Formation of Selfbound States in a One-Dimensional Nuclear Model – An RG based Density Functional Study

Sandra Kemler, Martin Pospiech and Jens Braun

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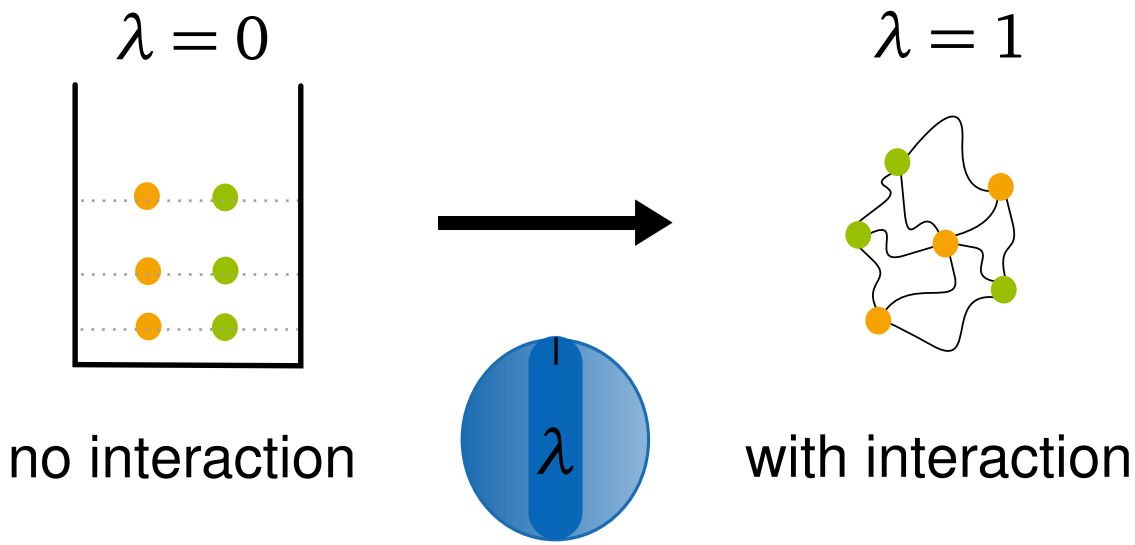

[S. Kemler and J. Braun, *2013*, *J. Phys. G: Nucl. Part. Phys.*]
[S. Kemler, M. Pospiech and J. Braun, *arxiv:1606.04388*]

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Hohenberg-Kohn Theorem

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- one-to-one correspondence between the wave functions and the density of a system [Hohenberg and Kohn, *1964*]

$$\left\langle \Psi[\rho_{\mathrm{gs}}] \left| \hat{\mathrm{O}} \right| \Psi[\rho_{\mathrm{gs}}] \right\rangle = \mathrm{O}[\rho_{\mathrm{gs}}]$$

- energy functional:

$$E_V[\rho] = E_{\mathrm{HK}}[\rho] + \int \mathrm{d}^3x \; V(x)\rho(x)$$

- theorem provides no recipe for the computation of E_{HK}

- take global ansatz for the energy density functional
- standard strategies:
  - solve Kohn-Sham equations selfconsistently
  - fit parameters of the functional to predict other nuclei [M. Kortelainen et. al., *2015*, *JPS Conf. Proc.*]

Hohenberg-Kohn Theorem

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- theorem provides no recipe for the computation of E_{HK}

- goal: calculate energy functional systematically from microscopic interactions

One-Dimensional Nuclear Model

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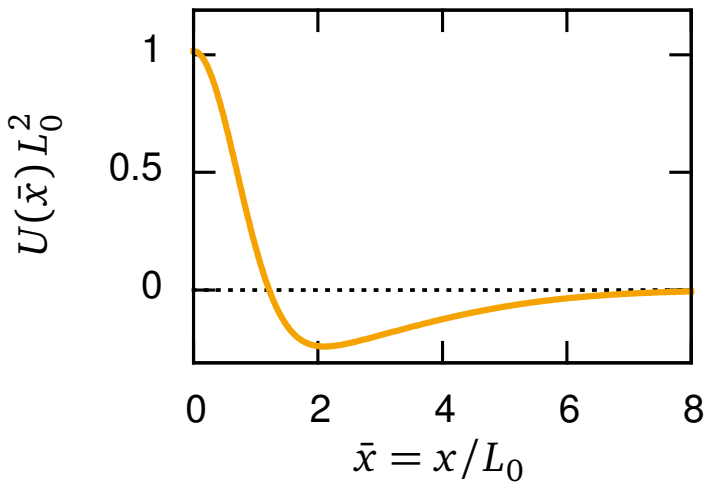
- ultimate goal: study realistic nuclei using short-range repulsive and long-range attractive interaction
- here: study simplified model of fermions with the following 2-body potential:

$$U(x) = \frac{g}{\sigma_1\sqrt{\pi}}\,\mathrm{e}^{\frac{-x^2}{\sigma_1^2}} - \frac{g}{\sigma_2\sqrt{\pi}}\,\mathrm{e}^{\frac{-x^2}{\sigma_2^2}}$$

with $L_0 \equiv \sigma_1 = 0.2$, $\sigma_2 = 4\,L_0$ and $g = 2.4/L_0$

[C. Alexandrou, J. Myczkowski and J. W. Negele, *1989*]



- parameter choice ensures that the one-dimensional saturation properties correspond to empirical three-dimensional properties in nuclear physics

One-Dimensional Model: Identical Fermions in a Box

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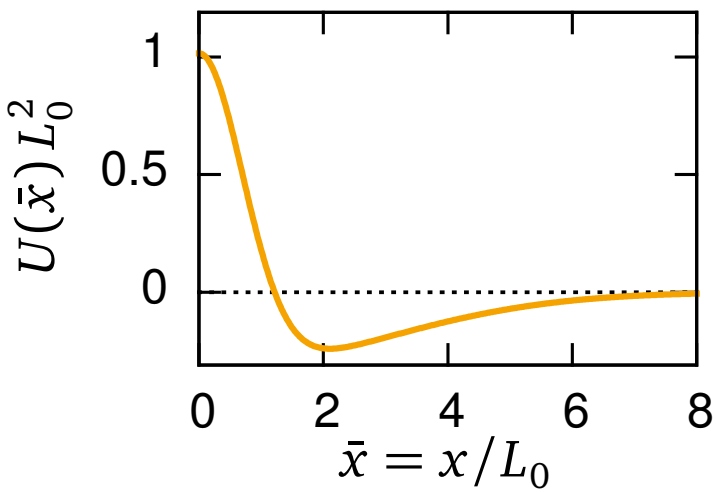
- classical action:

$$S = \int_\tau \int_x \psi^*(\tau,x)\left[\partial_\tau - \frac{1}{2}\partial_x^2\right]\psi(\tau,x) + \frac{1}{2}\int_\tau \int_x \int_y \psi^*(\tau,x)\,\psi^*(\tau,y)\,U(x-y)\,\psi(\tau,y)\,\psi(\tau,x)$$

- interaction:

$$U(x) = \frac{g}{\sigma_1\sqrt{\pi}}\,\mathrm{e}^{\frac{-x^2}{\sigma_1^2}} - \frac{g}{\sigma_2\sqrt{\pi}}\,\mathrm{e}^{\frac{-x^2}{\sigma_2^2}}$$



One-Dimensional Model: Identical Fermions in a Box

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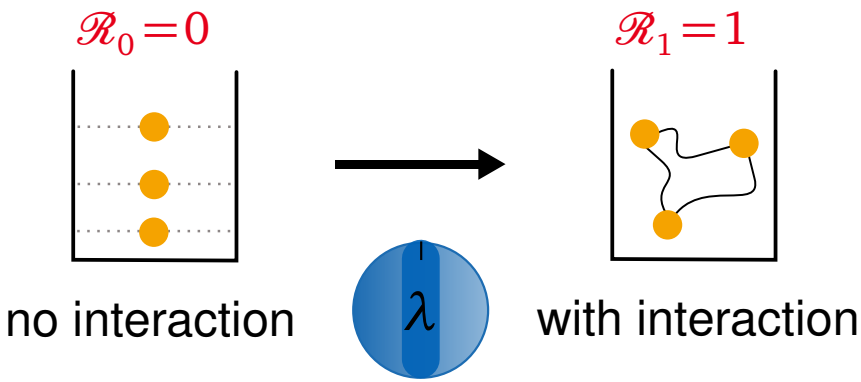
- idea: introduce control parameter λ:

$$S_\lambda = \int_\tau \int_x \psi^*(\tau,x)\left[\partial_\tau - \frac{1}{2}\partial_x^2\right]\psi(\tau,x)$$
$$+ \frac{1}{2}\int_\tau \int_x \int_y \psi^*(\tau,x)\,\psi^*(\tau,y)\,U(x-y)\,\mathscr{R}_\lambda(\tau,x,y)\,\psi(\tau,y)\,\psi(\tau,x)$$



- introduce a box with extent L to localize fermions in the non-interacting limit
- general form of $\mathscr{R}$ is at our disposal (e.g. to regularize the theory in 3d)
- for convenience we choose for 1d: $\mathscr{R} = \lambda$

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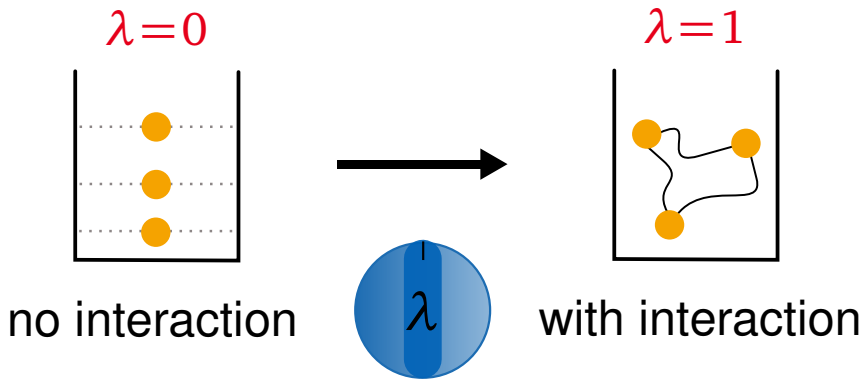

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Set up

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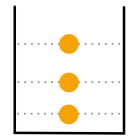
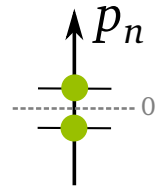
- starting point of the RG flow is a system of confined but non-interacting fermions



- anti-periodic boundary conditions for even particle numbers

$$p_n = (2n+1)\,\pi/L$$



- periodic boundary conditions for odd particle numbers

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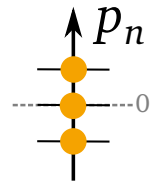

- density-correlation functions obey periodic boundary conditions in any case

- interaction is translation invariant in the continuum
- here: for convenience, we impose periodicity of the interaction also in the box

One-Dimensional Model: Identical Fermions in a Box

[J. Polonyi and K. Sailer, *2002, Phys. Rev. B*]
[A. Schwenk and J. Polonyi, *arxiv:nucl-th/0403011*]
[S. Kemler and J. Braun, *2013, J. Phys. G: Nucl. Part. Phys.*]

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- partition function:

$$Z_\lambda[J] = \int \mathscr{D}\psi^* \mathscr{D}\psi \;\; \mathrm{e}^{-S_\lambda + \int_\tau \int_x J(\tau,x)\psi^*(\tau,x)\psi(\tau,x)} \equiv \mathrm{e}^{W_\lambda[J]}$$

- exact flow equation:

$$\partial_\lambda W_\lambda[J] = -\frac{1}{2}\left[\frac{\delta W_\lambda}{\delta J}\cdot U \cdot \frac{\delta W_\lambda}{\delta J} + \mathrm{Tr}\, U \cdot \left(\frac{\delta^2 W_\lambda}{\delta J \delta J} - \frac{\delta W_\lambda}{\delta J}\cdot \mathbb{1}\right)\right]$$

- effective action (density functional):

$$\Gamma_\lambda[\rho] = \sup_J \left\{-W_\lambda[J] + \int_\tau \int_x J(\tau,x)\psi^*(\tau,x)\psi(\tau,x)\right\}$$

Flow Equations

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[S. Kemler, M. Pospiech and J. Braun, *arxiv:1606.04388*]

- expand density functional in terms of density-correlation functions
- obtain flow equations for density-correlation functions and energy:

$$\partial_\lambda E_{\mathrm{gs},\lambda} = \frac{1}{2}\rho_{\mathrm{gs},\lambda}\cdot U\cdot\rho_{\mathrm{gs},\lambda} + \frac{1}{2}\operatorname{Tr} U\cdot\left(G^{(2)}_\lambda - \rho_{\mathrm{gs},\lambda}\cdot\mathbb{1}\right)$$

$$\partial_\lambda \rho_{\mathrm{gs},\lambda} = -\rho_{\mathrm{gs},\lambda}\cdot U\cdot G^{(2)}_\lambda - \frac{1}{2}\operatorname{Tr} U\cdot\left(G^{(3)}_\lambda - G^{(2)}_\lambda\cdot\mathbb{1}\right)$$

$$\partial_\lambda G^{(2)}_\lambda = -G^{(2)}_\lambda\cdot U\cdot G^{(2)}_\lambda - \rho_{\mathrm{gs},\lambda}\cdot U\cdot G^{(3)}_\lambda - \frac{1}{2}\operatorname{Tr} U\cdot\left(G^{(4)}_\lambda - G^{(3)}_\lambda\cdot\mathbb{1}\right)$$

- density: $\rho(\tau,x) = \langle\psi^*(\tau,x)\psi(\tau,x)\rangle$
- density-density correlator: $G^{(2)}_\lambda(\tau,x,y) \sim \langle\psi^*(\tau,x)\psi(\tau,x)\,\psi^*(0,y)\psi(0,y)\rangle$

Flow Equations

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- simplified flow equations for density-correlation functions and energy:

$$\partial_\lambda E_{\mathrm{gs},\lambda} = \frac{1}{2} n_{\mathrm{gs}} \cdot U \cdot n_{\mathrm{gs}} + \frac{1}{2} \operatorname{Tr} U \cdot \left(G^{(2)}_\lambda - n_{\mathrm{gs}} \cdot \mathbb{1} \right)$$

$$\partial_\lambda \rho_{\mathrm{gs},\lambda} = 0$$

$$\partial_\lambda G^{(2)}_\lambda = - G^{(2)}_\lambda \cdot U \cdot G^{(2)}_\lambda - \frac{1}{2} \operatorname{Tr} U \cdot G^{(4)}_\lambda$$

- density: $\rho(\tau, x) = \langle \psi^*(\tau, x) \psi(\tau, x) \rangle$
- density-density correlator: $G^{(2)}_\lambda(\tau, x, y) \sim \langle \psi^*(\tau, x) \psi(\tau, x)\, \psi^*(0, y) \psi(0, y) \rangle$
- $n_{\mathrm{gs}} \equiv \rho_{\mathrm{gs},\lambda}(\tau, x) = N/L$ (not to be confused with the intrinsic density)

Flow Equations

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[S. Kemler, M. Pospiech and J. Braun, *arxiv:1606.04388*]

- leading order approximation: DFT-RG (LO)
  - use $G^{(2)}_{\lambda=0}$ in this flow equation

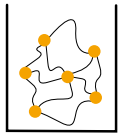
$$\partial_\lambda E_{\mathrm{gs},\lambda} = \frac{1}{2} n_{\mathrm{gs}} \cdot U \cdot n_{\mathrm{gs}} + \frac{1}{2} \mathrm{Tr}\, U \cdot \left(G^{(2)}_{\lambda=0} - n_{\mathrm{gs}} \cdot \mathbb{1} \right)$$

- next-to-leading order approximation: DFT-RG (NLO)
  - use $G^{(4)}_{\lambda=0}$ in these flow equations
  - introduce "Pauli-blocking function" $f_{\mathscr{P}}(\lambda)$
    to ensure Pauli principle in the truncated set of flow equations

$$\partial_\lambda E_{\mathrm{gs},\lambda} = \frac{1}{2} n_{\mathrm{gs}} \cdot U \cdot n_{\mathrm{gs}} + \frac{1}{2} \mathrm{Tr}\, U \cdot \left(G^{(2)}_{\lambda} - n_{\mathrm{gs}} \cdot \mathbb{1} \right)$$

$$\partial_\lambda G^{(2)}_{\lambda} = - G^{(2)}_{\lambda} \cdot U \cdot G^{(2)}_{\lambda} - \frac{1}{2} \mathrm{Tr}\, U \cdot f_{\mathscr{P}}(\lambda)\, G^{(4)}_{\lambda=0}$$

First Results
Perturbation Theory



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[S. Kemler, M. Pospiech and J. Braun, *arxiv:1606.04388*]

- extract perturbative results for any particle number from our DFT results
- for example: energy shifts for $L = 5L_0$:

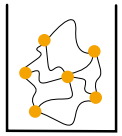
N	1	2	3	4	5	6	...
$\frac{\Delta E^{(1)}}{N}$ in $\frac{1}{L_0^2}$	0	-0.06209	-0.06752	-0.03788	0.00950	0.06628	...
$\frac{\Delta E^{(2)}}{N}$ in $\frac{1}{L_0^2}$	0	-0.00041	-0.00044	-0.00031	-0.00021	-0.00015	...

- agrees identically with conventional many-body perturbation theory

- no spurious fermion self-interactions
  - if we consider the flow equations order by order in the coupling constant
  - if we solve the infinite set of flow equations

  → guide the construction of truncations for our present framework

First Results
Fermions in a Box – Thermodynamic Limit



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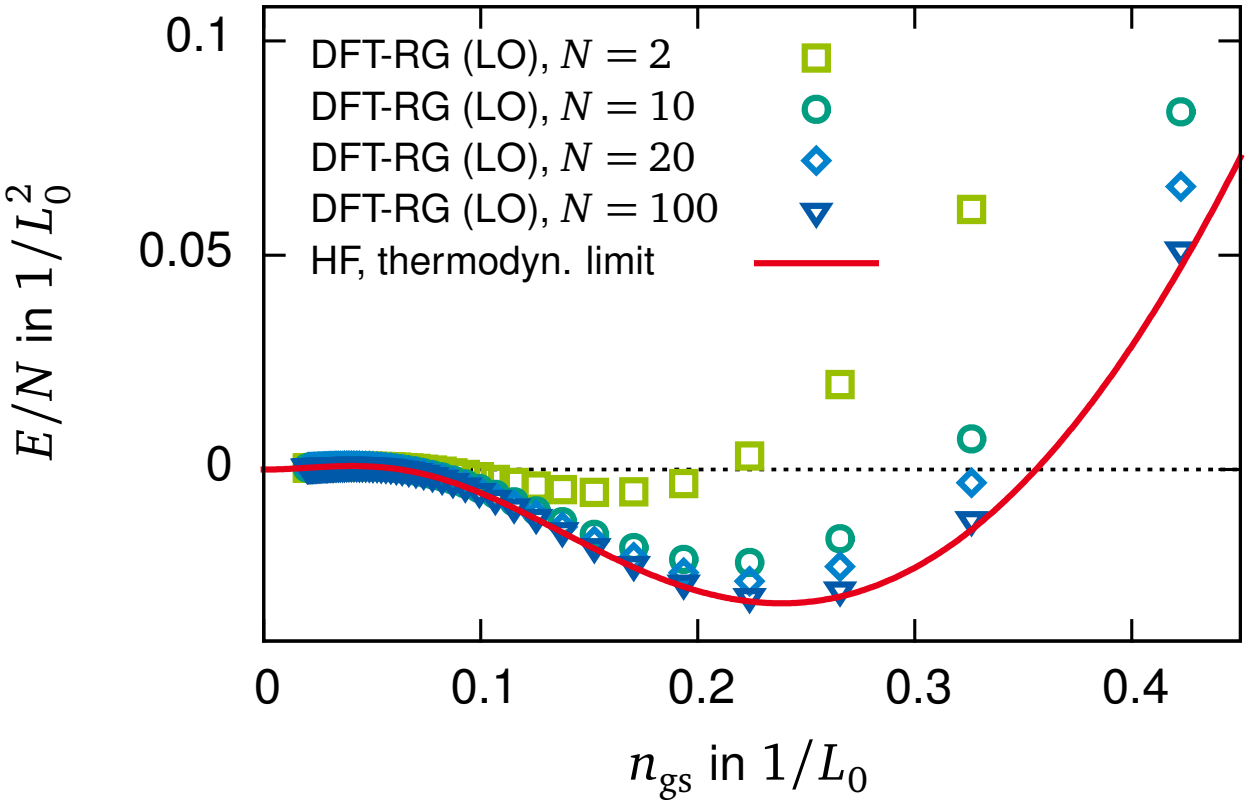
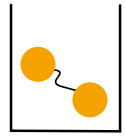


- energy obtained by DFT-RG (LO) corresponds to the Hartree-Fock approximation
- thermodynamic limit: $N \to \infty$ for fixed $n_{\mathrm{gs}} = N/L$

First Results
2 Fermions in a Box – Ground-State Energy



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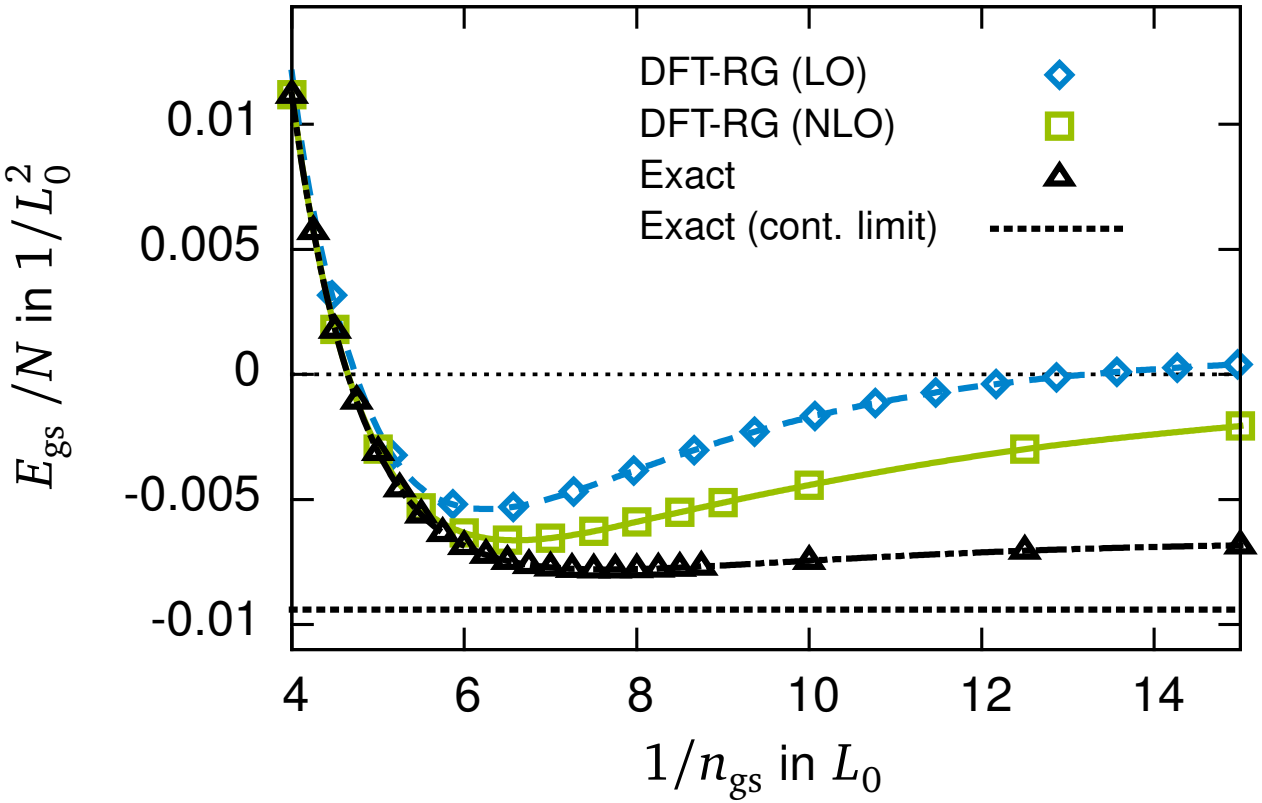

- full solution of the DFT equations (beyond perturbation theory)
- good agreement for small volumes or high densities (small $1/n_{gs}$)
- exact solution approaches the continuum limit (slowly) from above

First Results
2 Fermions in a Box – Relative Wave Function

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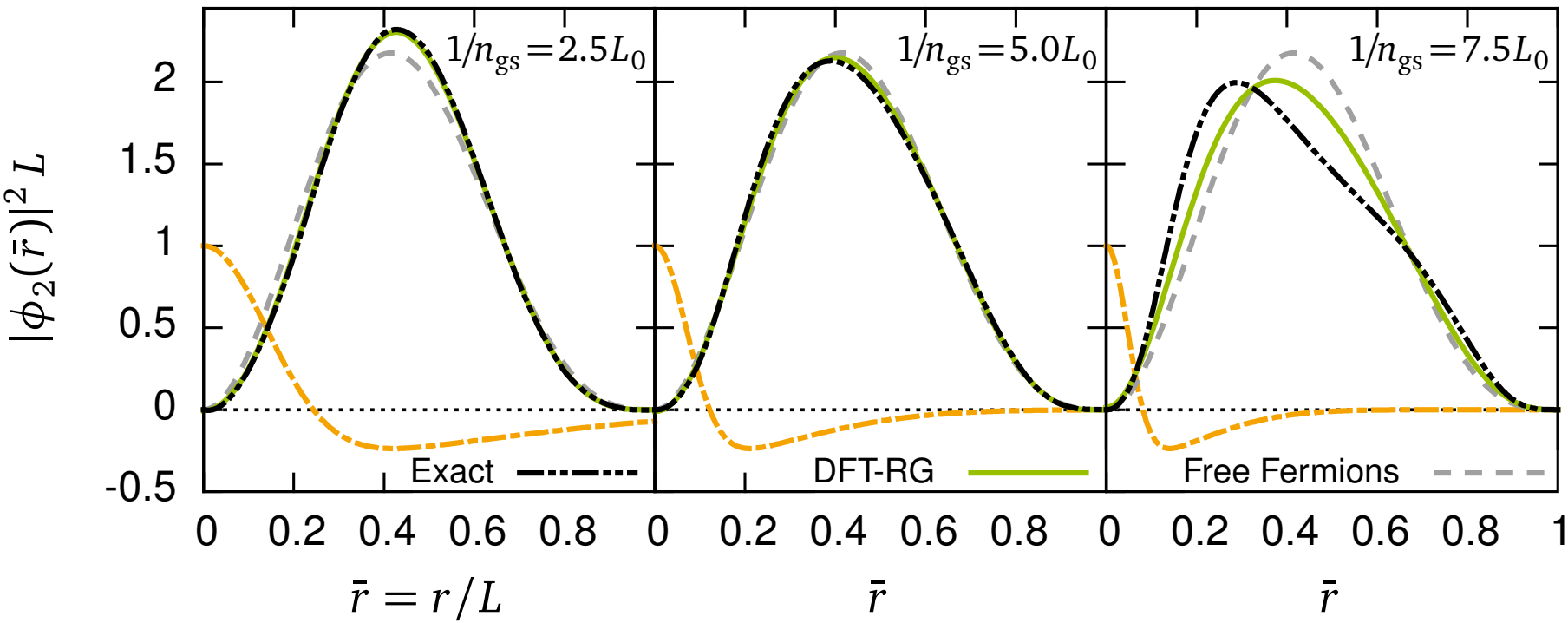
[S. Kemler, M. Pospiech and J. Braun, *arxiv:1606.04388*]



- absolute square of the wave-function $|\phi_2(\bar{r})|^2$ (intrinsic density) can be extracted from the density-density correlator:

$$|\Phi_{\mathrm{gs},\lambda}(x,y)|^2 = \frac{1}{2}\left(n_{\mathrm{gs}} n_{\mathrm{gs}} + G^{(2)}_{\lambda}(0,x,y) - n_{\mathrm{gs}}\delta(x-y)\right)$$

First Results
Fermions in a Box – Ground-State Energy

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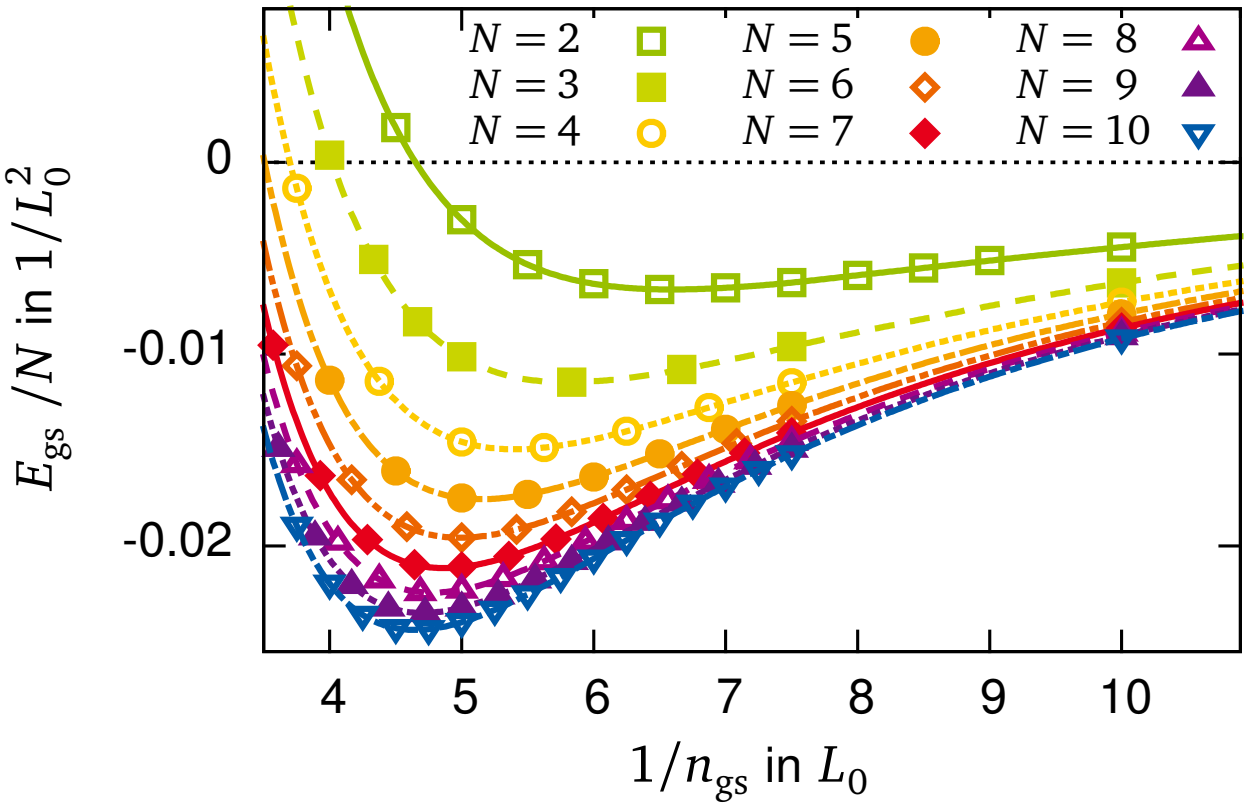
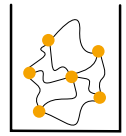


- results are similar on a qualitative level for all fermion numbers
- position of the minimum shifts to smaller $1/n_{\mathrm{gs}}$ for increasing N

First Results
Fermions in a Box – Continuum Limit



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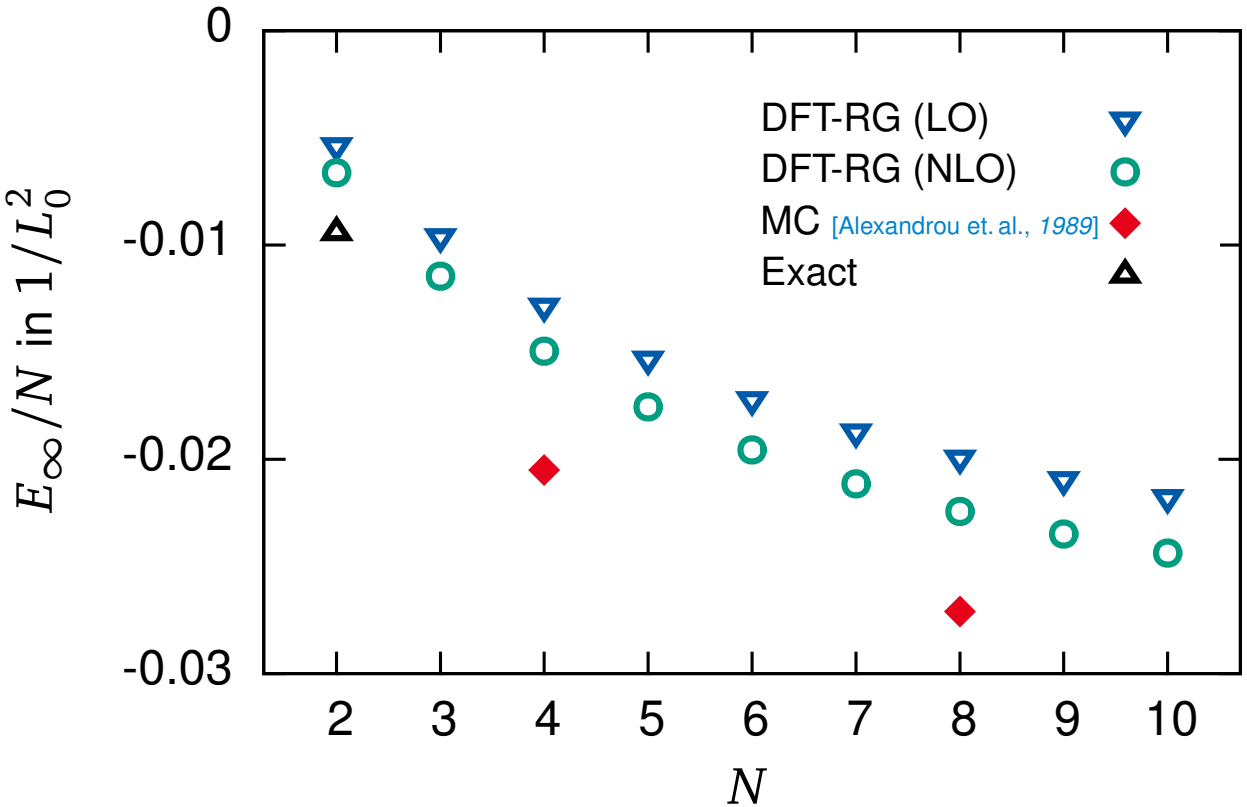

- estimate for the ground-state energy in the continuum limit: $E_\infty = \inf_L E(L)$
- DFT-RG (NLO) underestimates exact two-body result by about 30%
- DFT-RG (NLO) underestimates MC result by about 30%

Conclusions and Outlook

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Conclusions

- computation of ground state properties from microscopic interactions via the density functional is possible
- systematic expansion of the density functional in density-correlation functions
- very good results for small volumes or high densities (small $1/n_{\mathrm{gs}}$)

Outlook

- extract excited states from the time-dependent density-density correlator
- study fermions with spin (spin and/or mass imbalanced systems, ...)
- include higher order density-correlation functions
- extending the method to 3 dimensional systems
- long term: nuclei with realistic microscopic interactions