Formation of Selfbound States in One-Dimensional Models – an RG based Density Functional Study –

Martin Pospiech

Institut für Kernphysik, Technische Universität Darmstadt

with Sandra Kemler[1] and Jens Braun[1,2]

[1]TU Darmstadt, [2]ExtreMe Matter Institute EMMI, GSI

637. Wilhelm und Else Heraeus-Seminar: Understanding the LHC

Outline

TECHNISCHE UNIVERSITÄT DARMSTADT

Motivation

Hohenberg-Kohn Theorem

An RG Approach to Density Functional Theory

One-Dimensional Model Systems

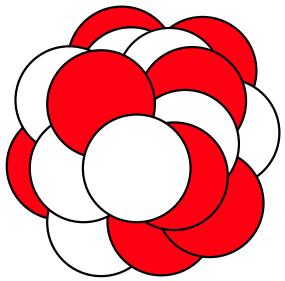
Conclusions

Motivation

TECHNISCHE UNIVERSITÄT DARMSTADT

Motivation

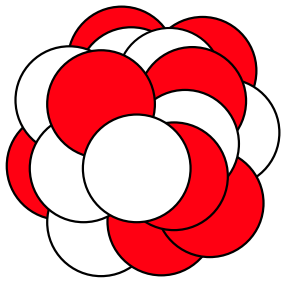
TECHNISCHE UNIVERSITÄT DARMSTADT



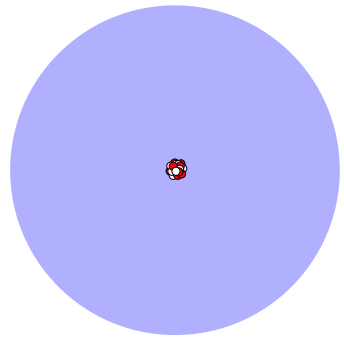
Nuclei

Motivation

TECHNISCHE UNIVERSITÄT DARMSTADT



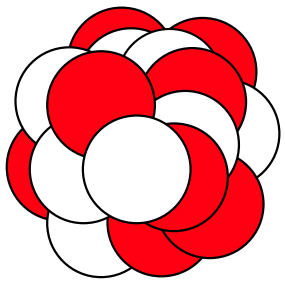
Nuclei



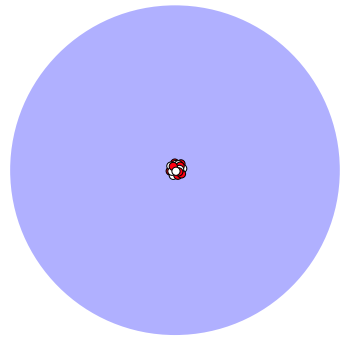
Atoms

Motivation

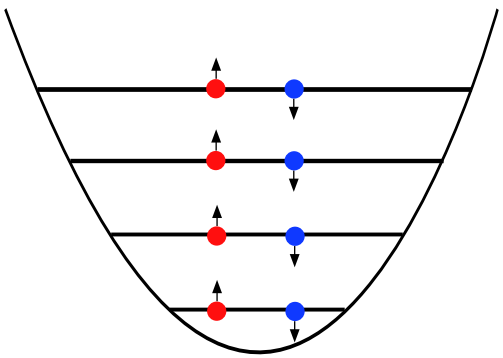
TECHNISCHE UNIVERSITÄT DARMSTADT

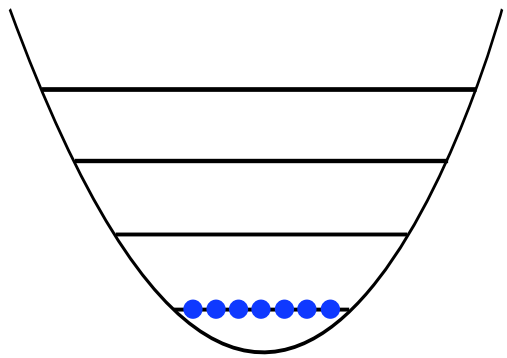


Nuclei



Atoms

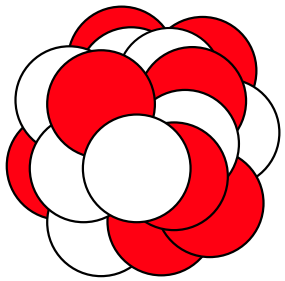




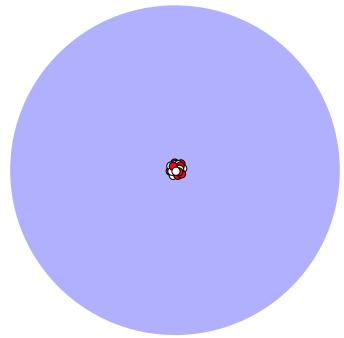
Ultracold Gases

Motivation

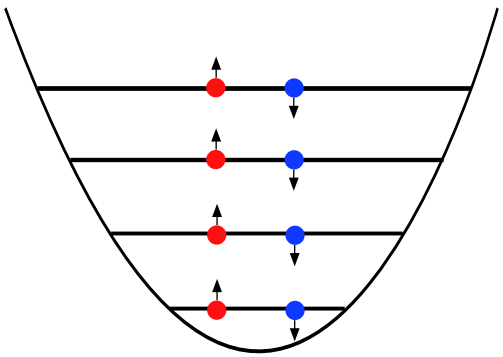
TECHNISCHE UNIVERSITÄT DARMSTADT

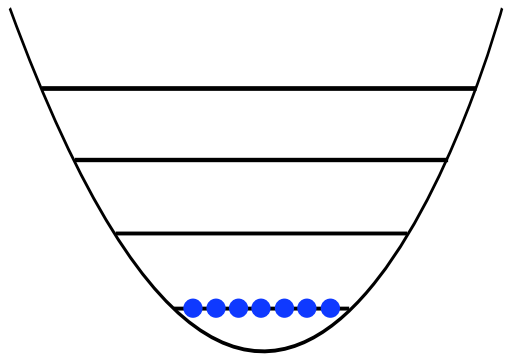


Nuclei

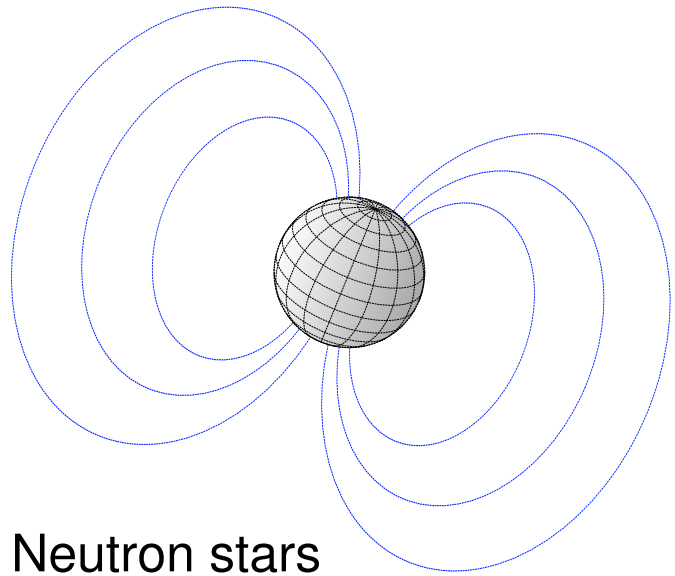


Atoms





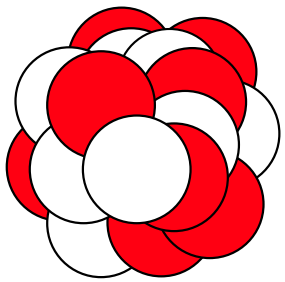
Ultracold Gases



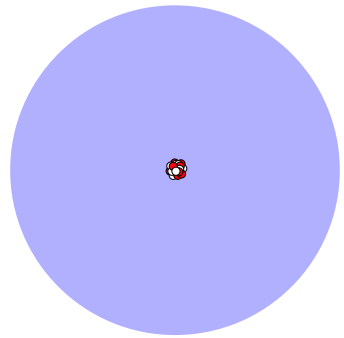
Neutron stars

Motivation

TECHNISCHE UNIVERSITÄT DARMSTADT



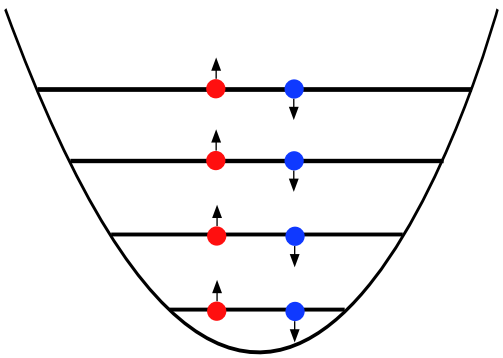
Nuclei

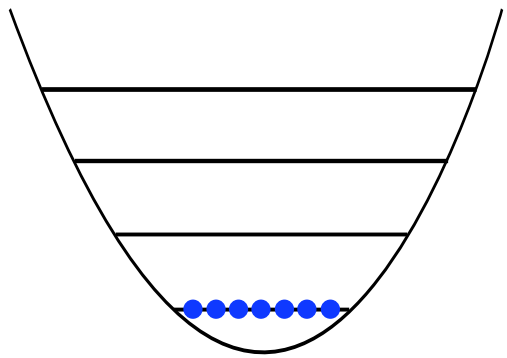


Atoms

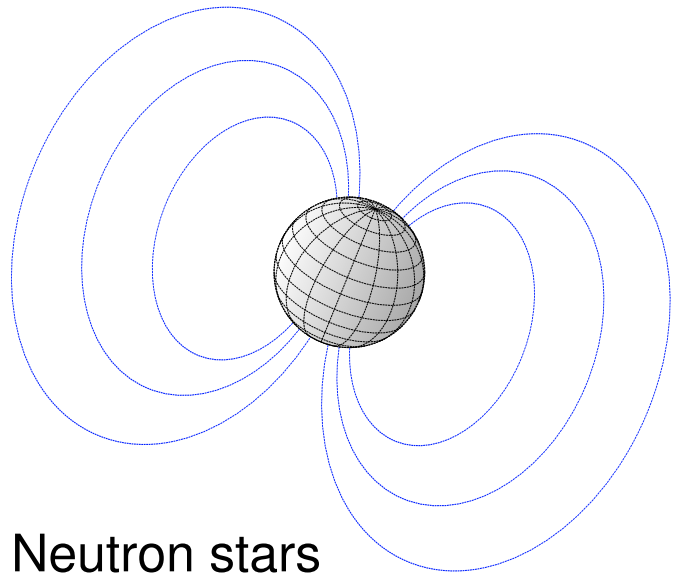
systems with many particles are difficult to solve

$\rightarrow$ density functional $O[\rho]$: density "good" degree of freedom ($3N \rightarrow 3$)





Ultracold Gases



Neutron stars

Hohenberg-Kohn Theorem

TECHNISCHE UNIVERSITÄT DARMSTADT

- HK: $\hat{O}$ can indeed be written as density functional:

$$O[\rho] = \langle \psi[\rho] | \hat{O} | \psi[\rho] \rangle \ .$$

P. Hohenberg und W. Kohn, Phys. Rev. 136, B864-B871 (1964)

Hohenberg-Kohn Theorem

TECHNISCHE UNIVERSITÄT DARMSTADT

- HK: $\hat{O}$ can indeed be written as density functional:

$$O[\rho] = \langle \psi[\rho] | \hat{O} | \psi[\rho] \rangle \ .$$

- e.g. energy functional: $E[\rho] = \langle \psi[\rho] | \hat{H} | \psi[\rho] \rangle$.

P. Hohenberg und W. Kohn, Phys. Rev. 136, B864-B871 (1964)

Hohenberg-Kohn Theorem

TECHNISCHE UNIVERSITÄT DARMSTADT

- HK: $\hat{O}$ can indeed be written as density functional:

$$O[\rho] = \langle \psi[\rho] | \hat{O} | \psi[\rho] \rangle \ .$$

- e.g. energy functional: $E[\rho] = \langle \psi[\rho] | \hat{H} | \psi[\rho] \rangle$.

- provides no recipe for computation:
  - nuclear physics: minimization of global ansatz for the energy density functional

P. Hohenberg und W. Kohn, Phys. Rev. 136, B864-B871 (1964)

Hohenberg-Kohn Theorem

TECHNISCHE UNIVERSITÄT DARMSTADT

- HK: $\hat{O}$ can indeed be written as density functional:

$$O[\rho] = \langle \psi[\rho] | \hat{O} | \psi[\rho] \rangle \ .$$

- e.g. energy functional: $E[\rho] = \langle \psi[\rho] | \hat{H} | \psi[\rho] \rangle$.

- provides no recipe for computation:
  - nuclear physics: minimization of global ansatz for the energy density functional

challenge: compute density functional from microscopic interactions

P. Hohenberg und W. Kohn, Phys. Rev. 136, B864-B871 (1964)

An RG Approach to Density Functional Theory

TECHNISCHE UNIVERSITÄT DARMSTADT

- start with partition function:

$$\mathcal{Z}_\lambda[J_\sigma] = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi \, \mathrm{e}^{-S_\lambda[\psi^\dagger,\psi]+\sum_\sigma \int_\tau \int_x J_\sigma(\tau,x)\,\left(\psi^\dagger_\sigma(\tau,x)\psi_\sigma(\tau,x)\right)}$$
$$\equiv \mathrm{e}^{W_\lambda[J_\sigma]}.$$

J. Polonyi und K. Sailer, Phys. Rev. B 66 155113 (2002) A. Schwenk und J. Polonyi nucl-th/0403011 (2004)

An RG Approach to Density Functional Theory

TECHNISCHE UNIVERSITÄT DARMSTADT

- start with partition function:

$$\mathcal{Z}_\lambda[J_\sigma] = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi \, e^{-S_\lambda[\psi^\dagger,\psi]+\sum_\sigma \int_\tau \int_x J_\sigma(\tau,x) \left(\psi^\dagger_\sigma(\tau,x)\psi_\sigma(\tau,x)\right)}$$
$$\equiv e^{W_\lambda[J_\sigma]} .$$

- flow parameter λ links free and interacting theory:

$$S \to S_\lambda .$$

J. Polonyi und K. Sailer, Phys. Rev. B 66 155113 (2002) A. Schwenk und J. Polonyi nucl-th/0403011 (2004)

An RG Approach to Density Functional Theory

TECHNISCHE UNIVERSITÄT DARMSTADT

- start with partition function:

$$\mathcal{Z}_\lambda[J_\sigma] = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi \, \mathrm{e}^{-S_\lambda[\psi^\dagger,\psi]+\sum_\sigma \int_\tau \int_x J_\sigma(\tau,x) \left(\psi^\dagger_\sigma(\tau,x)\psi_\sigma(\tau,x)\right)} \equiv \mathrm{e}^{W_\lambda[J_\sigma]} .$$

- flow parameter λ links free and interacting theory:

$$S \to S_\lambda .$$

- two-particle point-irreducible (2PPI) ansatz: $\psi^\dagger_\sigma(\tau,x)\psi_\sigma(\tau,x)$.

J. Polonyi und K. Sailer, Phys. Rev. B 66 155113 (2002) A. Schwenk und J. Polonyi nucl-th/0403011 (2004)

An RG Approach to Density Functional Theory

TECHNISCHE UNIVERSITÄT DARMSTADT

- "classical" action:

$$S_\lambda = \sum_\sigma \int_x \int_\tau \Psi^\dagger_\sigma(\tau, x) \left(\partial_\tau - \frac{1}{2}\partial_x^2 + V(x) \right) \Psi_\sigma(\tau, x)$$
$$+ \frac{\lambda}{2} \sum_{\sigma,\sigma'} \int_x \int_{x'} \int_\tau \int_{\tau'} \Psi^\dagger_\sigma(\tau, x) \Psi^\dagger_{\sigma'}(\tau', x') U_{\sigma\sigma'} \left(\tau, \tau', x, x'\right) \Psi_{\sigma'}(\tau', x') \Psi_\sigma(\tau, x) \,.$$

An RG Approach to Density Functional Theory

TECHNISCHE UNIVERSITÄT DARMSTADT

- "classical" action:

$$S_\lambda = \sum_\sigma \int_x \int_\tau \Psi^\dagger_\sigma(\tau, x) \left(\partial_\tau - \frac{1}{2}\partial_x^2 + V(x) \right) \Psi_\sigma(\tau, x)$$

$$+ \frac{\lambda}{2} \sum_{\sigma,\sigma'} \int_x \int_{x'} \int_\tau \int_{\tau'} \Psi^\dagger_\sigma(\tau, x) \Psi^\dagger_{\sigma'}(\tau', x') U_{\sigma\sigma'} \left(\tau, \tau', x, x'\right) \Psi_{\sigma'}(\tau', x') \Psi_\sigma(\tau, x) \,.$$

$$\boxed{W_\lambda = \ln \mathcal{Z}_\lambda}$$

$$\partial_\lambda \downarrow$$

An RG Approach to Density Functional Theory

TECHNISCHE UNIVERSITÄT DARMSTADT

- "classical" action:

$$S_\lambda = \sum_\sigma \int_x \int_\tau \Psi^\dagger_\sigma(\tau, x) \left(\partial_\tau - \frac{1}{2}\partial_x^2 + V(x) \right) \Psi_\sigma(\tau, x)$$
$$+ \frac{\lambda}{2} \sum_{\sigma,\sigma'} \int_x \int_{x'} \int_\tau \int_{\tau'} \Psi^\dagger_\sigma(\tau, x) \Psi^\dagger_{\sigma'}(\tau', x') U_{\sigma\sigma'} \left(\tau, \tau', x, x'\right) \Psi_{\sigma'}(\tau', x') \Psi_\sigma(\tau, x) \,.$$

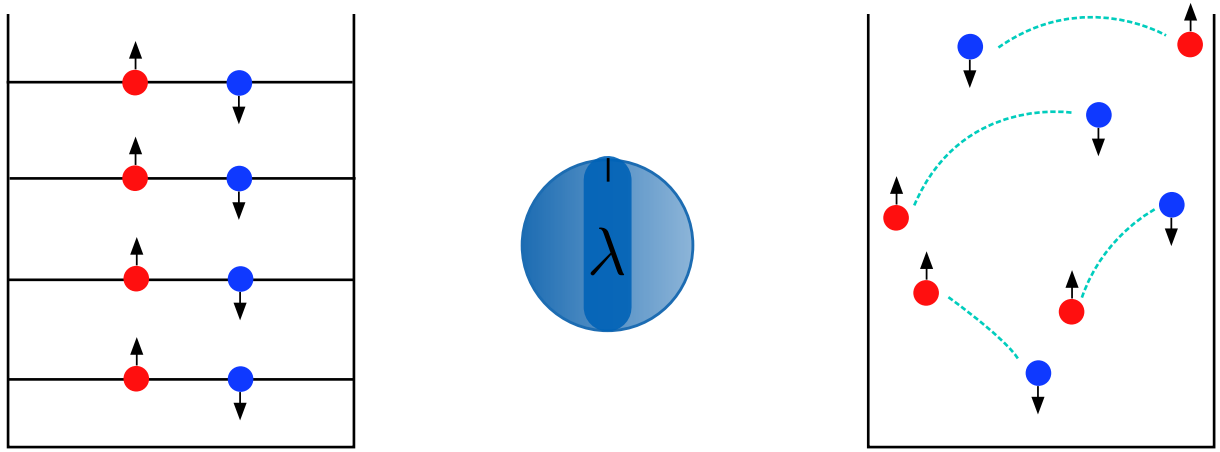
$$\boxed{W_\lambda = \ln \mathcal{Z}_\lambda}$$

$$\partial_\lambda \downarrow$$

$$\boxed{\partial_\lambda W_\lambda = -\frac{1}{2}\, \rho_\sigma \cdot U_{\sigma\sigma'} \cdot \rho_{\sigma'} - \frac{1}{2} \mathrm{Tr} \left[U_{\sigma\sigma'} \cdot \left(W^{(2)}_{\sigma'\sigma} + \rho_{\sigma'} \cdot \mathbb{1}_{(\sigma,x)} \right) \right] .}$$

An RG Approach to Density Functional Theory

TECHNISCHE UNIVERSITÄT DARMSTADT



$$\partial_\lambda W_\lambda = -\frac{1}{2}\,\rho_\sigma \cdot U_{\sigma\sigma'} \cdot \rho_{\sigma'} - \frac{1}{2}\,\mathrm{Tr}\left[U_{\sigma\sigma'} \cdot \left(W^{(2)}_{\sigma'\sigma} + \rho_{\sigma'} \cdot \mathbb{1}_{(\sigma,x)}\right)\right] .$$

An RG Approach to Density Functional Theory

TECHNISCHE UNIVERSITÄT DARMSTADT

- expanding $W_\lambda[J]$ about $J = 0$:

$$W_\lambda\left[J_\sigma\right] = W_\lambda[0] + \sum_\sigma \int_{\tau,x} W^{(1)}_{\lambda,\sigma}[0](\tau, x)\; J_\sigma(\tau, x) + \mathcal{O}\left({J_\sigma}^2\right) \; .$$

An RG Approach to Density Functional Theory

TECHNISCHE UNIVERSITÄT DARMSTADT

- expanding $W_\lambda[J]$ about $J = 0$:

$$W_\lambda[J_\sigma] = W_\lambda[0] + \sum_\sigma \int_{\tau,x} W^{(1)}_{\lambda,\sigma}[0](\tau, x)\, J_\sigma(\tau, x) + \mathcal{O}\left(J_\sigma^2\right) .$$

- expansion in n-density correlation functions

An RG Approach to Density Functional Theory

TECHNISCHE UNIVERSITÄT DARMSTADT

- expanding $W_\lambda[J]$ about $J = 0$:

$$W_\lambda\left[J_\sigma\right] = W_\lambda[0] + \sum_\sigma \int_{\tau,x} W^{(1)}_{\lambda,\sigma}[0](\tau, x)\, J_\sigma(\tau, x) + \mathcal{O}\left(J_\sigma^{\,2}\right) .$$

- expansion in n-density correlation functions
- coefficients depend on flow parameter λ

An RG Approach to Density Functional Theory

TECHNISCHE UNIVERSITÄT DARMSTADT

- expanding $W_\lambda[J]$ about $J = 0$:

$$W_\lambda[J_\sigma] = W_\lambda[0] + \sum_\sigma \int_{\tau,x} W^{(1)}_{\lambda,\sigma}[0](\tau, x)\, J_\sigma(\tau, x) + \mathcal{O}\left(J_\sigma^2\right) .$$

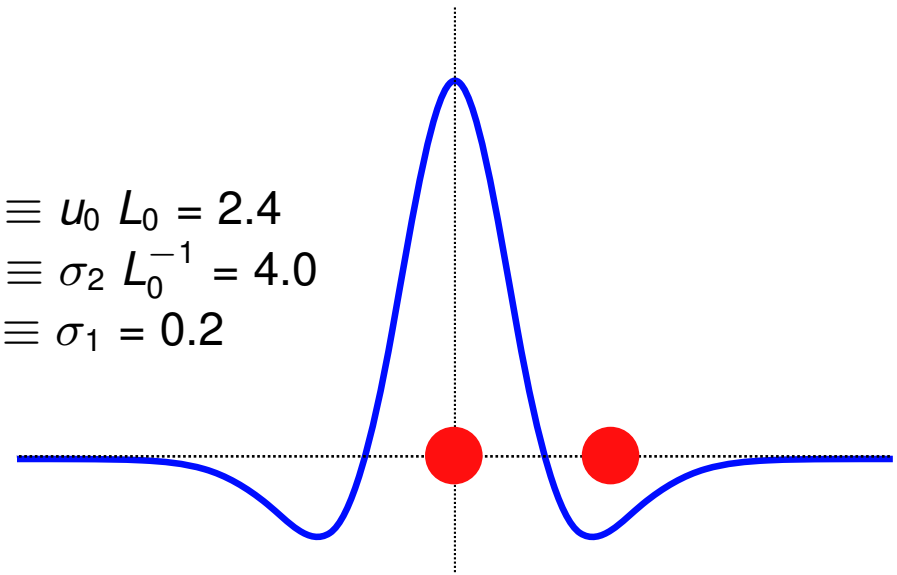
- expansion in n-density correlation functions
- coefficients depend on flow parameter λ

$$W_\lambda[0] \sim E_{\mathrm{gs},\lambda} ,$$
$$W^{(1)}_{\lambda,\sigma}[0](\tau, x) \sim \rho_{\mathrm{gs},\lambda,\sigma}(\tau, x) ,$$
$$W^{(2)}_{\lambda,\sigma\sigma'}[0](\tau, \tau', x, x') \sim G^{(2)}_{\lambda,\sigma\sigma'}(\tau, \tau', x, x') .$$

One-Dimensional Nuclear Model

TECHNISCHE UNIVERSITÄT DARMSTADT

$$\bar{u}_0 \equiv u_0 \, L_0 = 2.4$$
$$\bar{\sigma}_2 \equiv \sigma_2 \, L_0^{-1} = 4.0$$
$$L_0 \equiv \sigma_1 = 0.2$$

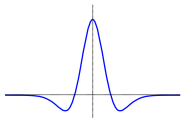


$$\frac{u_0}{\sigma_1 \sqrt{\pi}} \, e^{-\frac{(x_1 - x_2)^2}{\sigma_1^2}} - \frac{u_0}{\sigma_2 \sqrt{\pi}} \, e^{-\frac{(x_1 - x_2)^2}{\sigma_2^2}}$$

$\rightarrow$ parameter choice reflects saturation properties of real nuclei

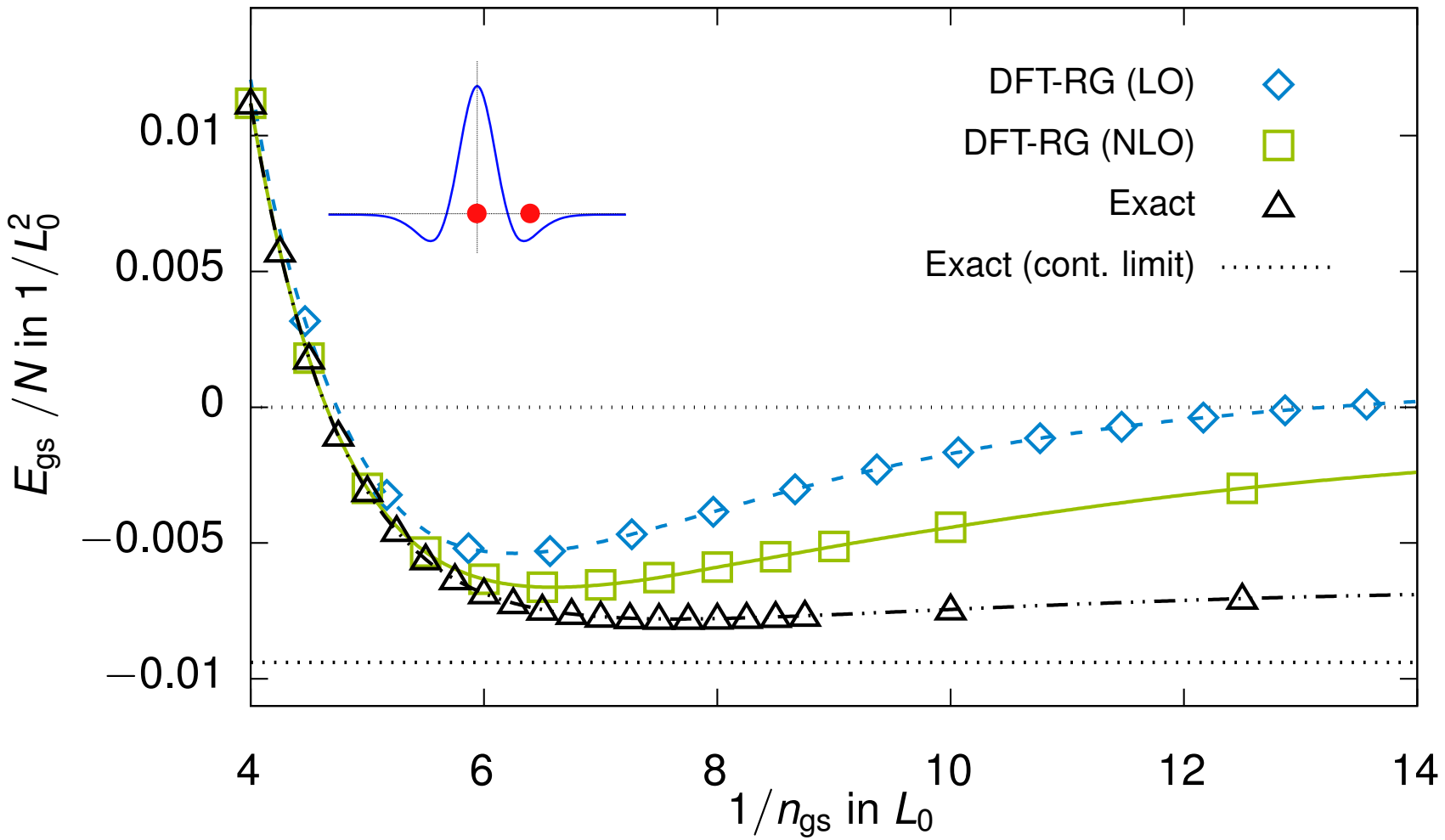
C. Alexandrou, J. Myczkowski und J. W. Negele, Phys. Rev. C 39, 1076 (1989)

One-Dimensional Nuclear Model:



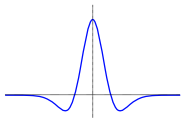
Two-Body

TECHNISCHE UNIVERSITÄT DARMSTADT



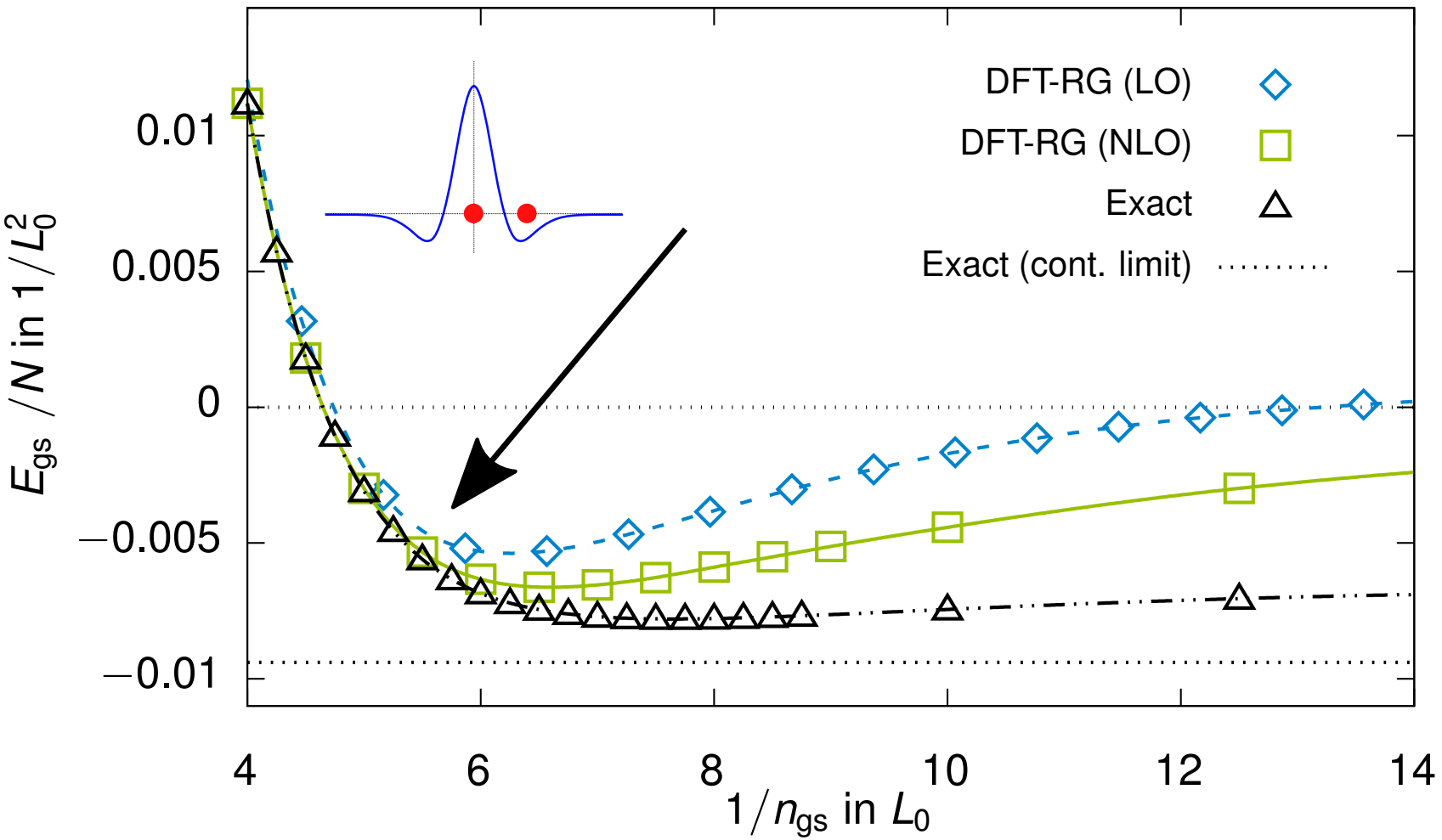
S. Kemler, MP, J. Braun, JPhys. G. Vol. 44 (2017)

One-Dimensional Nuclear Model:



Two-Body

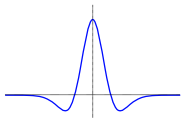
TECHNISCHE UNIVERSITÄT DARMSTADT



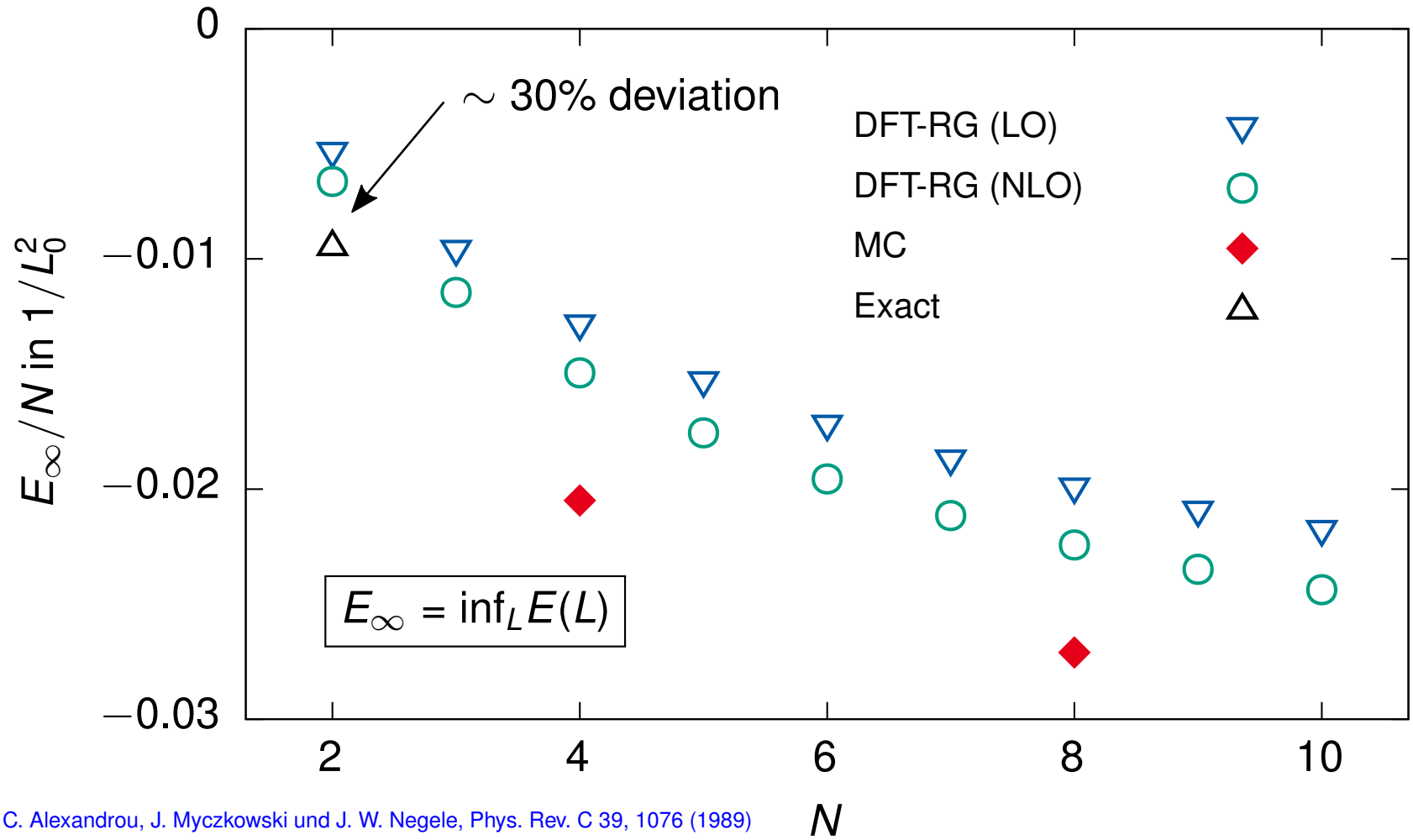
S. Kemler, MP, J. Braun, JPhys. G. Vol. 44 (2017)

One-Dimensional Nuclear Model:

From Two to Few

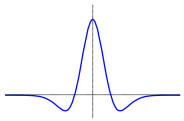


TECHNISCHE UNIVERSITÄT DARMSTADT



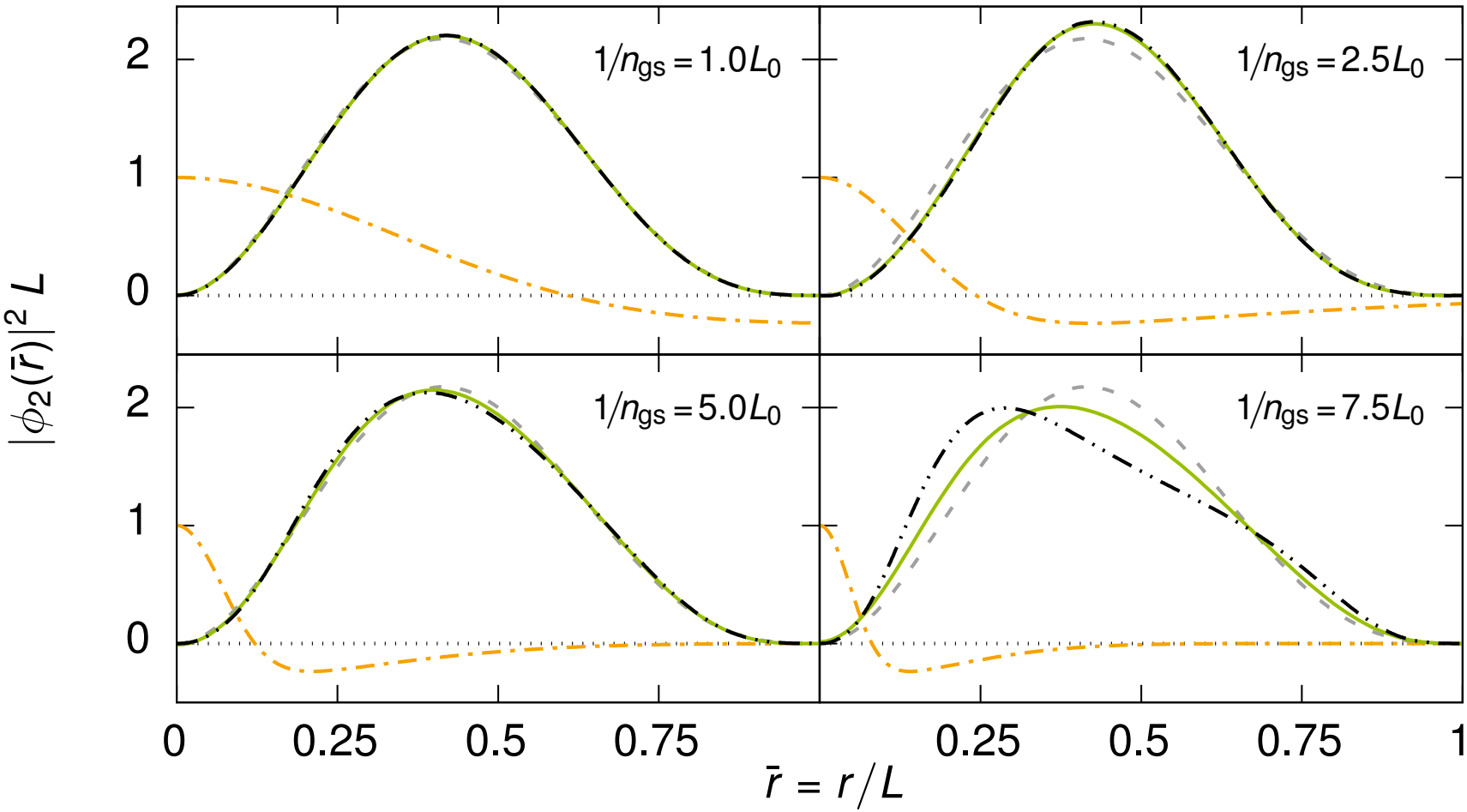
MC: C. Alexandrou, J. Myczkowski und J. W. Negele, Phys. Rev. C 39, 1076 (1989)
S. Kemler, MP, J. Braun, JPhys. G. Vol. 44 (2017)

One-Dimensional Nuclear Model:



Two-Body

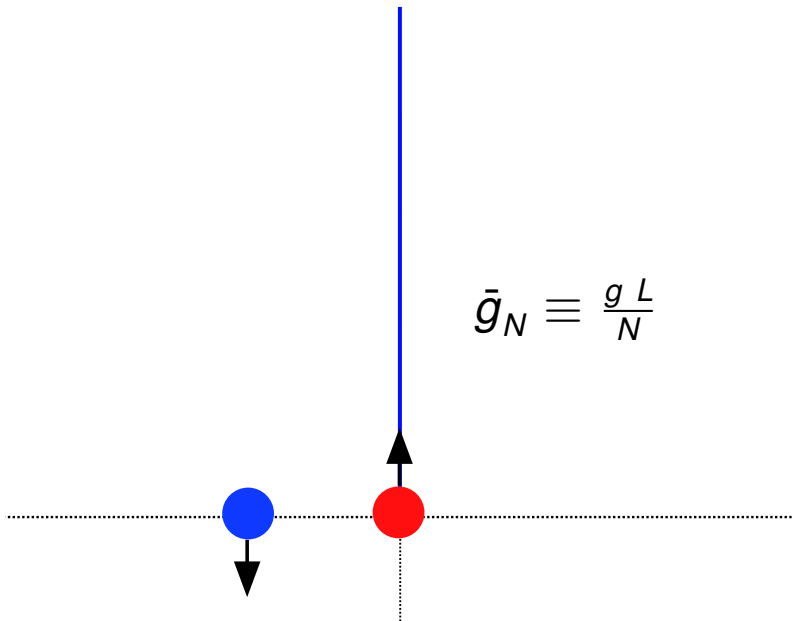
TECHNISCHE UNIVERSITÄT DARMSTADT



S. Kemler, MP, J. Braun, JPhys. G. Vol. 44 (2017)

One-Dimensional Ultracold Atoms

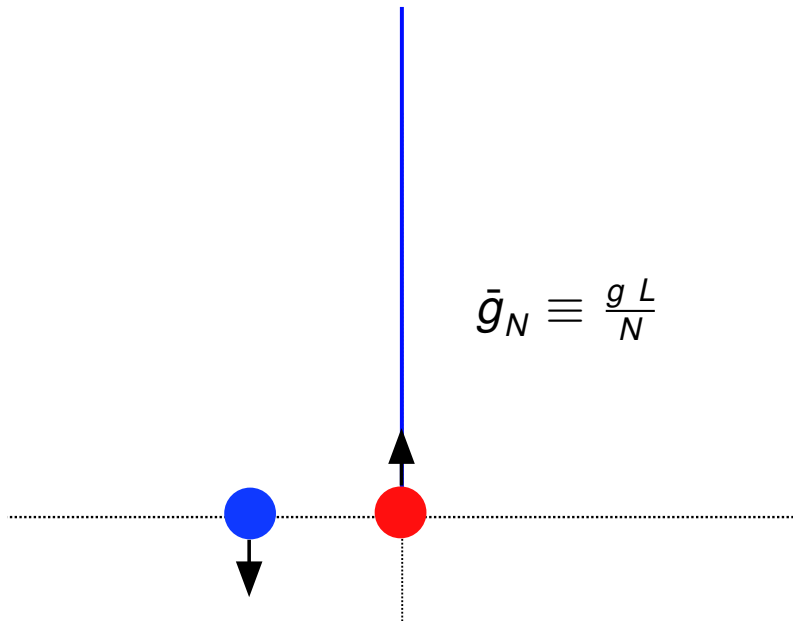
TECHNISCHE UNIVERSITÄT DARMSTADT



$$g\,\delta(x_1 - x_2)\,(1 - \delta_{\sigma\sigma'})$$

One-Dimensional Ultracold Atoms

TECHNISCHE UNIVERSITÄT DARMSTADT



$$g\,\delta(x_1 - x_2)\,(1 - \delta_{\sigma\sigma'})$$

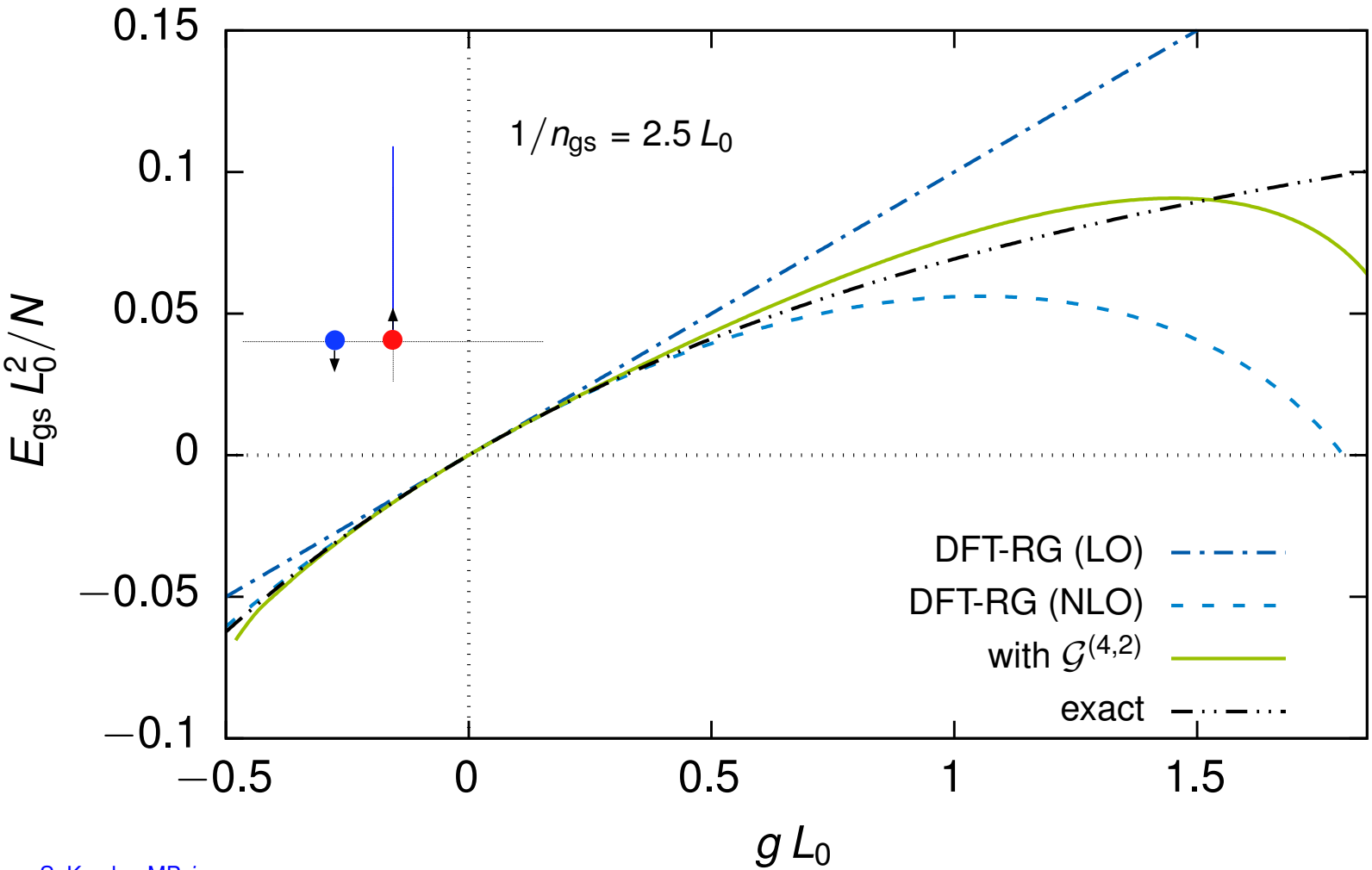
experimentally accessible!

$\longrightarrow$ G. Zürn et al. PRL 108, 075303 (2012)

One-Dimensional Ultracold Atoms:

Two-Body

TECHNISCHE UNIVERSITÄT DARMSTADT

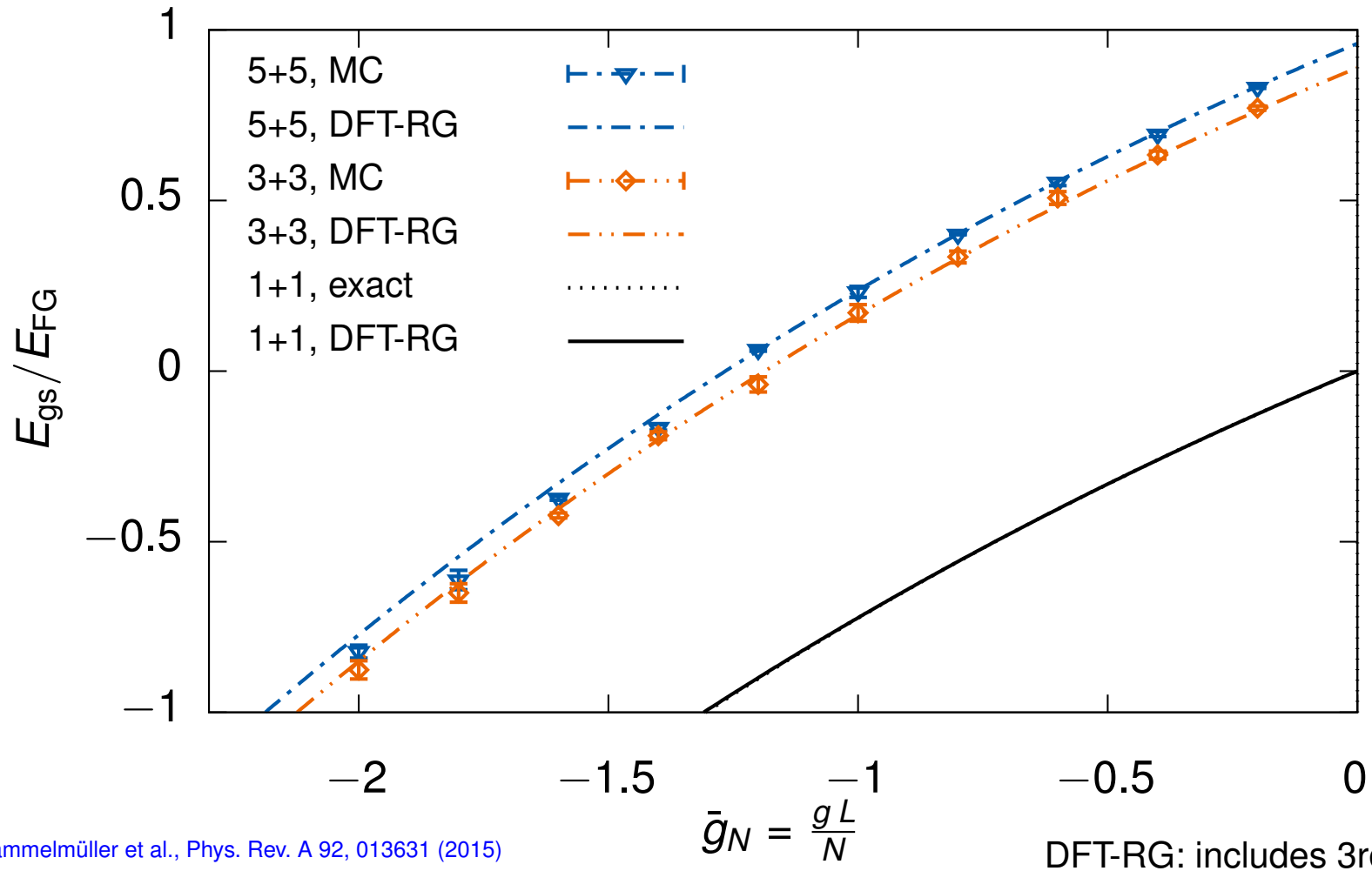


J. Braun, S. Kemler, MP, *in prep. . .*

One-Dimensional Ultracold Atoms:

Few-Body

TECHNISCHE UNIVERSITÄT DARMSTADT



MC: L. Rammelmüller et al., Phys. Rev. A 92, 013631 (2015)
J. Braun, S. Kemler, MP, *in prep. . .*

DFT-RG: includes 3rd order PT

Conclusions

TECHNISCHE UNIVERSITÄT DARMSTADT

- constructive scheme for density functionals from microscopic interactions:

$$\mathcal{Z}_\lambda \sim \int \mathcal{D}\psi^\dagger \mathcal{D}\psi \, e^{-S_\lambda + J\cdot(\psi^\dagger \psi)} \quad \longrightarrow \quad \partial_\lambda W_\lambda = \ldots \quad \longrightarrow \quad E_{gs}, \rho_{gs}, G^{(2)}$$

Conclusions

TECHNISCHE UNIVERSITÄT DARMSTADT

- constructive scheme for density functionals from microscopic interactions:

$$\mathcal{Z}_\lambda \sim \int \mathcal{D}\psi^\dagger \mathcal{D}\psi \, e^{-S_\lambda + J\cdot(\psi^\dagger \psi)} \quad \longrightarrow \quad \partial_\lambda W_\lambda = \ldots \quad \longrightarrow \quad E_{gs}, \rho_{gs}, G^{(2)}$$

- computation of n-density correlation functions $\langle \rho(x_1)\rho(x_2)\ldots \rangle$

Conclusions

TECHNISCHE UNIVERSITÄT DARMSTADT

- constructive scheme for density functionals from microscopic interactions:

$$\mathcal{Z}_\lambda \sim \int \mathcal{D}\psi^\dagger \mathcal{D}\psi \, e^{-S_\lambda + J\cdot(\psi^\dagger \psi)} \quad \longrightarrow \quad \partial_\lambda W_\lambda = \ldots \quad \longrightarrow \quad E_{\mathrm{gs}}, \rho_{\mathrm{gs}}, G^{(2)}$$

- computation of n-density correlation functions $\langle \rho(x_1)\rho(x_2)\ldots \rangle$
- RG approach to density functional theory contains many-body perturbation theory

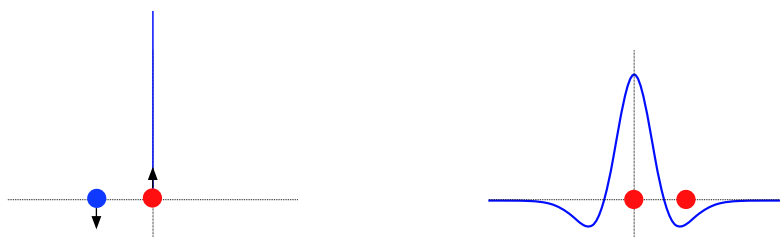
Conclusions

TECHNISCHE UNIVERSITÄT DARMSTADT

- constructive scheme for density functionals from microscopic interactions:

$$\mathcal{Z}_\lambda \sim \int \mathcal{D}\psi^\dagger \mathcal{D}\psi \, e^{-S_\lambda + J\cdot(\psi^\dagger \psi)} \quad \longrightarrow \quad \partial_\lambda W_\lambda = \ldots \quad \longrightarrow \quad E_{gs}, \rho_{gs}, G^{(2)}$$

- computation of n-density correlation functions $\langle \rho(x_1)\rho(x_2)\ldots \rangle$
- RG approach to density functional theory contains many-body perturbation theory
- local and non-local interaction types:



TECHNISCHE
UNIVERSITÄT
DARMSTADT

Thank you for your attention!