Psi | W_P | \Psi \rangle$$

Variational principle:

$$\mathcal{F}_{\text{exact}} \leq \mathcal{F}_G$$

Exact in leading order
in BEC regime



$$\begin{aligned}
 \mathcal{F}_G(\mathbf{n}) &= \min_{\{\sigma_{\mathbf{p}}=\pm 1\}} \langle \Psi | \hat{W}_P | \Psi \rangle \\
 &= \min_{\{\sigma_{\mathbf{p}}=\pm 1\}} \left\{ \sum_{\mathbf{p} \neq \mathbf{0}} \left[\frac{n_0}{V} W_{\mathbf{p}} + \frac{1}{2} I_2(\mathbf{p}, \mathbf{n}) \right] n_{\mathbf{p}} \right. \\
 &\quad \left. - \sigma_{\mathbf{p}} \left[\frac{n_0}{V} W_{\mathbf{p}} - \frac{1}{2} I_1(\mathbf{p}, \mathbf{n}, \boldsymbol{\sigma}) \right] \sqrt{n_{\mathbf{p}}(n_{\mathbf{p}} + 1)} \right\}
 \end{aligned}$$

$$I_1(\mathbf{p}, \mathbf{n}, \boldsymbol{\sigma}) \equiv \frac{1}{V} \sum_{\mathbf{p}' \neq \mathbf{0}} W_{\mathbf{p}-\mathbf{p}'} \sigma_{\mathbf{p}'} \sqrt{n_{\mathbf{p}'}(n_{\mathbf{p}'} + 1)},$$

$$I_2(\mathbf{p}, \mathbf{n}) \equiv \frac{1}{V} \sum_{\mathbf{p}' \neq \mathbf{0}} W_{\mathbf{p}-\mathbf{p}'} n_{\mathbf{p}'}, \quad n_0 = N - \sum_{\mathbf{p} \neq \mathbf{0}} n_{\mathbf{p}}$$

} negligible close to complete BEC

Bogoliubov functional:

Close to complete BEC:

$$\sigma_{\mathbf{p}} = \text{sgn}(W_{\mathbf{p}}), \quad \forall \mathbf{p} \neq \mathbf{0}$$



$$\mathcal{F}_B(\mathbf{n}) = n \sum_{\mathbf{p} \neq \mathbf{0}} W_{\mathbf{p}} \left[n_{\mathbf{p}} - \text{sgn}(W_{\mathbf{p}}) \sqrt{n_{\mathbf{p}}(n_{\mathbf{p}} + 1)} \right]$$

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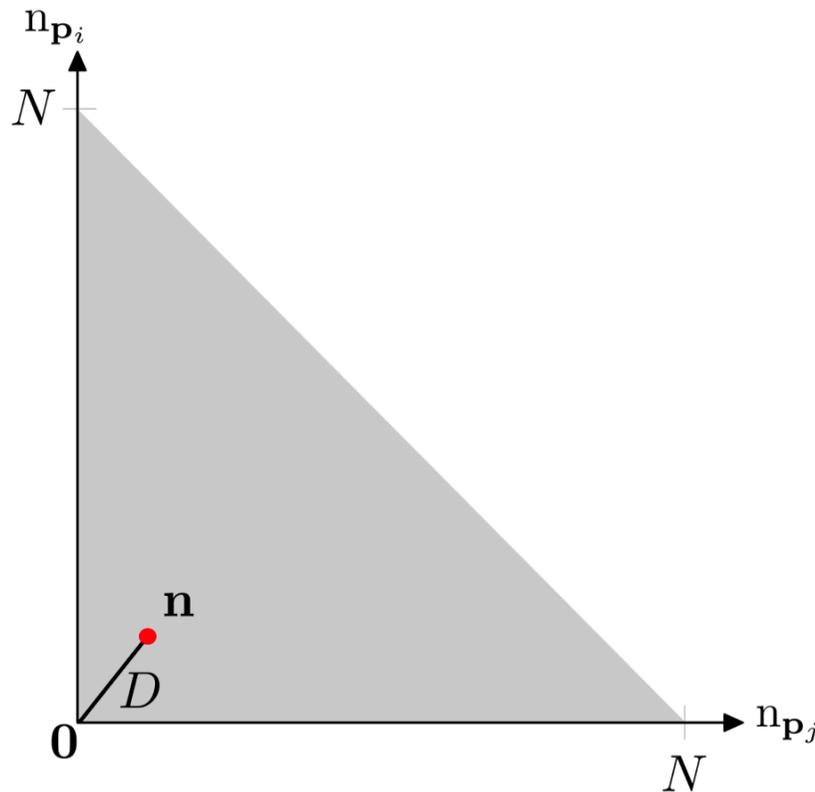


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- Valid for **arbitrary** pair interaction close to complete BEC
- Phase dilemma is solved
- Overall sign of the second term is negative independent of $W_{\mathbf{p}}$

III) Novel concept: BEC force

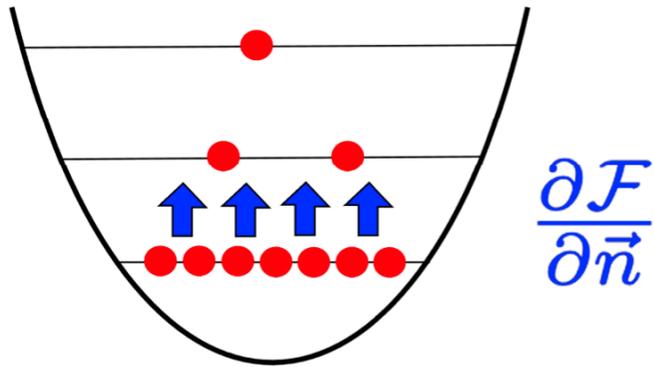
Degree of quantum depletion: $D \equiv 1 - N_{\text{BEC}}/N = \frac{1}{N} \sum_{\mathbf{p} \neq 0} n_{\mathbf{p}}$



\Rightarrow

$$\frac{d\mathcal{F}}{dD} \propto -\frac{1}{\sqrt{D}}$$

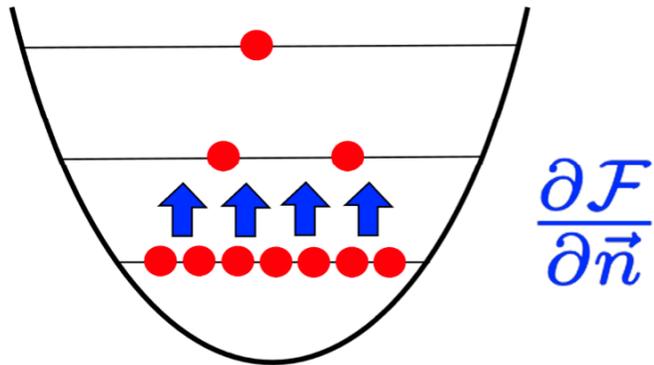
Bose-Einstein force



**Universal
explanation for
quantum depletion** !

[J. Liebert, C. Schilling, Phys. Rev. Research **3**, 013282 (2021)]

Bose-Einstein force



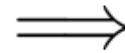
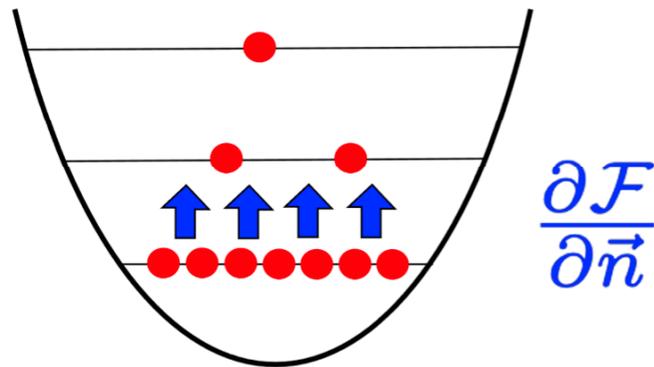
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Generalization to inhomogeneous Bose gases:

T. Maciażek, Repulsively diverging gradient of the density functional in the reduced density matrix functional theory, New J. Phys. **23**, 113006 (2021)

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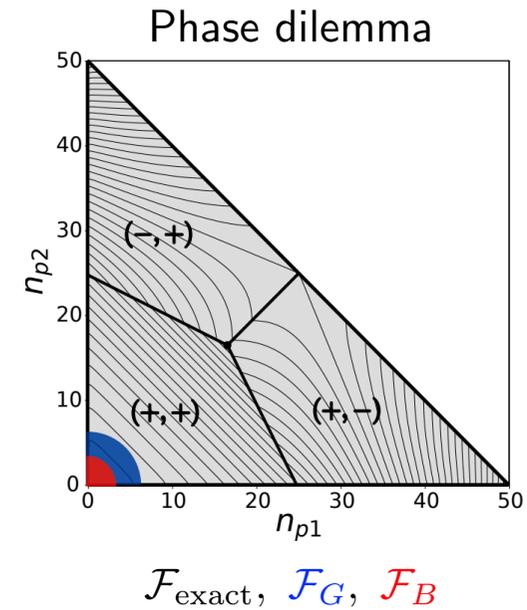
IV) Applications and illustrations

Hubbard model for 5 lattice sites:

Hamiltonian: $H = t + UW$



e. g. different hopping processes,
hopping strengths, ...



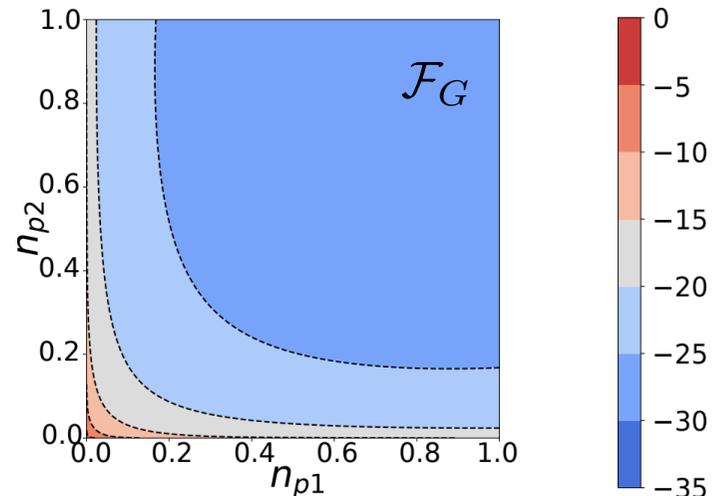
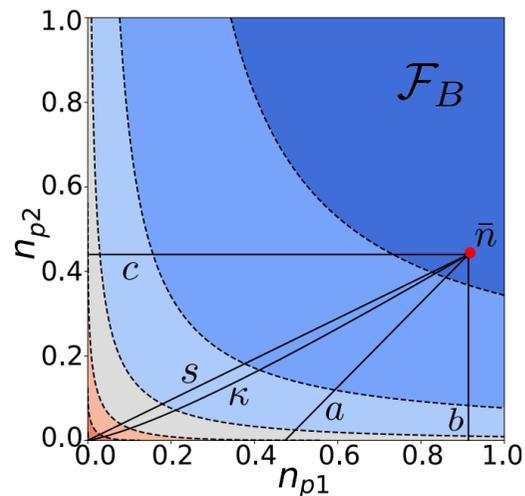
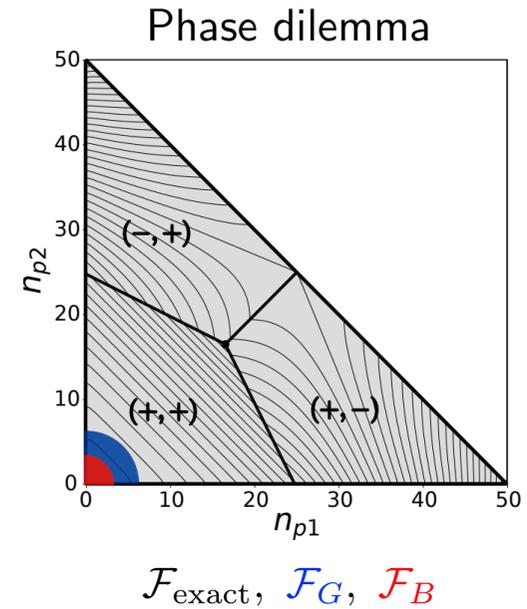
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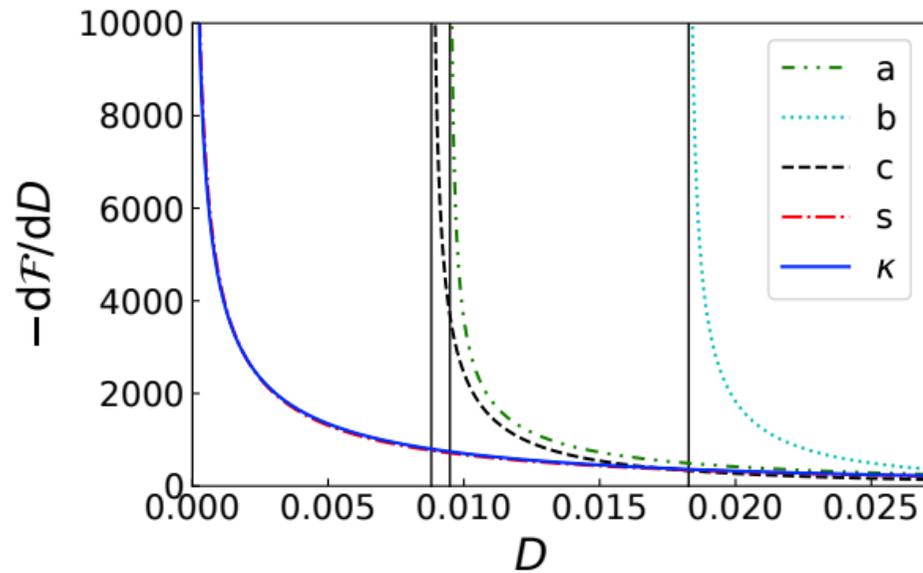
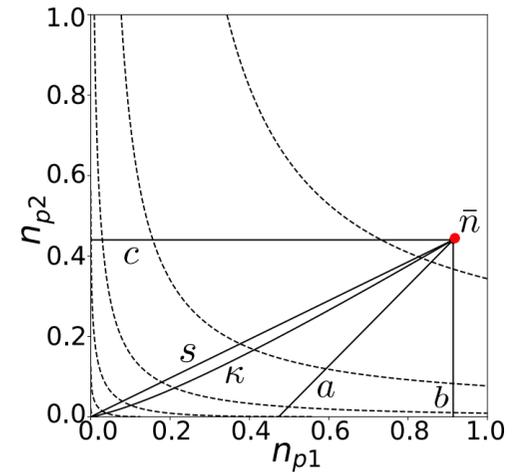
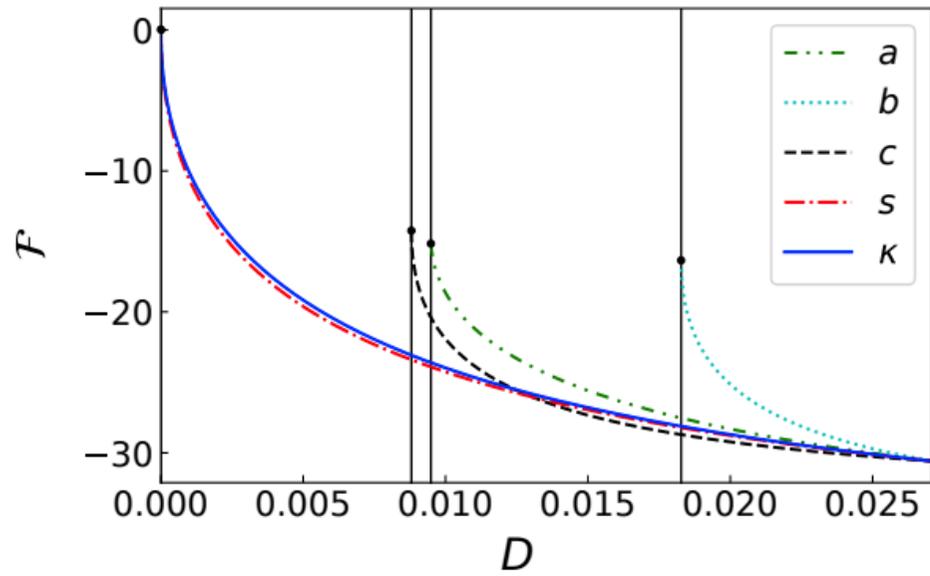
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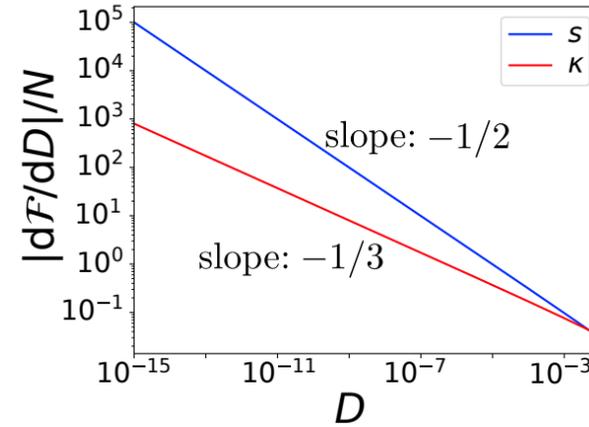
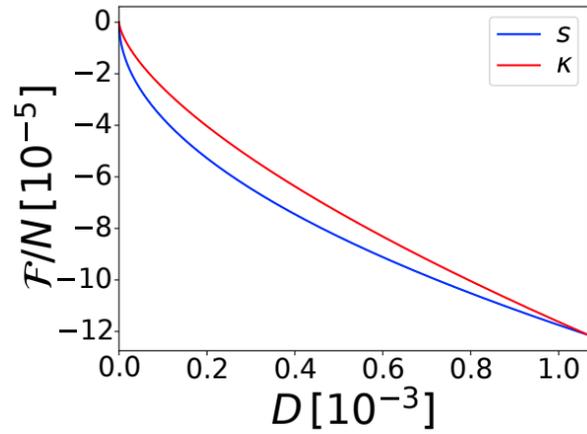
e. g. different hopping processes,
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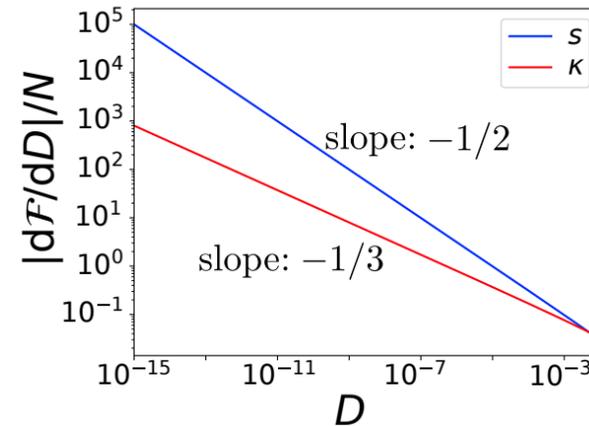
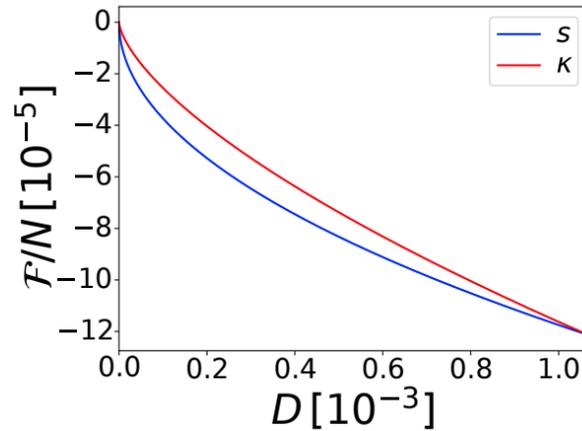


$$\Rightarrow \frac{d\mathcal{F}}{d(\text{dist}(\mathbf{n}, \partial\Delta))} \propto -\frac{1}{\sqrt{\text{dist}(\mathbf{n}, \partial\Delta)}}$$

Dilute Bose gas in 3D:



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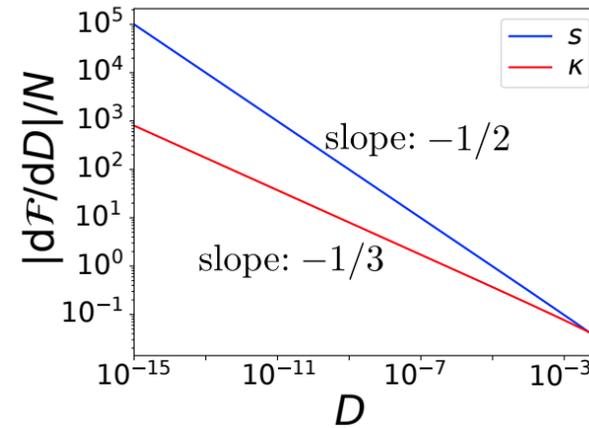
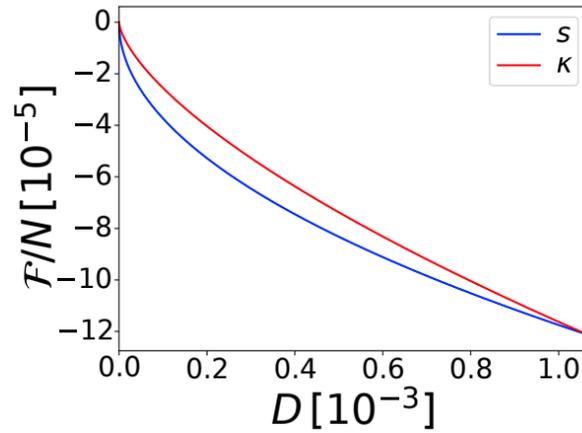


Charged Bose gas in 3D: (+ uniform background charge)

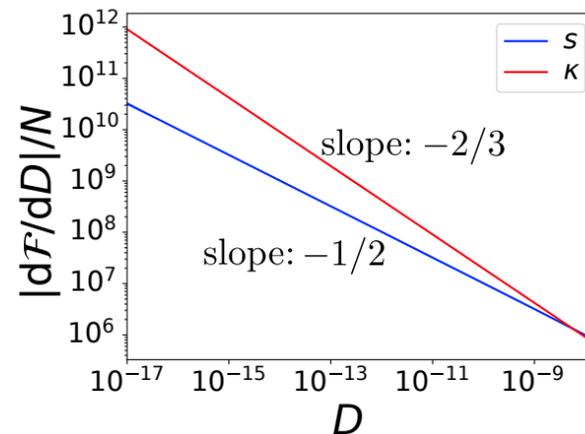
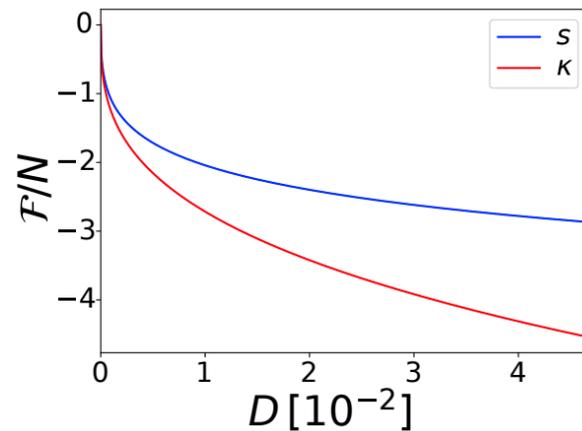
- $W_0 = 0, \quad W_{\mathbf{p}} = \frac{4\pi e^2}{p^2} \quad \forall \mathbf{p} \neq \mathbf{0}$
- Bogoliubov theory becomes exact in the high-density limit

[L. L. Foldy, Phys. Rev. **124**, 649-651 (1961),
E. H. Lieb, J. Solovej, Comm. Math. Phys. **217**, 127-163 (2001)]

Dilute Bose gas in 3D:



Charged Bose gas in 3D: (+ uniform background charge)



Summary

- RDMFT potentially ideal approach to describe BEC

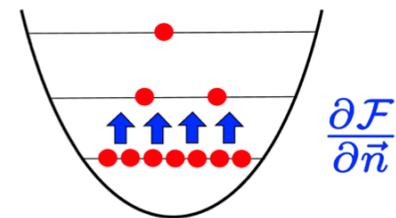
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Summary

- RDMFT potentially ideal approach to describe BEC
- Derivation of the universal functional in the Bogoliubov regime
- Gradient of \mathcal{F} diverges repulsively in the regime of complete BEC
 - ⇒ Novel concept: Universal Bose-Einstein force
 - ⇒ Most fundamental explanation of quantum depletion
 - ⇒ Bosonic analogue of fermionic exchange force

Bose-Einstein force



[C. Schilling, R. Schilling, Phys. Rev. Lett. **122**, 013001 (2019)]

Outlook

- Generalization to excited states

J. Liebert, C. Schilling, An exact one-particle theory of bosonic excitations: From a generalized Hohenberg-Kohn theorem to convexified N-representability, arXiv:2204.12715 (2022),

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Experimental visualization of BEC force?

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Mathematical rigorous derivations of \mathcal{F} and its diverging gradient

(Inspired by the work of E. H. Lieb, R. Seiringer, P. Pickl, ...)

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Derivation of more advanced functionals

Schilling group: Theoretical Quantum Physics



Thank you!

References:

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7. J. Liebert, C. Schilling, arXiv:2210.00964 (2022)