Many interacting fermions in a 1D harmonic trap: a quantum chemist's perspective

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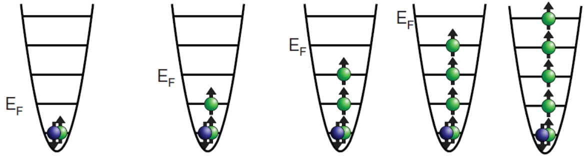
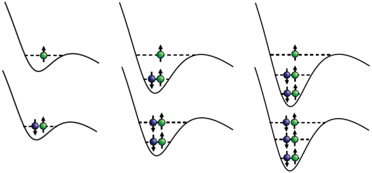
Motivation

- Selim Jochim's experiments[1]

1. 

2. 

- transition between two-, few- and many-body physics
- pursuit of high accuracy predictions

[1] S. Jochim *et al.* Science, **342** 457 (2013) and S. Joachim *et al.* Phys. Rev. Lett. **111**, 175302 (2013)

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The Hamiltonian

The model Hamiltonian describing N structureless spin-1/2 fermions in a one-dimensional harmonic trap reads

$$\hat{H} = -\frac{1}{2m}\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2} + \frac{1}{2}m\omega^2\sum_{i=1}^{N}x_i^2 + g\sum_{i<j}\delta(x_i - x_j) \tag{1}$$

where m is the mass of the atom, ω is the frequency of the trap and g is the interaction strength.

Methods

- algebraic approximation $\rightarrow$ finite (n_b) number of single-particle functions of the form:

$$\varphi_n(x_i) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi}\right)^{1/4} e^{-\frac{m\omega x_i^2}{2}} H_n\left(\sqrt{m\omega} x_i\right) \tag{2}$$

- full configuration interaction method also known as the exact diagonalization,
- coupled cluster methods

Full Configuration Interaction

Wave function of the form:

$$\Psi = (1 + \hat{C})\Phi = \Phi + c_{\rho_i}^{\alpha_i} e_{\alpha_i}^{\rho_i} \Phi + \ldots + \frac{1}{(N!)^2} c_{\rho_1 \ldots \rho_N}^{\alpha_1 \ldots \alpha_N} e_{\alpha_1 \ldots \alpha_N}^{\rho_1 \ldots \rho_N} \Phi \tag{3}$$

were Φ is the Slater determinant, $e_{\alpha_1 \ldots \alpha_k}^{\rho_1 \cdots \rho_k}$ are the k-tuple excitation operators and coefficients $c_{\rho_1 \ldots \rho_k}^{\alpha_1 \cdots \alpha_k}$ are variationally optimized.

$$E = \frac{\langle \Psi | \hat{H} \Psi \rangle}{\langle \Psi | \Psi \rangle} \tag{4}$$

Cutting the number of excitations resulting in the loss of size-consistency.

Coupled Cluster

Full CC equivalent to full CI, as the wave function is of the form:

$$\Psi = e^{\hat{T}}\Phi, \quad \text{where} \quad e^{\hat{T}} = 1 + \hat{C} \tag{5}$$

Possible cutoff in included excitations (preserving size-consistency):

- $\hat{T} = \hat{T}_1 + \hat{T}_2$ — CCSD,
- $\hat{T} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3$ — CCSDT,
- $\hat{T} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3 + \hat{T}_4$ — CCSDTQ.

Energy expression (nonvariational):

$$E = \langle \Phi | e^{-\hat{T}} \hat{H} e^{\hat{T}} \Phi \rangle \tag{6}$$

Equations for $\hat{T}$:

$$0 = \left\langle e^{\rho_k \cdots \rho_k}_{\alpha_k \ldots \alpha_k} \Phi | e^{-\hat{T}} \hat{H} e^{\hat{T}} \Phi \right\rangle , \quad k = 1, \ldots, N \tag{7}$$

Extrapolation to the infinite basis set

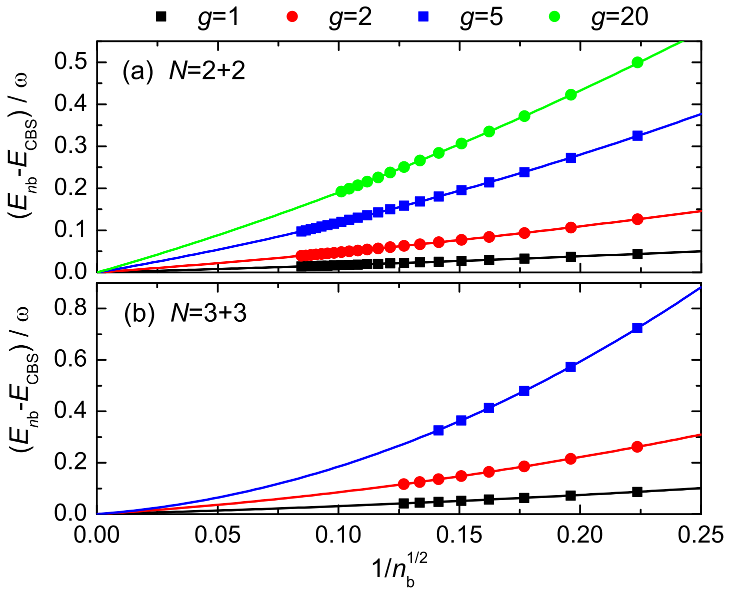
- typical electronic Schrödinger equation: L^{-3}, where L – highest angular momentum present in the basis set
- this Hamiltonian, rigorously proven two-body behaviour

$$E_\infty - E_{n_b} = \mathrm{const} \times \left(\frac{1}{\sqrt{n_b}} + \frac{g}{\pi} \frac{1}{n_b} \right) + \mathcal{O}\left(n_b^{-\frac{3}{2}} \right). \tag{8}$$

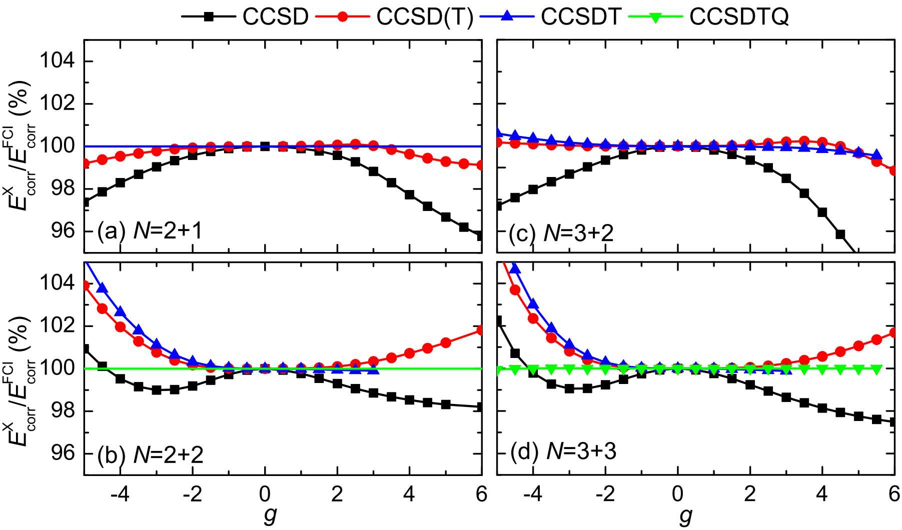
- many-body case: three-terms extrapolation formula

$$E_\infty - E_{n_b} = \frac{A}{\sqrt{n_b}} + \frac{B}{n_b} \tag{9}$$

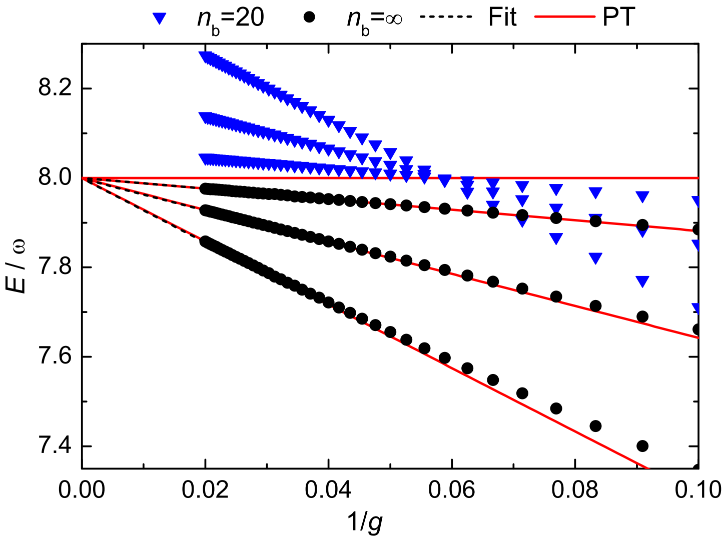
Convergence of the FCI results with the basis set size



Convergence of the CC results with the level of excitation

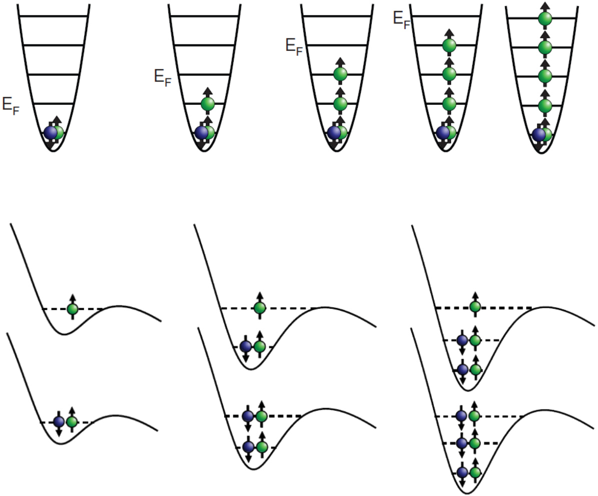


Comparison with the previous *state-of-the-art*[2]

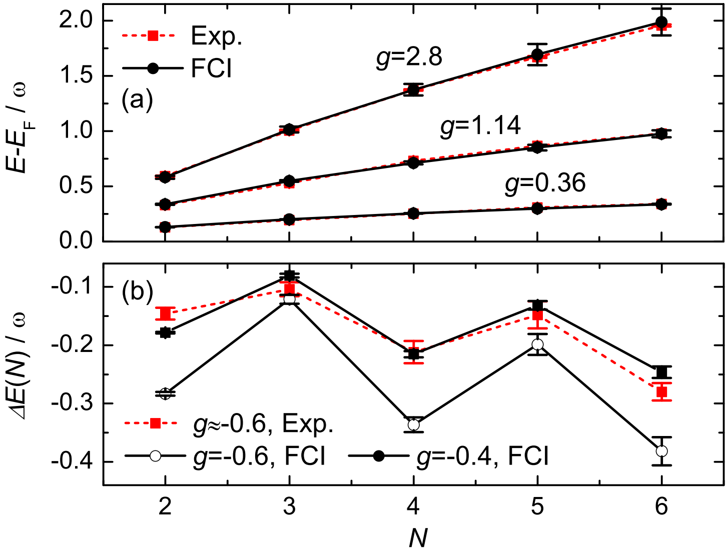


[2]M. Lewenstein *et al.* , Phys. Rev. A **88** 033607 (2013)

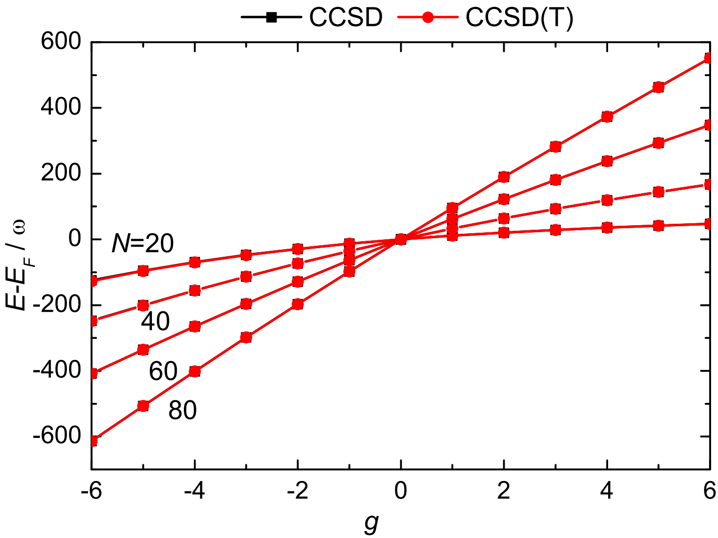
Comparison with Jochim's experiments



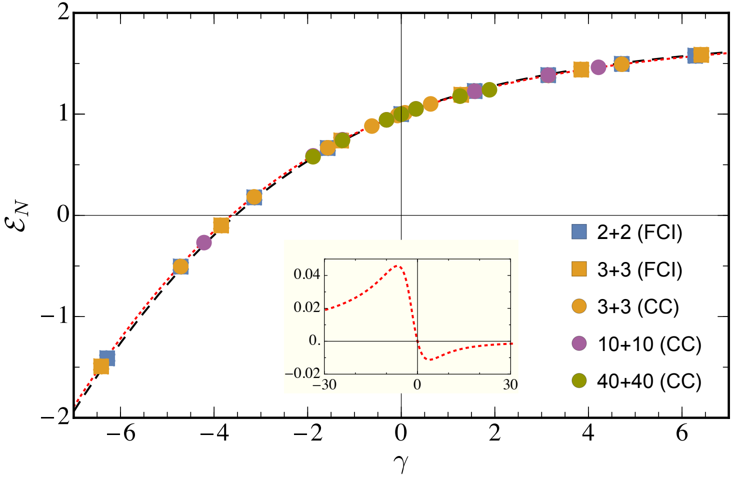
Comparison with Jochim's experiments



What is possible with the coupled cluster methods

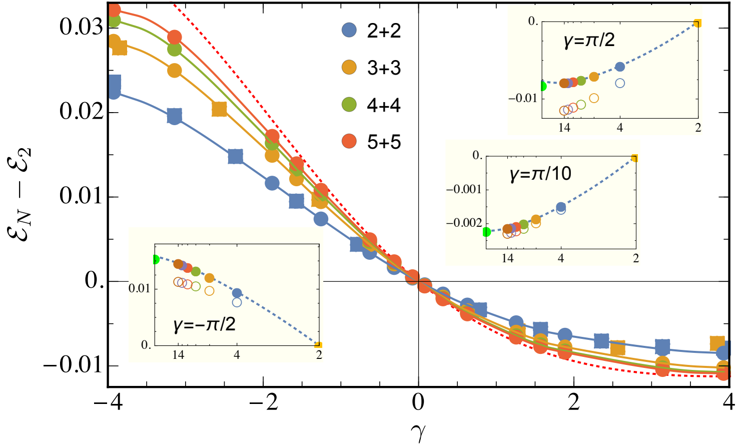


Approaching the thermodynamic limit, rescaled energies

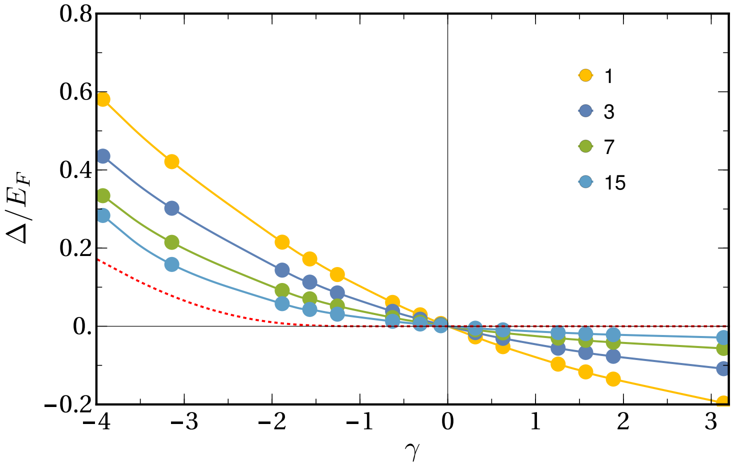


$$\mathcal{E}_N = E_N / E_N^{(0)}, \qquad \gamma = \pi g / \sqrt{N}$$

Thermodynamic limit, rescaled many-body contributions



Thermodynamic limit, BCS pairing gap



$$\Delta_N = E_N - (E_{N+1} + E_{N-1})/2, \qquad \Delta_\infty = 8E_F\sqrt{-\frac{\gamma}{2\pi^3}}\exp\left(\frac{\pi^2}{\gamma}\right)$$

Summary

1. Successful implementation of the quantum chemical methods in quantum gas physics.
2. Pushing the boundary of what is possible in the numerical calculations for 1D Fermi gases.
3. Importance of the extrapolation to the infinite set of one-particle functions.
4. Accurate predictions for the past and future experiments.
5. Unprecedented description of the transition to the thermodynamical limit.