# Many interacting fermions in a 1D harmonic trap: a quantum-chemical treatment

Tomasz Grining, Michał Tomza, Michał Lesiuk, Pietro Massignan, Maciej Lewenstein, Robert Moszynski

University of Warsaw, Poland
ICFO - The Institute of Photonic Sciences, Spain

KITP, Santa Barbara, 2.12.2016

# Application of quantum chemistry methods to trapped Fermi gases

- T. Grining, M. Tomza, M. Lesiuk, M. Przybytek, M. Musial, P. Massignan, M. Lewenstein, R. Moszynski, *Many interacting fermions in a one-dimensional harmonic trap: a quantum-chemical treatment*, New J. Phys. 17, 115001 (2015)
- T. Grining, M. Tomza, M. Lesiuk, M. Przybytek, M. Musial, R. Moszynski, M. Lewenstein, P. Massignan, *Crossover between few and many fermions in a harmonic trap*, Phys. Rev. A 92, 061601(R) (2015)

# The Hamiltonian

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

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

where $m$ is the mass of the atom, $\omega$ is the frequency of the trap and $g$ is the interaction strength.

# Fundamentals of the many-body method

- If a set of one-particle functions $\{\phi_n\}$ spans the one-particle Hilbert space $L^2(\mathbb{R}^3)$, then the set of all $N$-particle determinants constructed from this one-particle set $\{\Phi_I\}$ span the antisymmetric part of the $N$ particle Hilbert space $\mathcal{A}L^2(\mathbb{R}^{3N})$
- Algebraic approximation
  $\{\phi_n\}_{n=1}^{n_b} \rightarrow \{\Phi_I\}_{I=1}^{\approx n_b!}$
  accuracy critically depends on $n_b$ and analytical structure of $\phi_n$ as compared to the two-body solution

# Basis set, convergence, and extrapolation

- finite ($n_b$) number of single-particle functions of the form:

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

- rigorously proven for two-body Hamiltonian

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

- many-body case: three-terms extrapolation formula

$$E_\infty - E_{n_b} = \frac{A}{\sqrt{n_b}} + \frac{B}{n_b} \qquad (4)$$

# Full Configuration Interaction

Wave function of the form:

$$\Psi = (1 + \hat{C})\Phi = \Phi + c_{\rho_i}^{\alpha_i} e_{\alpha_i}^{\rho_i} \Phi + \ldots + \frac{1}{(N!)^2} c_{\rho_1 \ldots \rho_N}^{\alpha_1 \ldots \alpha_N} e_{\alpha_1 \ldots \alpha_N}^{\rho_1 \ldots \rho_N} \Phi \quad (5)$$

were $\Phi$ is the Slater determinant, $e_{\alpha_1 \ldots \alpha_k}^{\rho_1 \ldots \rho_k}$ are the $k$-tuple excitation operators (e.g. $e_\alpha^\rho = a_\rho^\dagger a_\alpha$, $a_\rho^\dagger, a_\alpha$ defined with respect to the Fermi vacuum $\Phi$) and coefficients $c_{\rho_1 \ldots \rho_k}^{\alpha_1 \ldots \alpha_k}$ are variationally optimized.

$$E = \frac{\langle \Psi | \hat{H} \Psi \rangle}{\langle \Psi | \Psi \rangle} \quad (6)$$

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:

$$\Psi = e^{\hat{T}}\Phi, \quad \text{where} \quad e^{\hat{T}} = 1 + \hat{C} \tag{7}$$

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.

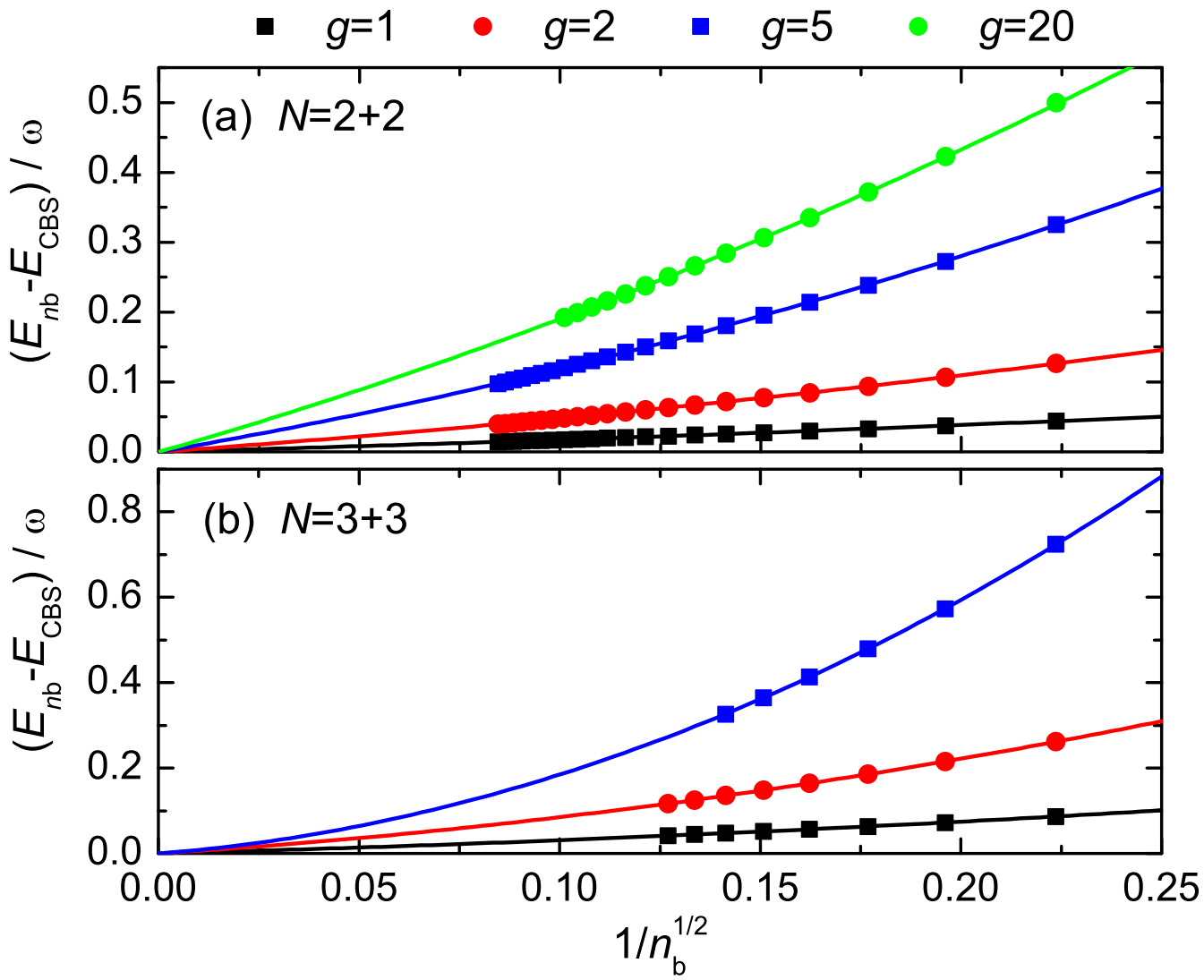
Energy expression (nonvariational):

$$E = \langle \Phi | e^{-\hat{T}} \hat{H} e^{\hat{T}} \Phi \rangle \tag{8}$$

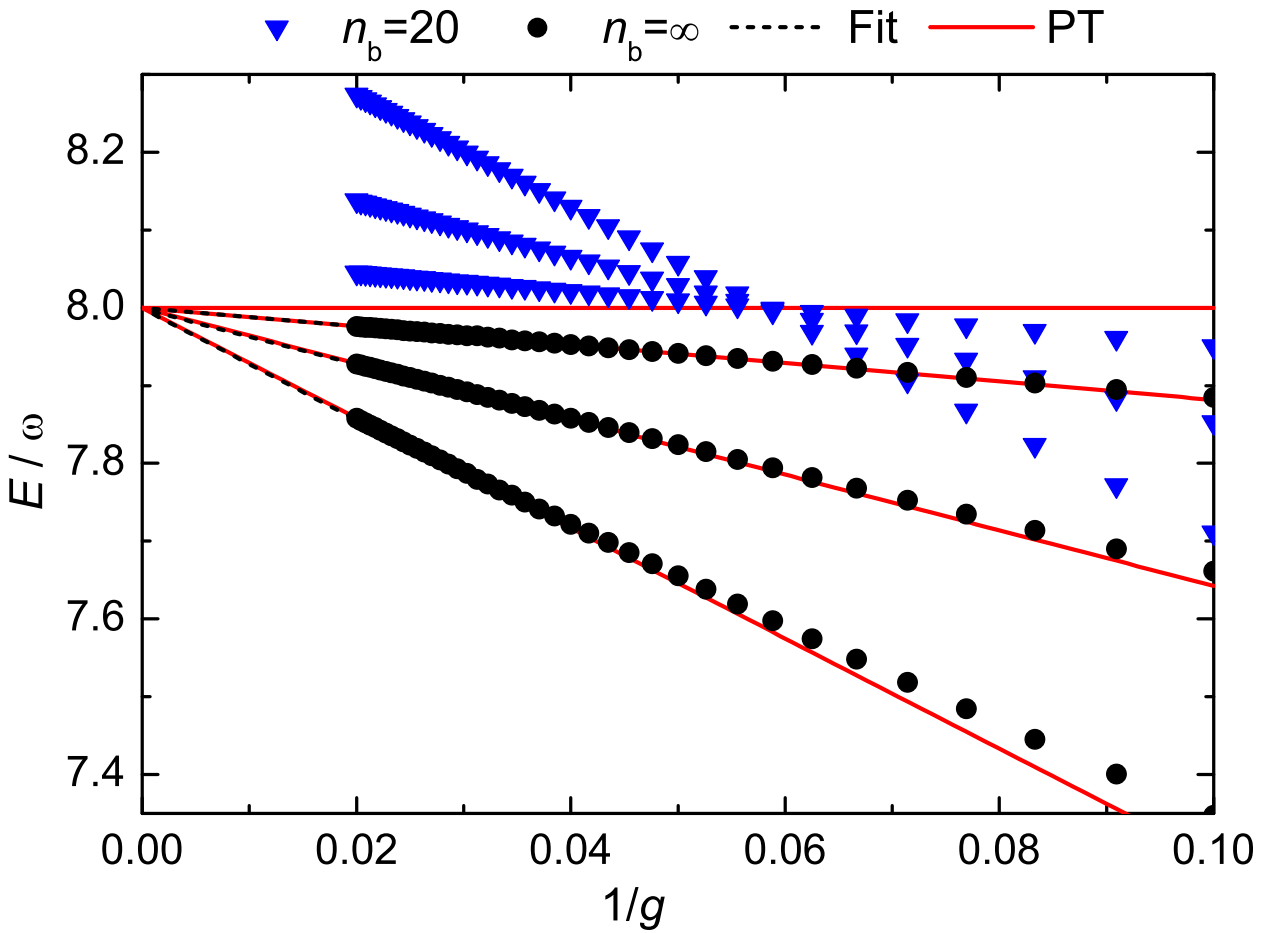
Equations for $\hat{T}$:

$$0 = \left\langle e^{\rho_k \cdots \rho_k}_{\alpha_k \ldots \alpha_k} \Phi | e^{-\hat{T}} \hat{H} e^{\hat{T}} \Phi \right\rangle, \quad k = 1, \ldots, N \tag{9}$$

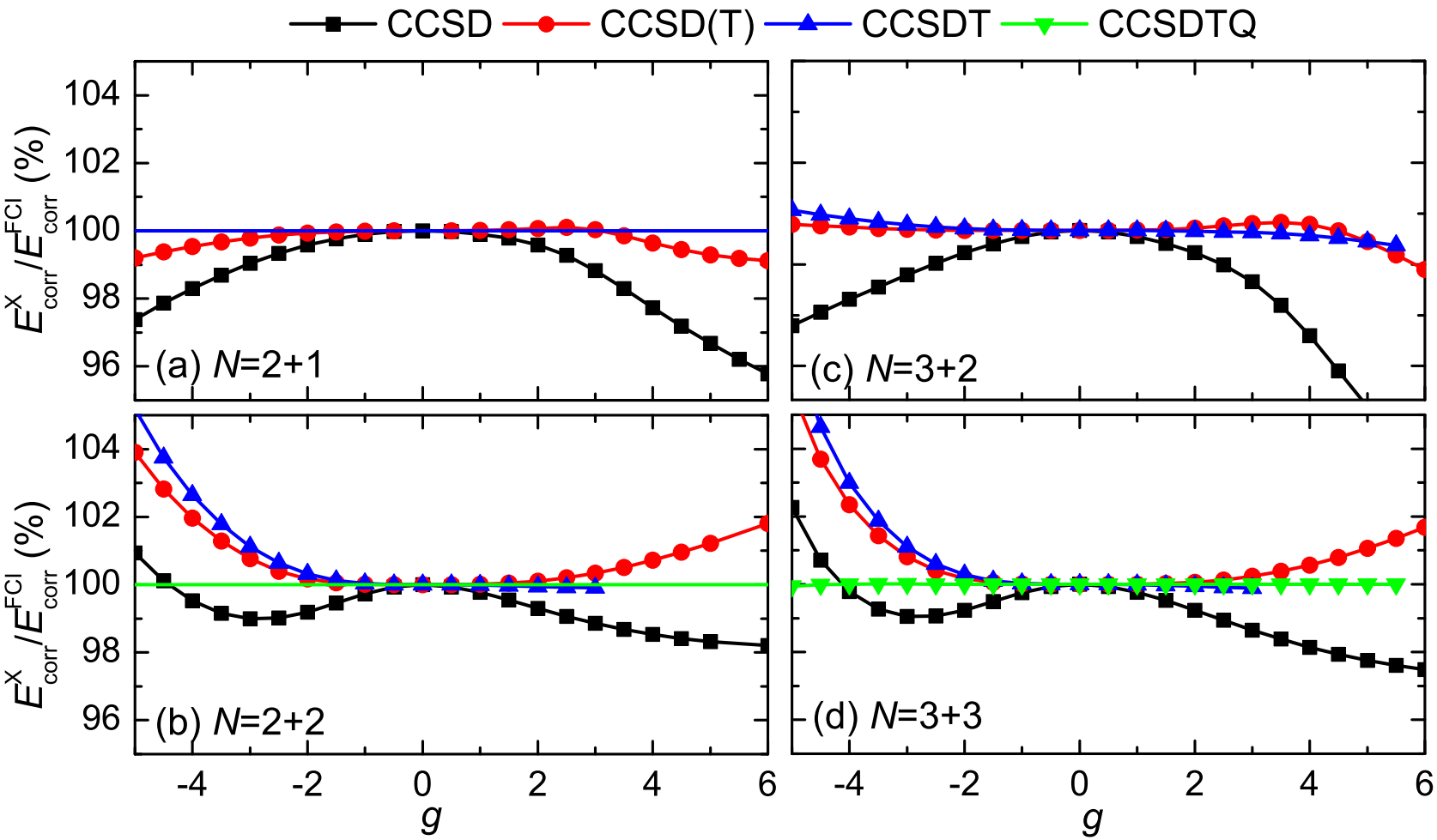
# Convergence of the FCI results with the basis set size



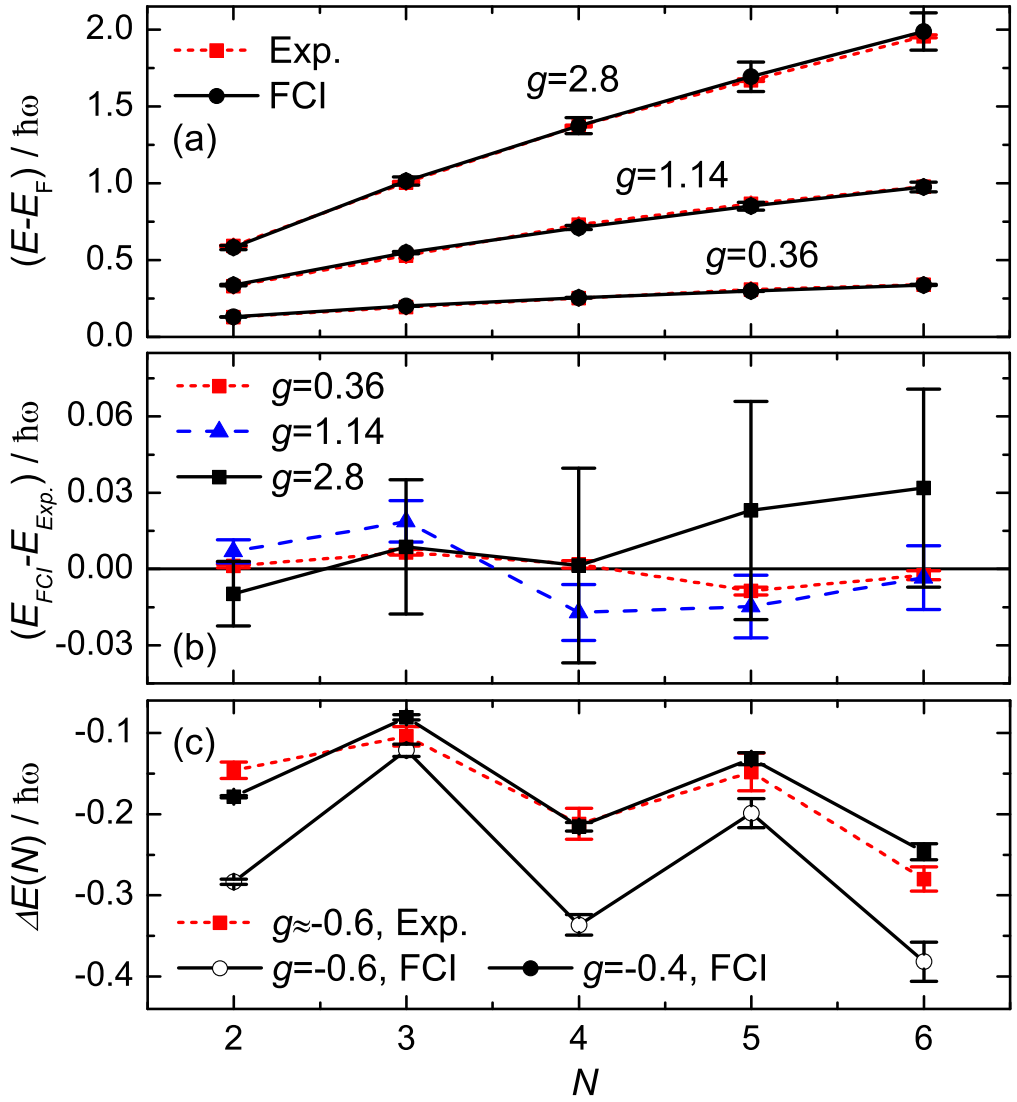
# Importance of the convergence in the unitary limit



# Convergence of the CC results with the level of excitation

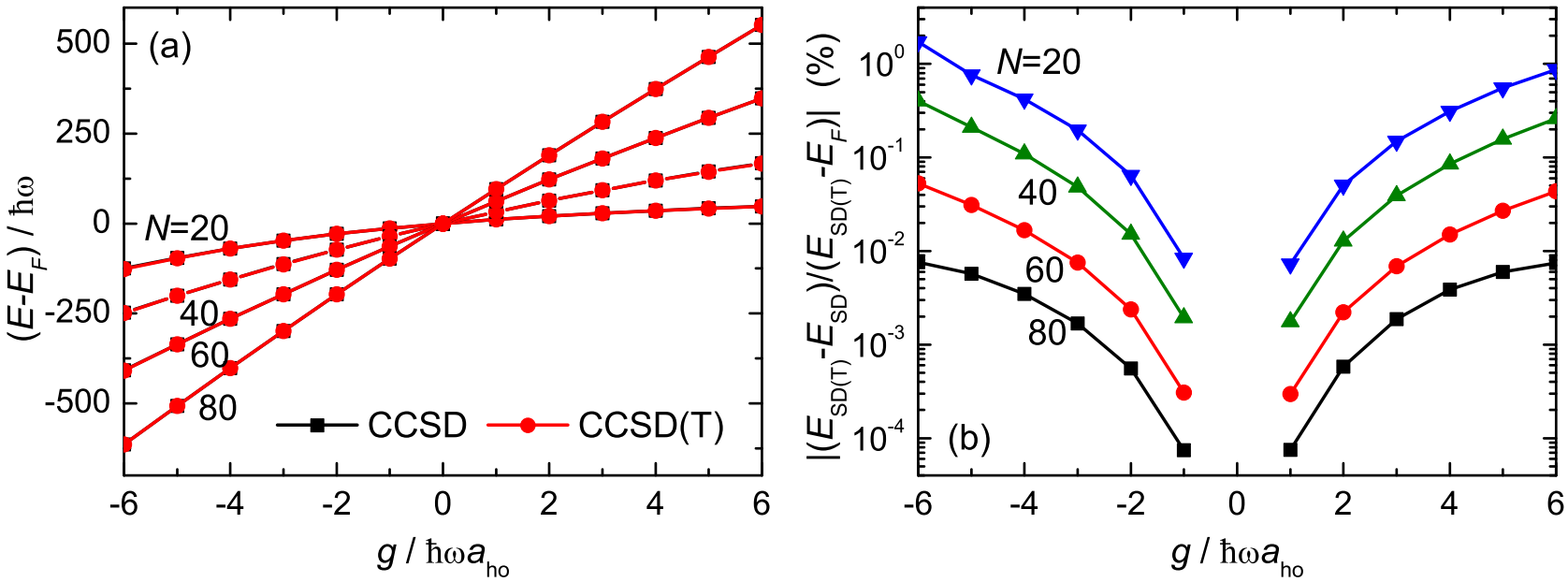


# Comparison with Jochim Selim's experiments

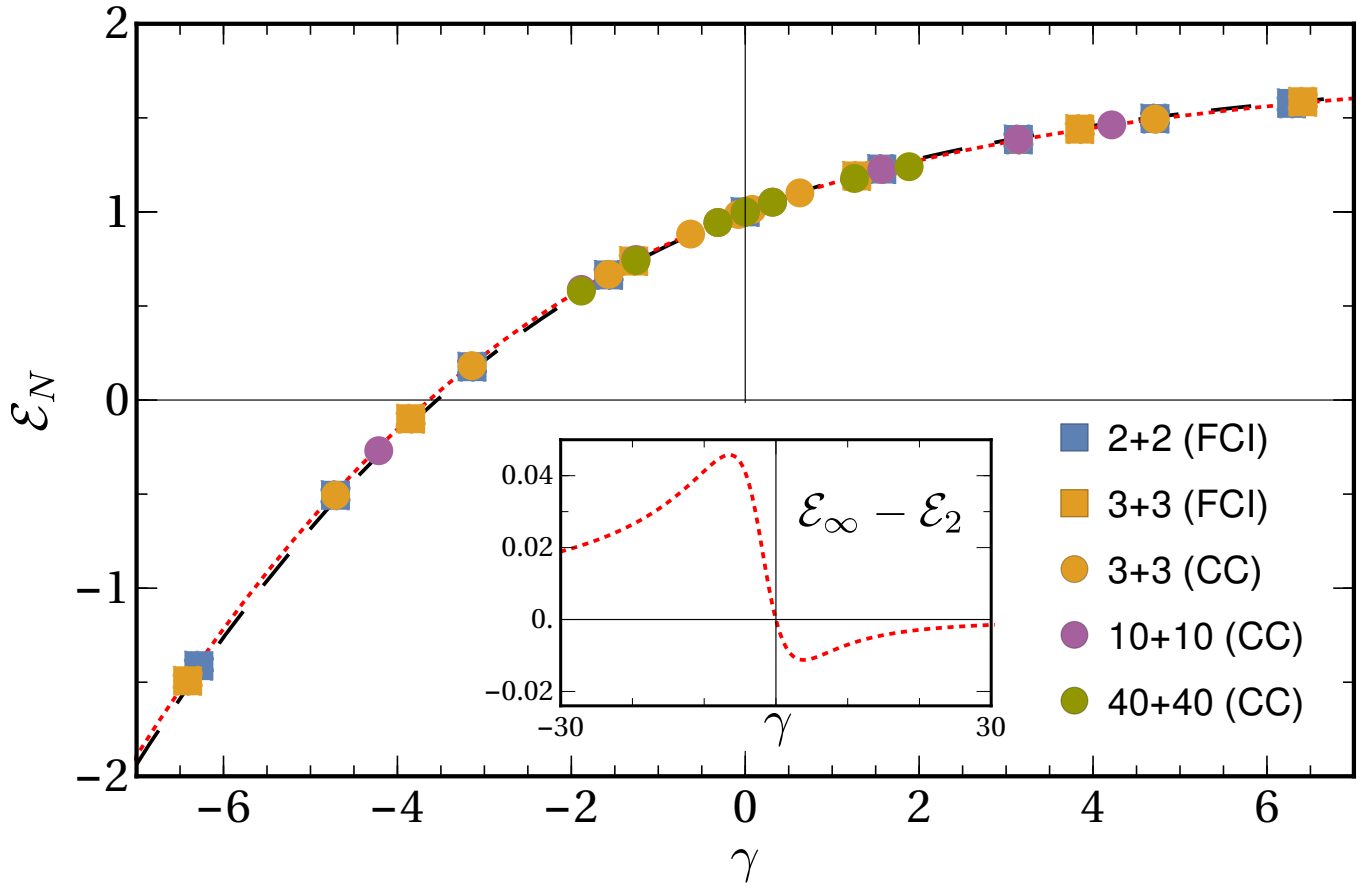



Wenz et al., Science 342, 457 (2013); Zürn et al., Phys. Rev. Lett. 111, 175302 (2013)

# Approaching many-body limit

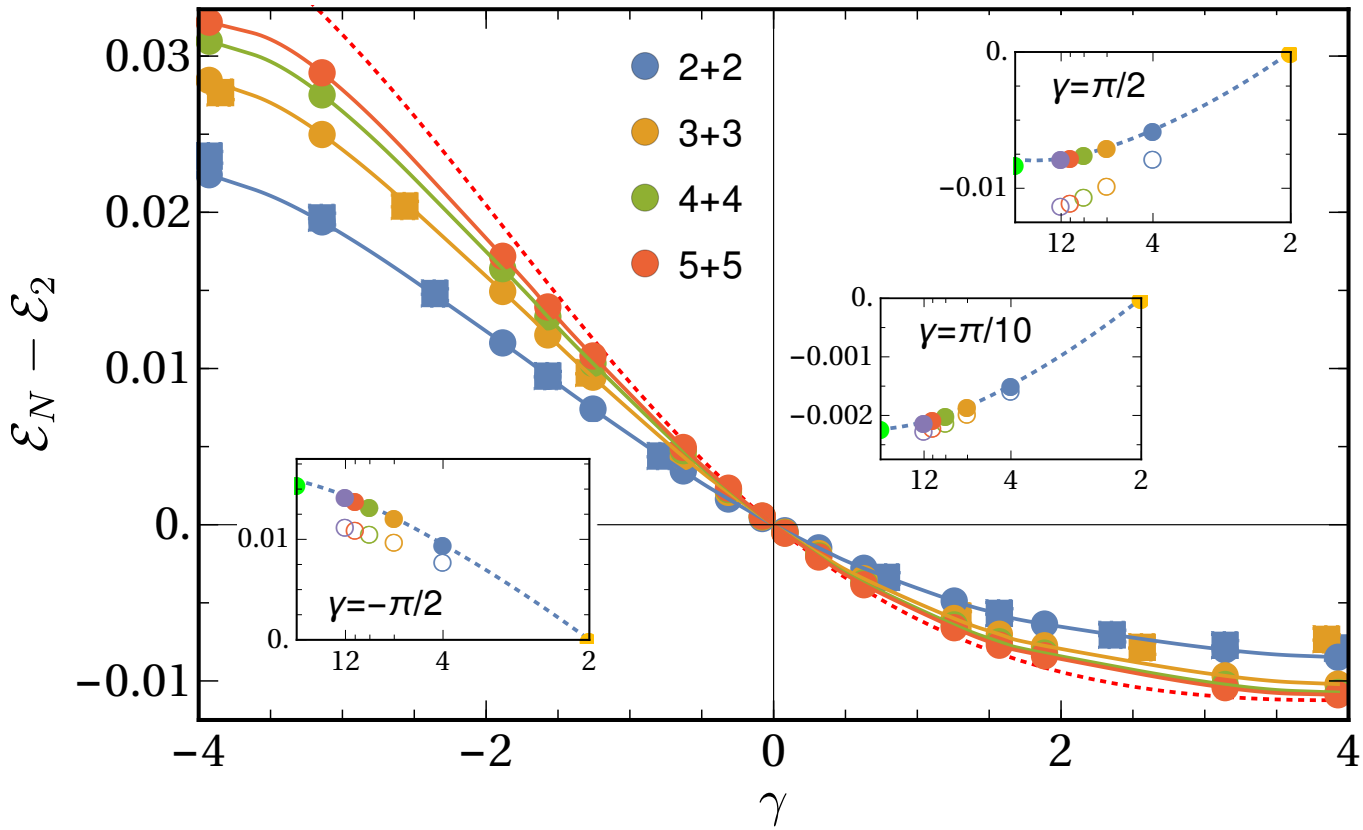


# Crossover between few and many fermions

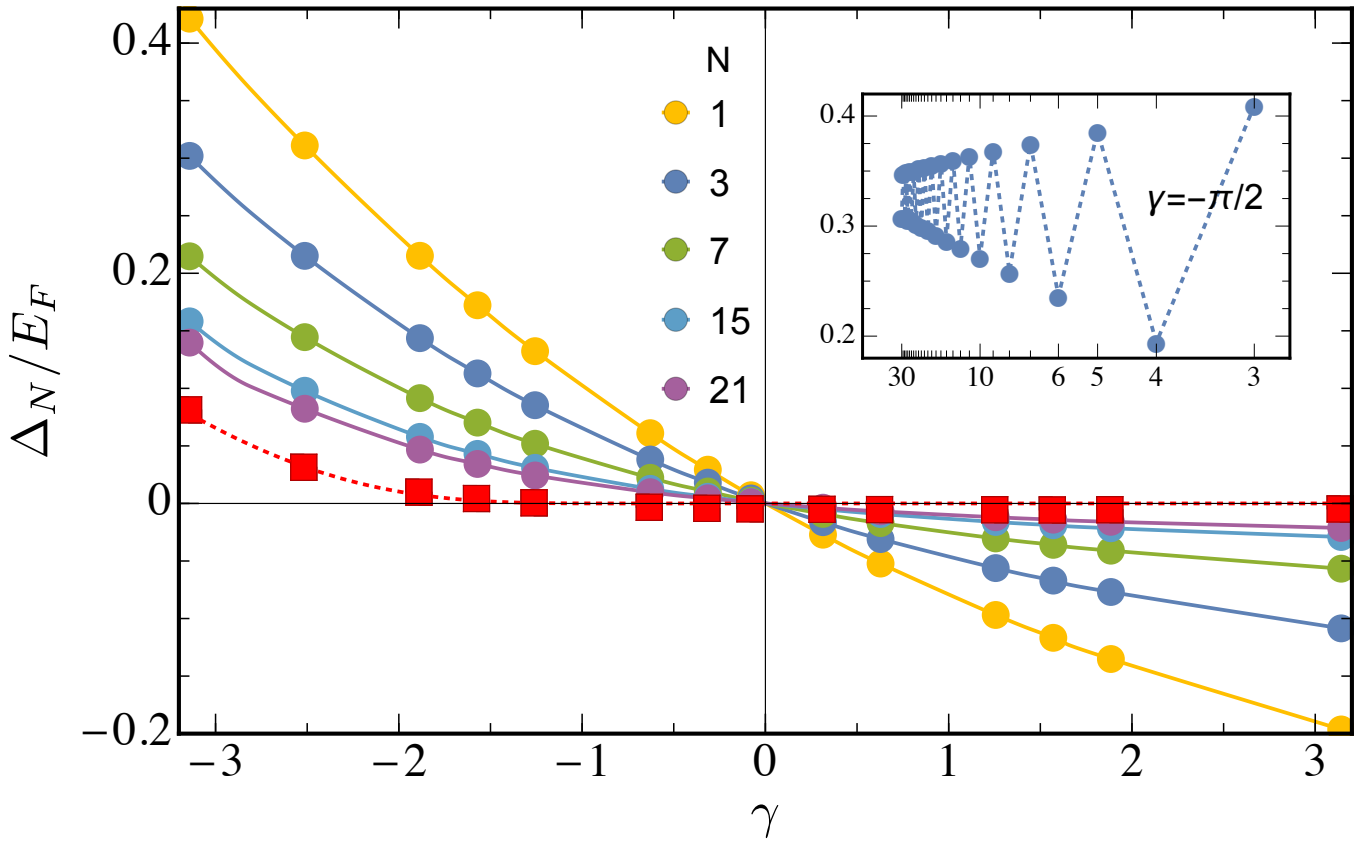



$$\mathcal{E}_N = E_N / E_N^{(0)}, \qquad \gamma = \pi g / \sqrt{N}$$

# Crossover between few and many fermions



# BCS pairing gap and chemical potential




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

$$\mu_N = E_{N+1} - E_N$$

# Open questions (work in progress)

Can coupled cluster methods in many-fermion physics describe:

- Explicitly correlated approaches?
- Degenerate systems?
- Unitary limit?
- 2D and 3D?
- Periodic systems?
- Excited states?