Rigorous analysis of *ab initio* calculations for parabolic quantum dots

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Confrontation and convergence in nuclear theory
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Outline

1. Background and formalism
   - Overview and motivation
   - Quantum dots as artificial nuclei
   - The Harmonic oscillator and model spaces
2. The full configuration interaction method
   - Formulation
   - How to analyze FCI
   - Numerical results
3. Coupled cluster methods (CC)
   - Brief outline of method
   - “Imagined” convergence analysis

Outline

Overview of this talk

- The ultimate goal of this work is to understand coupled cluster methods (CC) applied to nuclei. One may consider (parabolic) quantum dots as minimal model for nuclei, in a sense "artificial nuclei"
- We will analyze the full configuration interaction (FCI) method for quantum dots
- We will also see some illuminating numerical results
- Finally, we will discuss CC methods and discuss how these may be analyzed rigorously for quantum dots
- Very little physics, only method talk: an outline of rigorous mathematical analysis

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Motivation

Why do all this rigorous analysis?

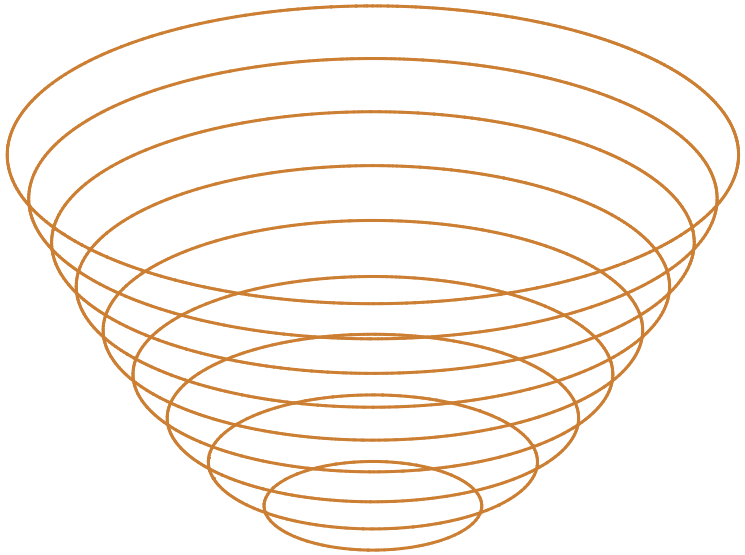
- People disagree on published results.
- Curse of dimensionality $\Rightarrow$ computational constraints:

$$\text{dim. of Hilbert space} \quad \sim \quad \exp(A), \quad A = \text{no. particles}$$

- If we don't understand FCI/CC for quantum dots, then what with nuclei? (See next slides.)
- Understanding might also lead to new or better methods, or make them easier to implement

Parabolic quantum dots

- A harmonic oscillator (HO) trap.
- We place A electrons in the trap
- They interact via Coulomb repulsion
- This gives us the Hamiltonian ($\hbar = m = 1$ etc)



$$H = H_0 + V = \sum_{i=1}^{A} h(i) + \frac{1}{2}\sum_{i\neq j} u(i,j)$$

with

$$h(i) = -\frac{1}{2}\nabla_i^2 + \frac{1}{2}\mathbf{r}_i^2 \qquad u(i,j) = \frac{\lambda}{\|\mathbf{r}_i - \mathbf{r}_j\|} \tag{1}$$

$$\lambda = \mathcal{O}(1) \text{ to } \mathcal{O}(10)$$

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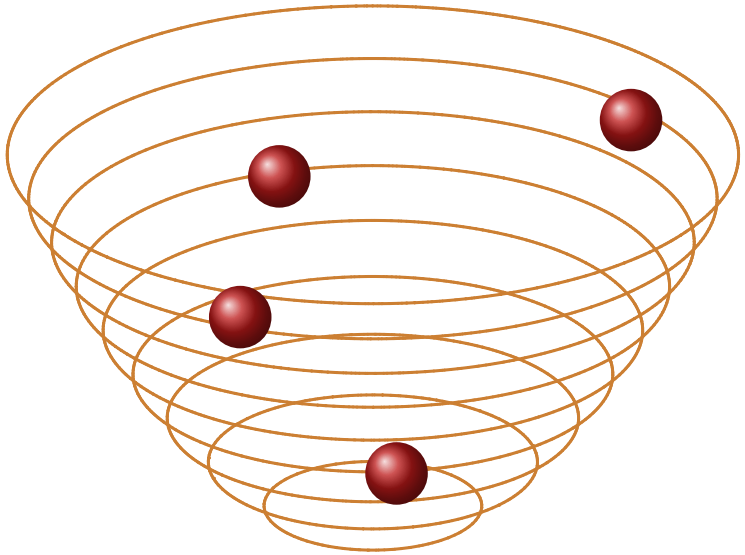

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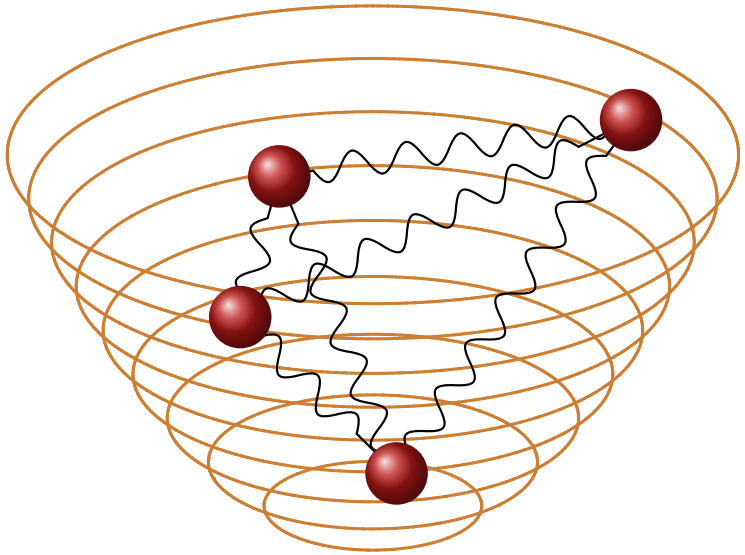

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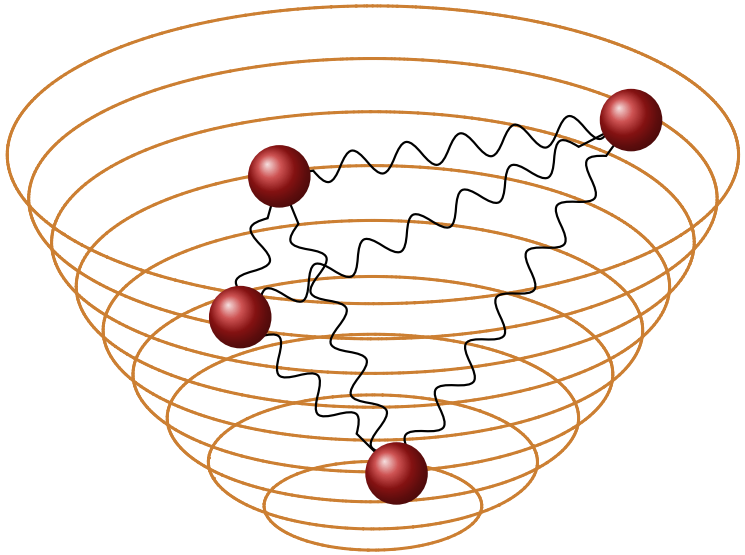

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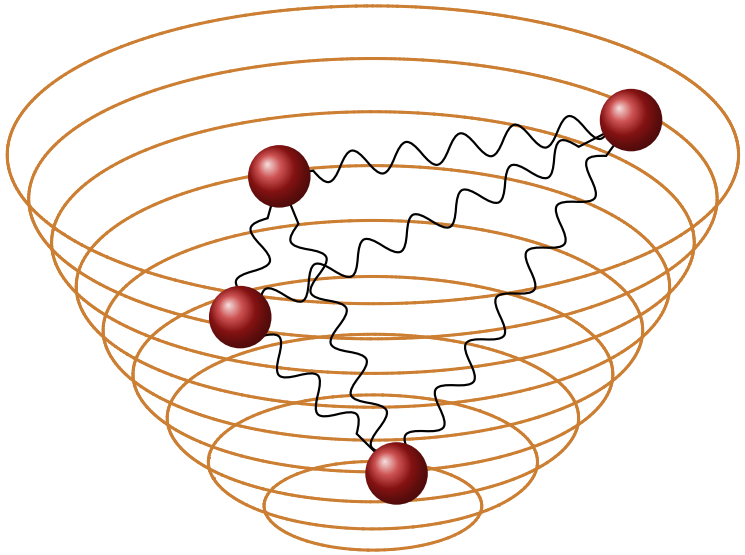

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Quantum dots *vs.* nuclei

There are strong similarities between no-core shell model approach to nuclei and parabolic quantum dots:

Quantum dots:

- $\mathbb{R}^d$, $d = 1, 2, 3$, spin-$\frac{1}{2}$
- HO confinement, $\hbar\omega$ fixed
- Singluar two-body interaction $\lambda/\|\mathbf{r}_{ij}\|$
- Purely discrete spectrum

Nuclei:

- $\mathbb{R}^3$, spin-$\frac{1}{2}$, isospin
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Multi-indices

We need the concept of a multi-index to ease notation.

Definition (Multi-index)

A tuple of d integers n_j:

$$\mathbf{n} = (n_1, n_2, \cdots, n_d), \quad n_j \geq 0.$$

We think of it as a vector of integers.
The "length" of $\mathbf{n}$:

$$|\mathbf{n}| = n_1 + n_2 + \cdots + n_d.$$

We will use the multi-index to specify q.n.'s in each spatial direction x, y, z, ...

The harmonic oscillator Hamiltonian

- I suppose we all know the HO and it's eigenfunctions:

$$H_0 = \sum_{i=1}^{A} h(i) = \sum_{\alpha} \epsilon_\alpha c_\alpha^\dagger c_\alpha$$

- Here,

$$\alpha \equiv (\mathbf{n}, \sigma) = (\text{space q.n.}, \text{spin q.n.})$$

- Single-particle functions $\phi_\alpha(x)$:

$$\phi_\alpha(x) = \underbrace{\phi_{\mathbf{n}}(\mathbf{r})}_{\text{space w.f.}} \underbrace{\chi_\sigma(s)}_{\text{spin w.f.}}, \qquad \epsilon_\alpha = \underbrace{|\mathbf{n}|}_{\text{shell}} + \frac{d}{2}$$

- Separation of variables:

$$\phi_{\mathbf{n}}(\mathbf{r}) \equiv \phi_{n_1}(r_1) \cdots \phi_{n_d}(r_d)$$

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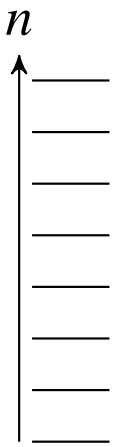
Examples of quantum numbers and shells



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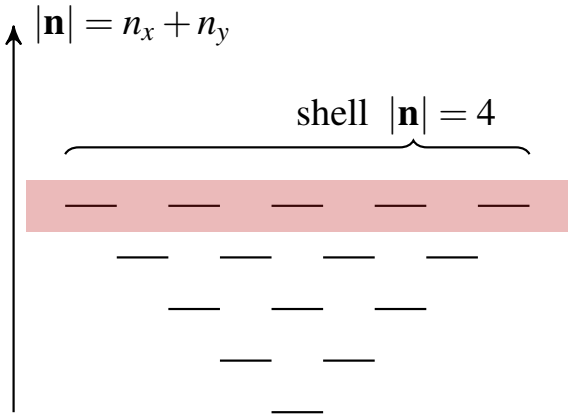

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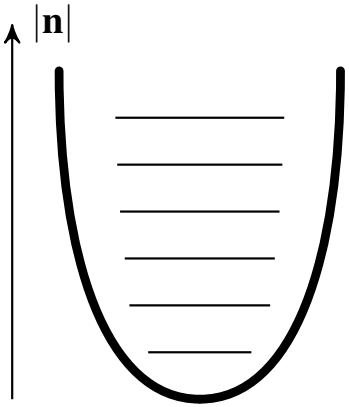

general case

- Finally, $c^\dagger_\alpha$ creates particle in orbital α

$$c^\dagger_{\alpha_1} c^\dagger_{\alpha_2} \cdots c^\dagger_{\alpha_A} |-\rangle \equiv \underbrace{|\alpha_1 \alpha_2 \cdots \alpha_A\rangle}_{\text{Slater determinant}}$$

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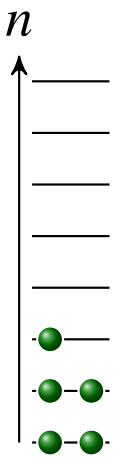

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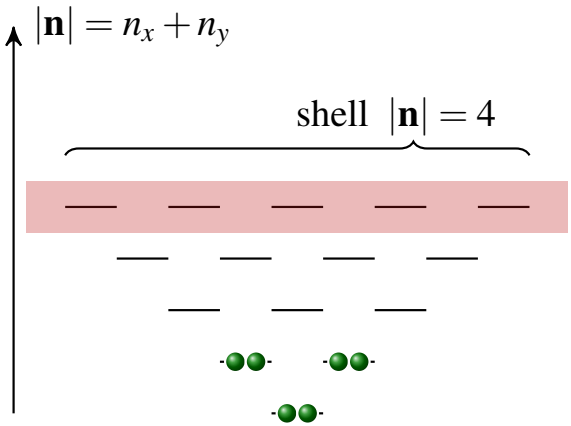

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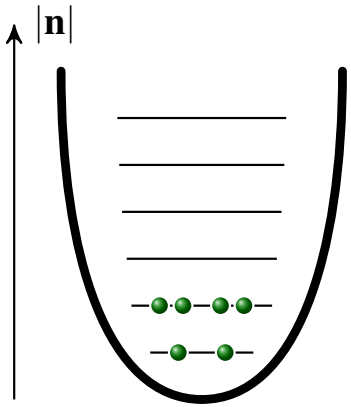

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Single-particle function expansions

- Arbitrary single-particle functions expanded in HO functions:

$$\begin{aligned} |\psi\rangle &= \sum_\alpha |\alpha\rangle \langle\alpha|\psi\rangle = \sum_\alpha c_\alpha |\alpha\rangle \\ \psi(x) &= \langle x|\psi\rangle = \sum_\alpha c_\alpha \phi_\alpha(x) \end{aligned}$$

- Expansion in eigenspaces:

Projects onto space with HO energy $N + d/2$

$$|\psi\rangle = \sum_{N=0}^{\infty} P_N |\psi\rangle$$

- We define shell-probability $p(N)$:

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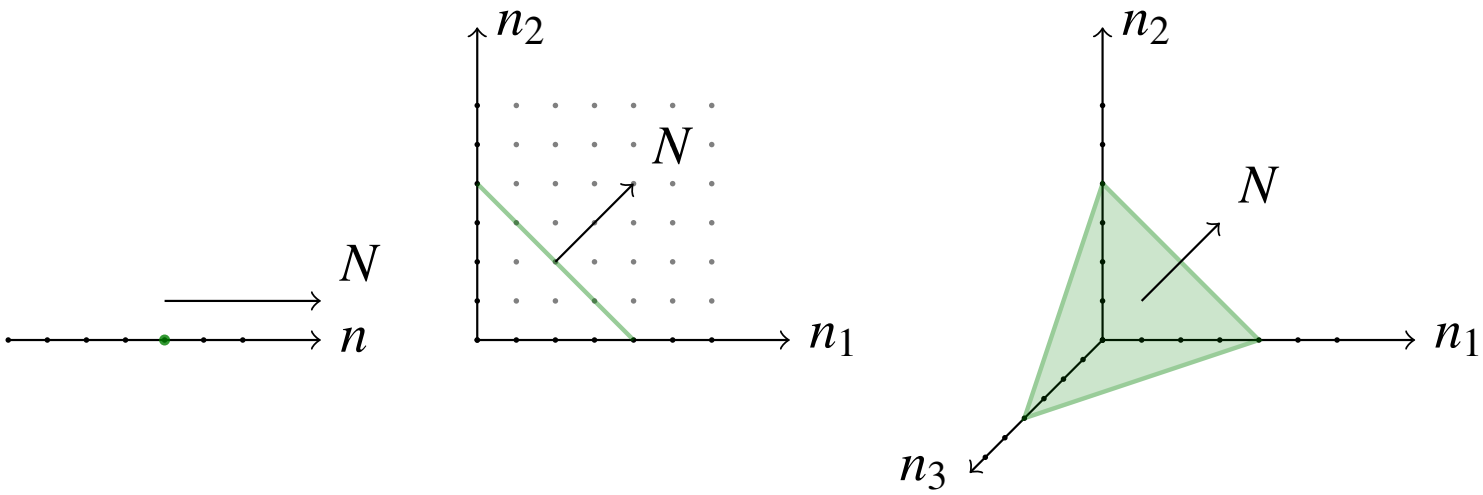
The shell-probability

- Recall the shell-probability $p(N)$:

$$p(N) \equiv \langle \psi | P_N | \psi \rangle \,, \quad P_N \text{ projects onto } N\text{'th shell}$$

- We have:

$$p(N) = \sum_{|\mathbf{n}|=N} |c_{\mathbf{n}}|^2$$



Many-body harmonic oscillator

It is important to keep in mind that:

- Mathematically, we may treat the many-body $|\Psi\rangle$ as a higher-dimensional one-body function!
- Trivial separation property of HO gives:

$$H_0 = \sum_{i=1}^{A} h(i) = -\frac{1}{2}\nabla_{\mathbf{R}}^2 + \frac{1}{2}\mathbf{R}^2, \quad \mathbf{R} = (\mathbf{r}_1, \cdots, \mathbf{r}_A) \in \mathbb{R}^{Ad}$$

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$$H_0 |\alpha_1 \cdots \alpha_A\rangle = (\epsilon_{\alpha_1} + \cdots + \epsilon_{\alpha_A}) |\alpha_1 \cdots \alpha_A\rangle$$

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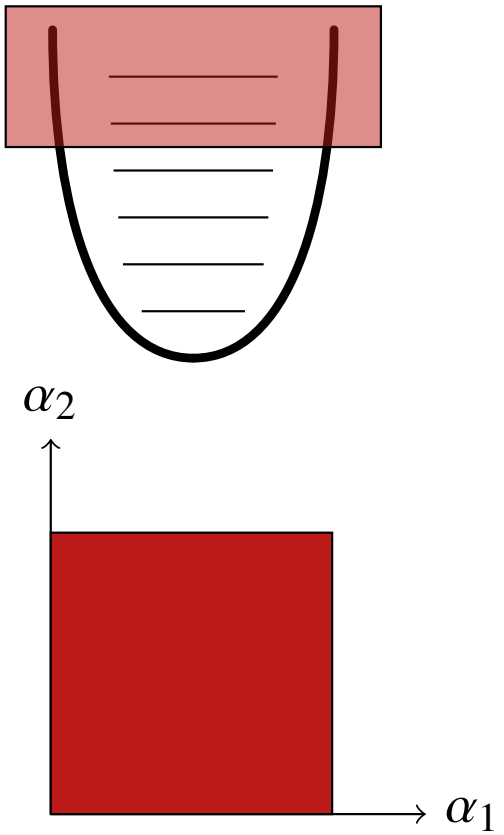
Model spaces: cutting down ∞ dimensions



Direct product space:

Allow only $|\mathbf{n}| \leq N_{\max}$ in *single-particle space.*

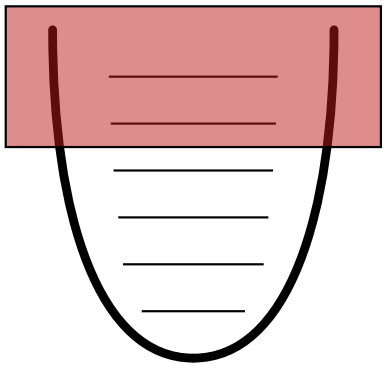
$$\mathscr{V}_{\rm DP} = \text{Span}\left\{|\alpha_1 \cdots \alpha_A\rangle \mid \max|\mathbf{n}_i| \leq N_{\max}\right\}$$
$$\subset \mathscr{H}_A \quad \leftarrow \text{(complete } A\text{-body Hilbert space)}$$

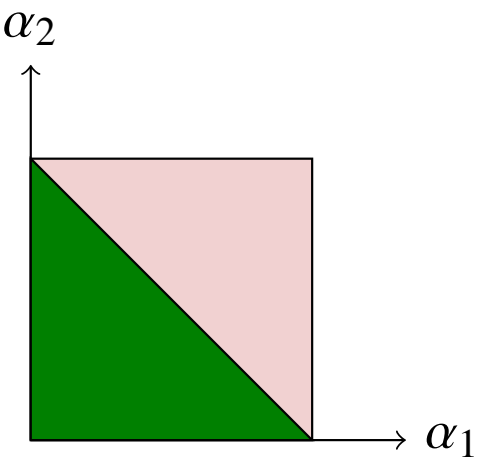
Energy cut space:

Restrict *total* HO energy instead:

$$\mathscr{V}_{\rm EC} = \text{Span}\left\{|\alpha_1 \cdots \alpha_A\rangle \mid \sum_i |\mathbf{n}_i| = N \leq N_{\max}\right\}$$
$$= (P_0 + P_1 + \cdots + P_{N_{\max}})\mathscr{H}_A$$

Model spaces: cutting down ∞ dimensions





Direct product space:

Allow only $|\mathbf{n}| \leq N_{\max}$ in *single-particle space.*

$$\mathscr{V}_{\rm DP} = \mathrm{Span}\left\{ |\alpha_1 \cdots \alpha_A\rangle \mid \max |\mathbf{n}_i| \leq N_{\max} \right\}$$
$$\subset \mathscr{H}_A \quad \leftarrow \text{ (complete } A\text{-body Hilbert space)}$$

Energy cut space:

Restrict *total* HO energy instead:

$$\mathscr{V}_{\rm EC} = \mathrm{Span}\left\{ |\alpha_1 \cdots \alpha_A\rangle \mid \sum_i |\mathbf{n}_i| = N \leq N_{\max} \right\}$$
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Outline

Configuration Interaction (CI)

- Variational formulation of eigenvalue problem:

  Find the $|\Psi\rangle \in \mathscr{H}$ that minimizes the energy:

$$E = \min_{|\Psi\rangle \in \mathscr{H}} \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

- Rayleigh-Ritz: Restrict to model space $\mathscr{V} \subset \mathscr{H}$:

  Find the $|\Psi_h\rangle \in \mathscr{V}$ that minimizes the energy:

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- This is CI with respect to $\mathscr{V}$, using $\mathscr{V}_{\mathrm{DP}}$ or $\mathscr{V}_{\mathrm{EC}}$ gives FCI.
- Let $|\Phi_i\rangle$ be basis for $\mathscr{V}$. We obtain the matrix formulation

$$\mathbf{H}\mathbf{u}_\mathbf{h} = E_h \mathbf{u}_\mathbf{h}, \qquad \mathbf{H}_{ij} = \langle \Phi_i | H | \Phi_j \rangle$$

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Questions of accuracy and convergence

When studying convergence,
accuray, etc., norms are useful:

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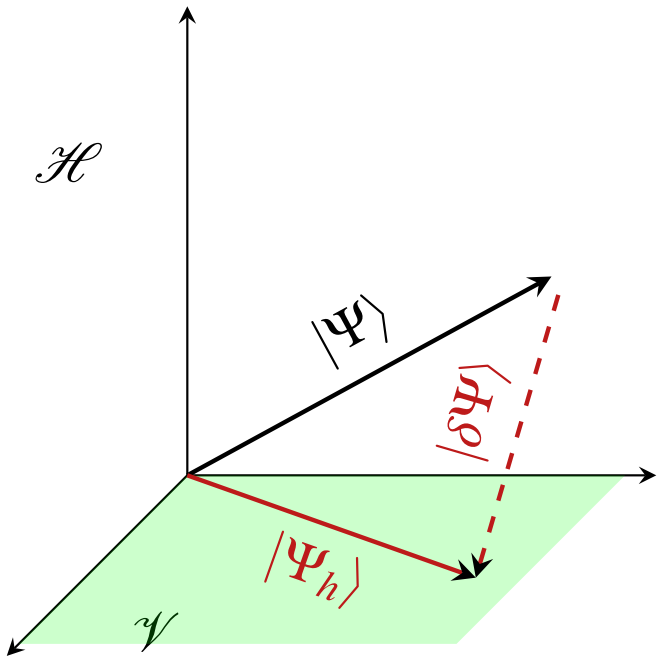

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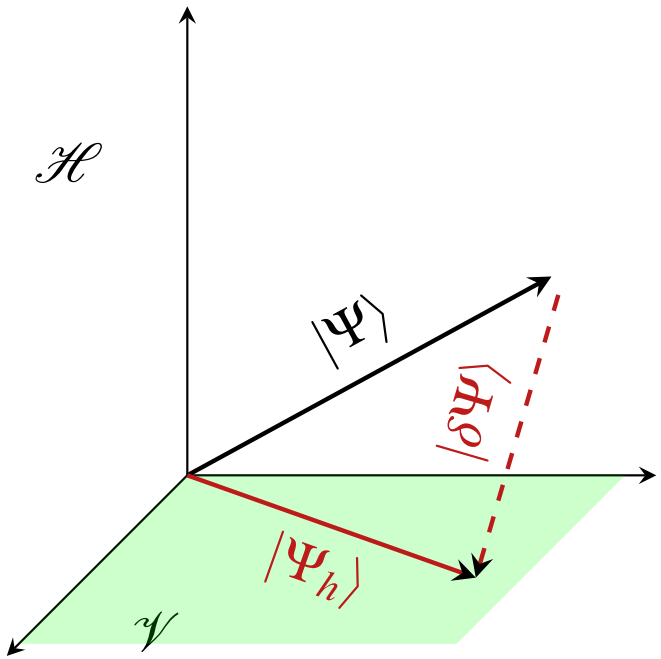

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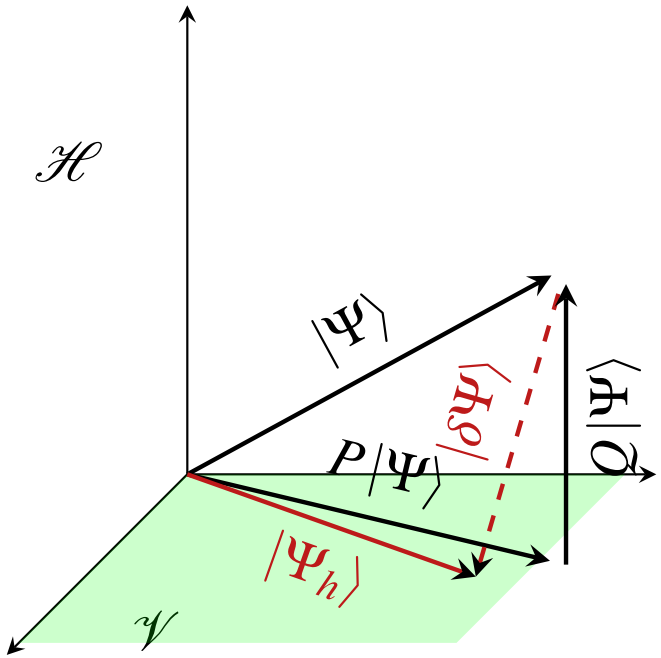

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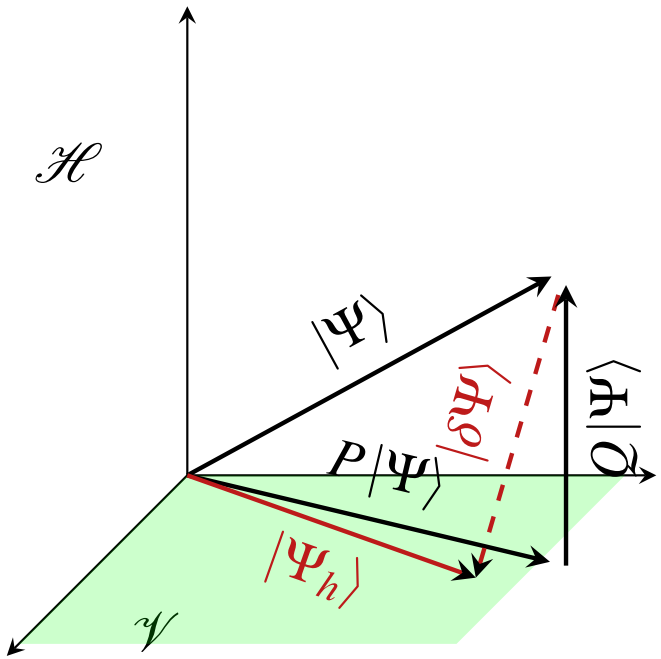

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There exists a constant C_1, dependent on $u(i,j)$ only, such that the error $|\delta\Psi\rangle$ is bounded by

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Properties of basis functions

- Already seen: $|\Phi_i\rangle$ are harmonic oscillator eigenfunctions in Ad dimensions.
- Let P project onto $\mathscr{V} = \mathscr{V}_{\mathrm{EC}}$, and $Q = 1 - P$:

$$P = P_0 + P_1 + \cdots + P_{N_{\max}}$$

- Consider expansion of some wave function $|\Psi\rangle$:

$$|\Psi\rangle = (P+Q)\sum_i c_i |\Phi_i\rangle = \sum_{i=1}^{D} c_i |\Phi_i\rangle + \sum_{i=D+1}^{\infty} c_i |\Phi_i\rangle$$

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Properties of basis functions for $A = d = 1$

- For $A = d = 1$, we have $\langle x|\Phi_i(x)\rangle \longrightarrow \phi_n(x)$:

$$\phi_n(x) = (2^n n!\sqrt{\pi})^{-1/2} H_n(x) e^{-x^2/2}$$

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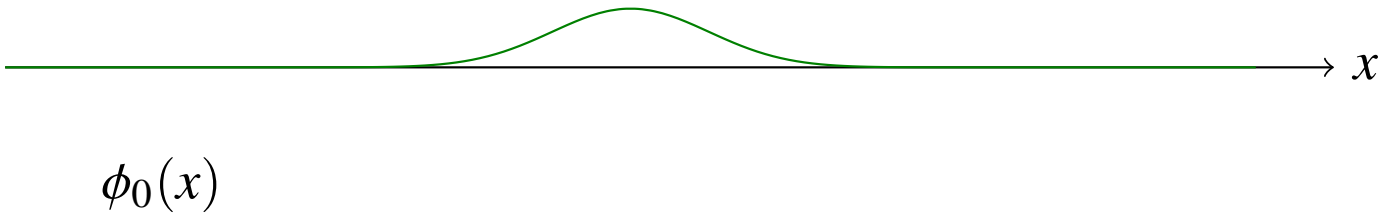

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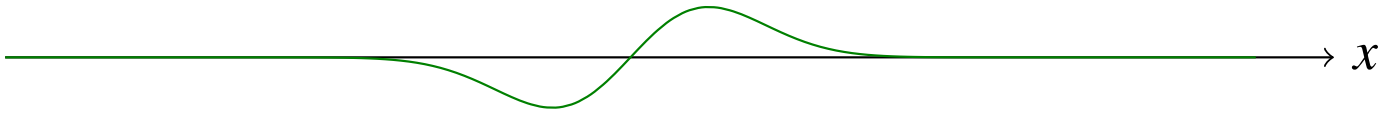

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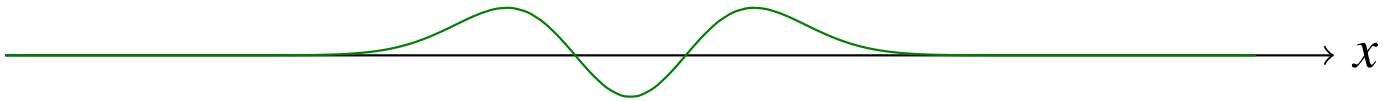

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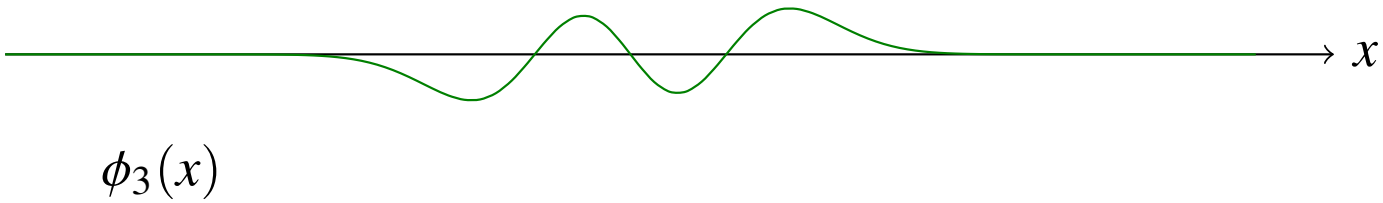

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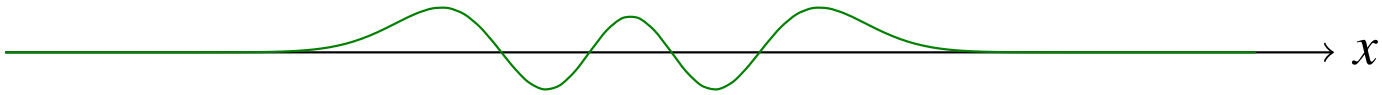

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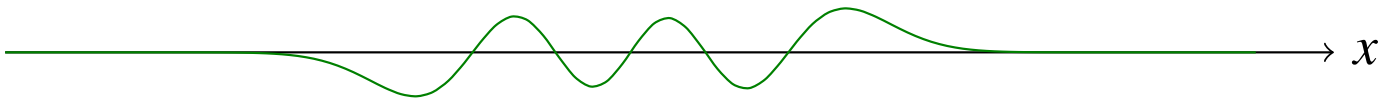

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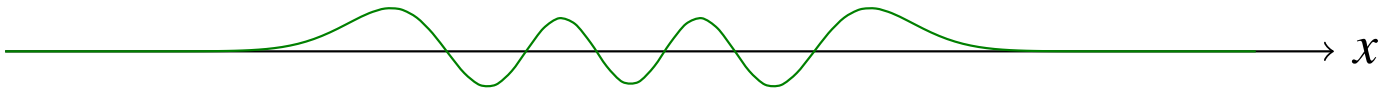

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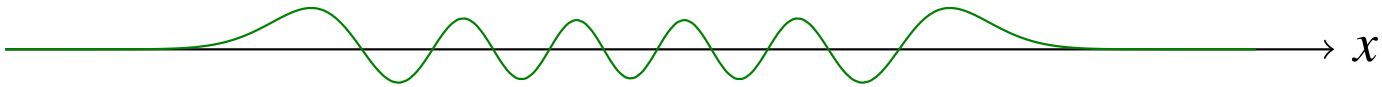

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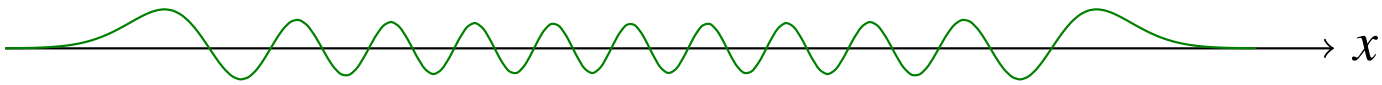

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Hermite function approximation: 1D result

Consider the expansion

$$\psi(x) = \sum_{n=0}^{\infty} c_n \phi_n(x).$$

Theorem (Approximation by Hermite functions (See S.K. '09))

Assume $\psi(x)$ falls off exponentially. Then $\psi(x) \in H^k(\mathbb{R})$ if and only if

$$\sum_{n=0}^{\infty} |c_n|^2 n^k \quad < \quad +\infty$$

- That is,

$$p(n) = |c_n|^2 \sim n^{-(k+1)}.$$

- What is $H^k(\mathbb{R})$? All (weak) partial derivatives up to order k exist and are L^2-integrable
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$$p(n) = |c_n|^2 \sim n^{-(k+1)}.$$
- What is $H^k(\mathbb{R})$? All (weak) partial derivatives up to order k exist and are L^2-integrable
- Rapid fall-off of $p(n)$ (and c_n) $\Leftrightarrow \psi(x)$ is smooth

Hermite function approximation: 1D result

Consider the expansion

$$\psi(x) = \sum_{n=0}^{\infty} c_n \phi_n(x).$$

Theorem (Approximation by Hermite functions (See S.K. '09))

Assume $\psi(x)$ falls off exponentially. Then $\psi(x) \in H^k(\mathbb{R})$ if and only if

$$\sum_{n=0}^{\infty} |c_n|^2 n^k \quad < \quad +\infty$$

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Numerical calculation

- We consider

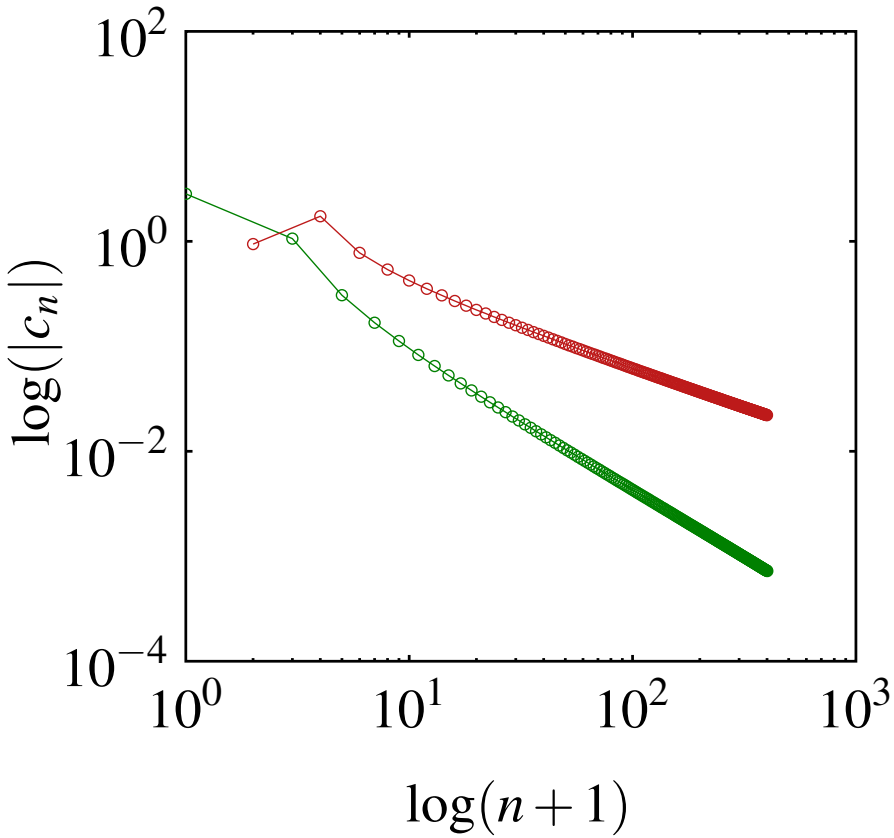
$$f(x) = (1+2|x|)e^{-x^2/2}$$
$$g(x) = f'(x)$$

- We have:

$$|c_n| \sim n^{-1.28}$$

$$|c_n| \sim n^{-0.74}$$

- Notice: k not necessarily an integer!



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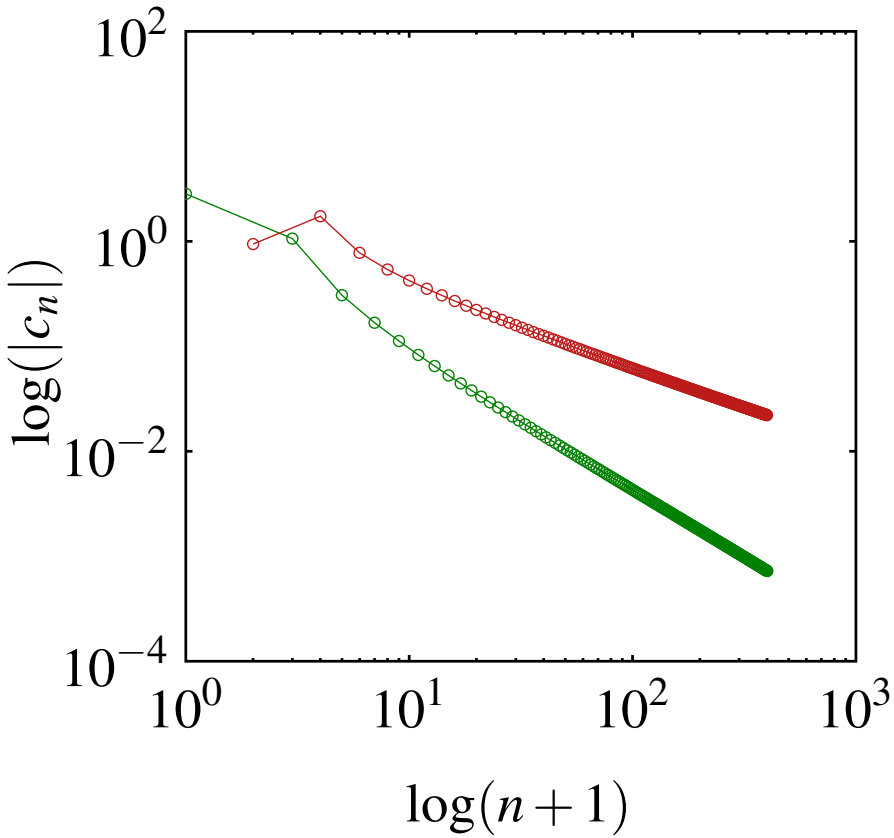

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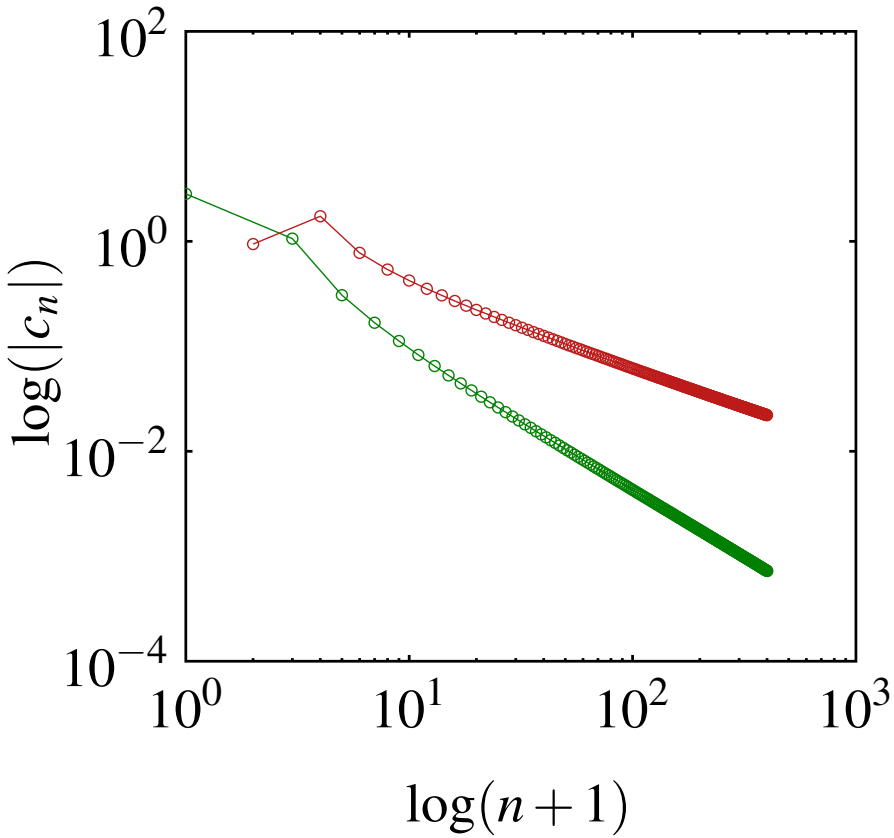

Weak differentiability, again

- Would it be sufficient to consider standard derivatives of $\psi(x)$?
- No! The concept of weak differentiability is essential to this result.
- Both the below functions are smooth everywhere except at $x = 0$. But the jump discontinuity distinguishes the two.

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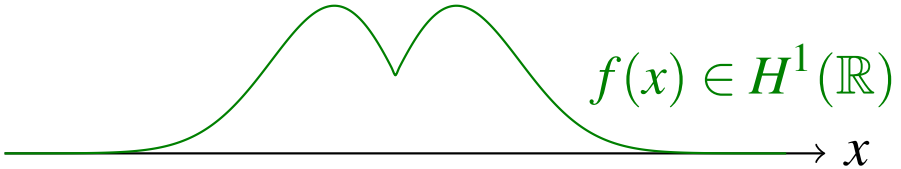

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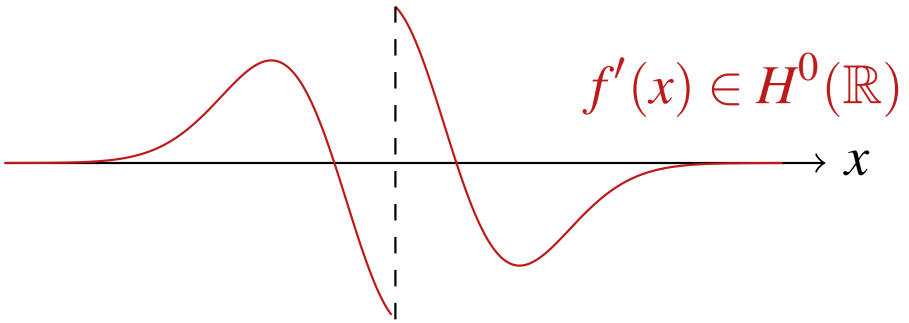
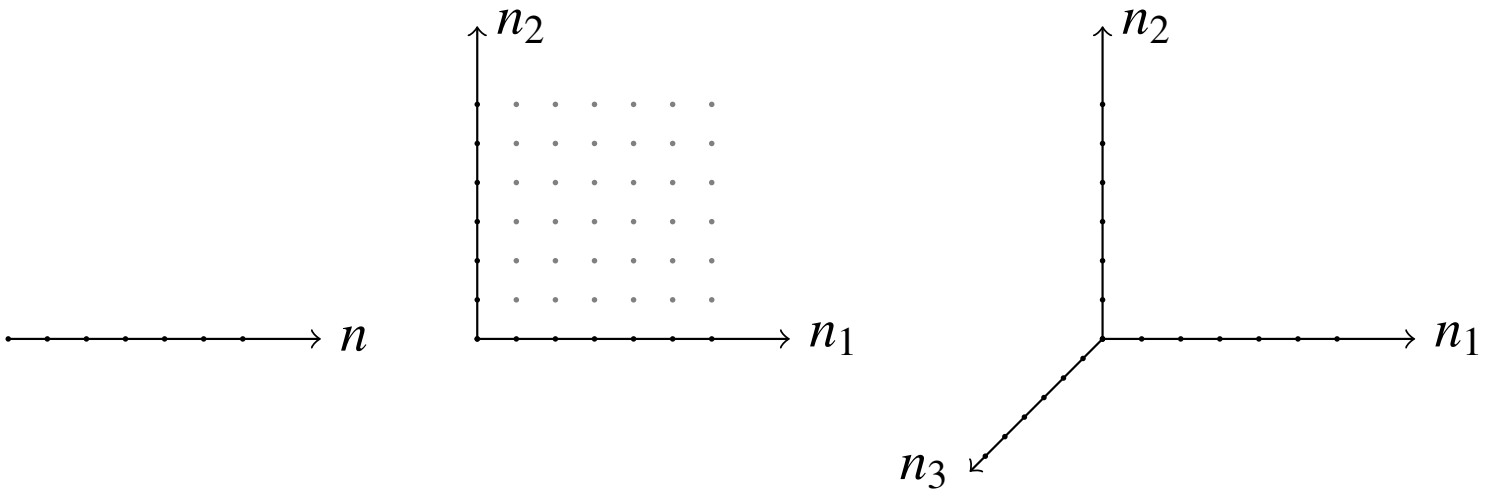


Generalization to d dimensions

- Consider expansion of $\psi(\mathbf{r})$,

$$\begin{aligned}\psi(\mathbf{r}) &= \sum_{\mathbf{n}} c_{\mathbf{n}}\,\phi_{\mathbf{n}}(\mathbf{r}) \\ &= \sum_{n_1=0}^{\infty}\cdots\sum_{n_d=0}^{\infty} c_{n_1\cdots n_d}\phi_{n_1}(r_1)\cdots\phi_{n_d}(r_d)\end{aligned}$$

- How do we study the limit "large $\mathbf{n}$" as we have a d-dimensional *array* of coefficients?



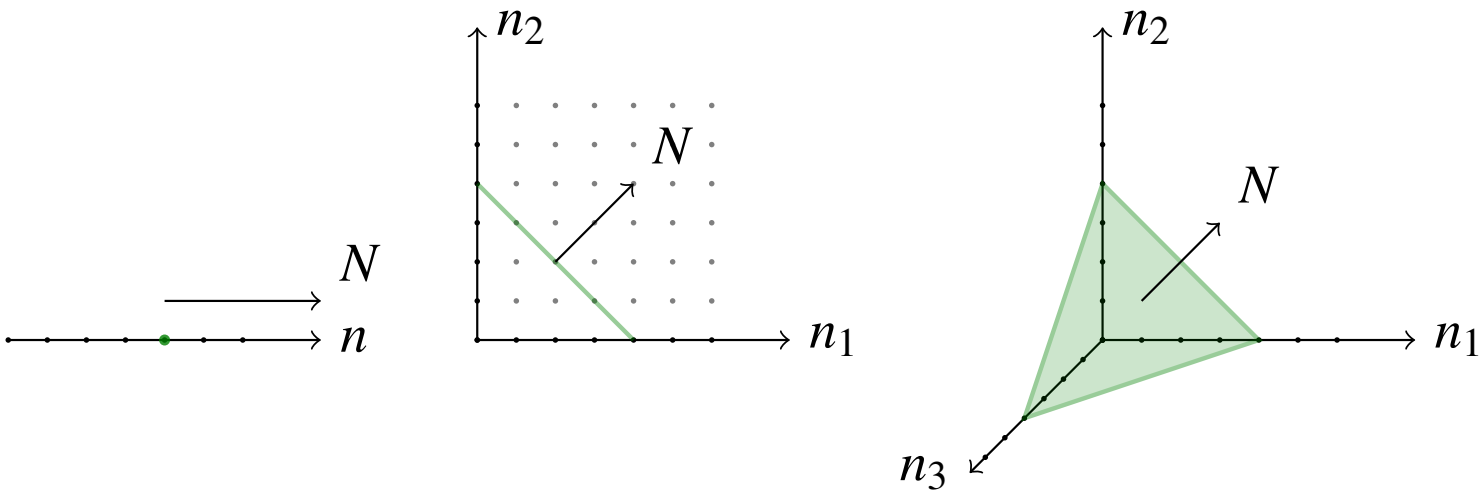
Generalization to d dimensions *II*

- Solution: Study behaviour of shell probability $p(N)$:

$$p(N) \equiv \langle \psi | P_N | \psi \rangle \,, \quad P_N \text{ projects onto } N\text{'th shell}$$

- We have:

$$p(N) = \sum_{|\mathbf{n}|=N} |c_{\mathbf{n}}|^2$$



Harmonic oscillator function approximation: general result

Consider the expansion

$$\psi(\mathbf{r}) = \sum_{\mathbf{n}} c_{\mathbf{n}}\, \phi_{\mathbf{n}}(\mathbf{r}).$$

Theorem (Approximation by h.o. functions (See S.K. '09))

Assume $\psi(\mathbf{r})$ falls off exponentially. Then $\psi(\mathbf{r}) \in H^k(\mathbb{R}^d)$ if and only if

$$\sum_{N=0}^{\infty} p(N) N^k \quad < \quad +\infty$$

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- Notice: Valid for many-body wave-functions as well!

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Approximation in model space

- Let's recall the "hyper-pyramid"/energy cut model space $\mathscr{V}_{\mathrm{EC}}$:

$$\mathscr{V}_A = \mathrm{Span}\left\{\text{Slater det's with h.o. energy} \leq E_{\max}\right\}$$

- As the Slater determinants are Ad-dimensional h.o. eigenfunctions,

$$\begin{aligned}\mathscr{V}_A &= \mathrm{Span}\left\{\text{Slater det's with h.o. energy} \leq N_{\max} + Ad/2\right\} \\ &= \underbrace{\left(P_0 + P_1 + \cdots + P_{N_{\max}}\right)}_{\equiv P}\mathscr{H}\end{aligned}$$

- We obtain for the error in the norm

$$\|Q\Psi\|^2 = \sum_{N=N_{\max}+1}^{\infty} p(N) \sim N_{\max}^{-k}$$

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Approximation using Slater determinants

Using this information, we obtain the following:

Theorem (Accuracy of FCI calculations)

Suppose we solve the many-body problem with FCI using HO basis functions in an energy cut model space with parameter $E_{max} = N_{max} + Ad/2$. Assume that the exact solution $|\Psi\rangle \in H^k(\mathbb{R}^{Ad}) \otimes \mathbb{C}^{q^A}$. Then:

$$\|\delta\Psi\|_1 \leq C_1 N_{max}^{-(k-1)/2}$$

and

$$\delta E \leq C_2 N_{max}^{-(k-1)}$$

The constants depends roughly linearly on the strength of the interactions.

Behaviour of exact wave function

- Singular potential $u(i,j) \Rightarrow$ well-known cusp conditions on wave functions across singularities (see Hoffmann-Ostenhof *et al.)*
- Ground state for two-electron dot with $\lambda = 1$:

$$\Psi_0(\mathbf{r}_1, \mathbf{r}_2) = (1 + cr_{12})e^{-(r_1^2 + r_2^2)/2}$$

- Pauli principle $\Rightarrow$ smoothness varies for different wave functions
- Also some other interesting results are available: Work of Yserentant, Hackbush, Hoffmann-Ostenhof and others

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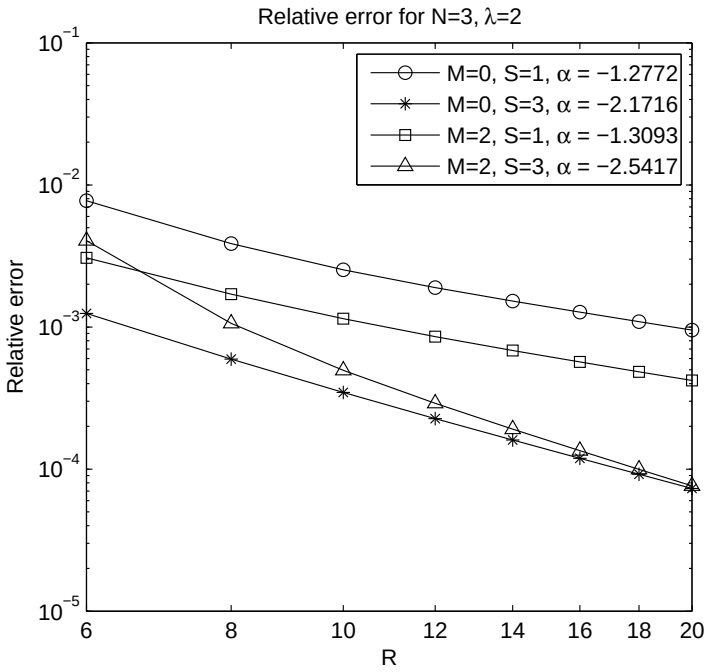
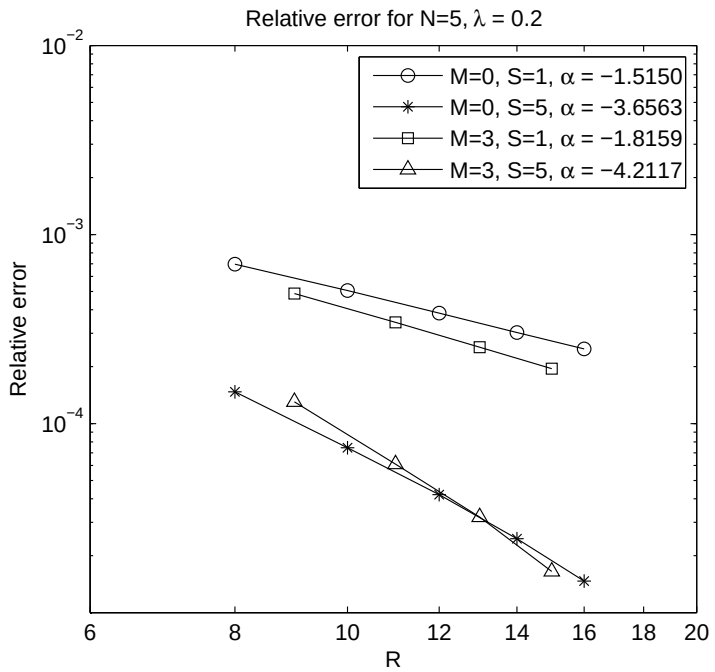
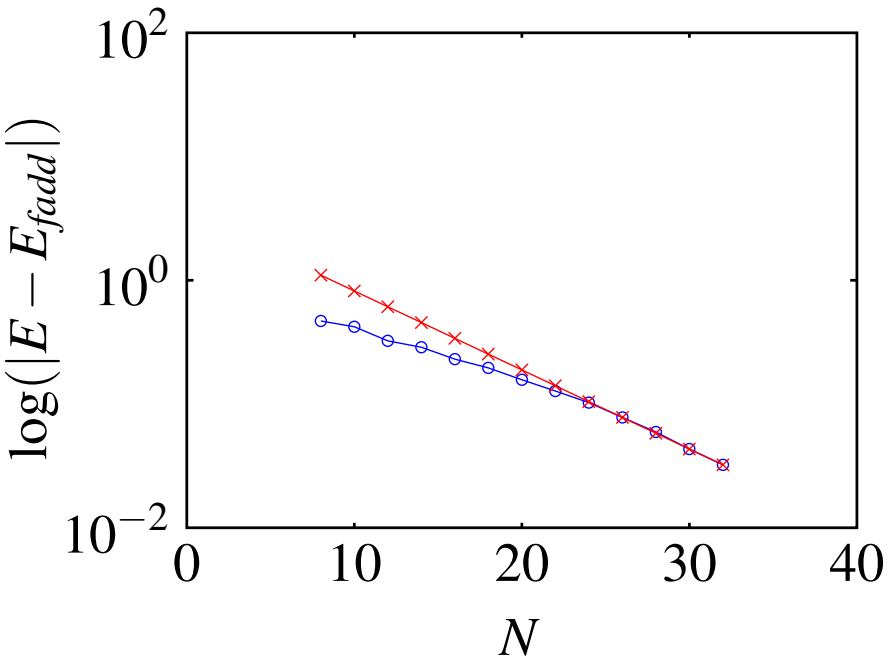
Convergence of parabolic dot FCI

N is number of particles, $R = N_{\max}$, M is total angular momentum, S is total electron spin. Curves show $\delta E/E$.

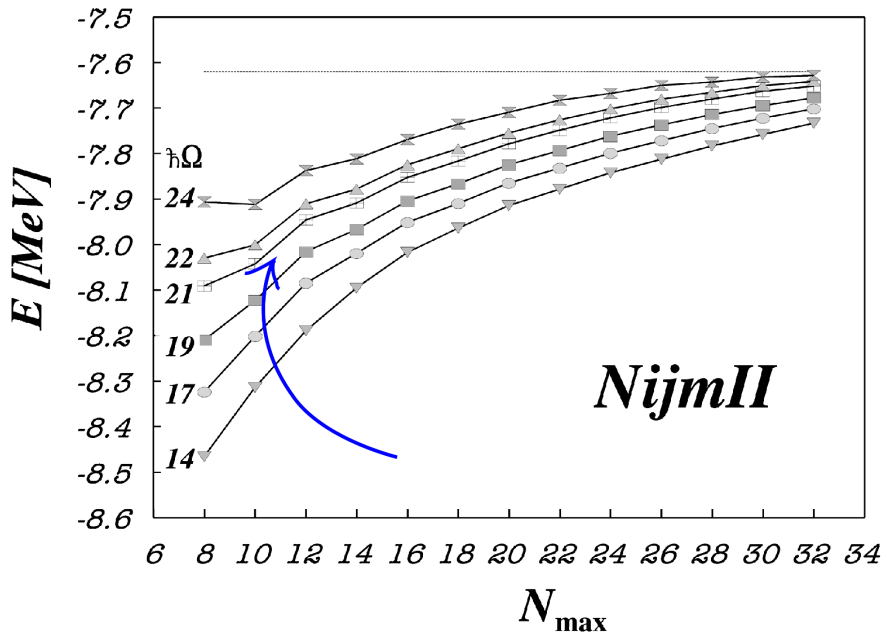




Exponential (?) convergence in NCSM calculations



$\hbar\omega = 24$ MeV, $|E - E_{\text{fadd}}| \sim Ce^{-0.15N}$



From Navratil & Barrett, PRC **57**, p. 562 (1998). Convergence test of NCSM for ^{3}H, Nijmegen II effective interaction.

Outline

From CI to coupled cluster (CC)

- CI is a variational search within a linear space $\mathscr{V}$.
- CC is a non-variational search within a non-linear space $\mathscr{X}\,(\subset \mathscr{V})$
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True ground state; ansatz always valid

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Excitation operators

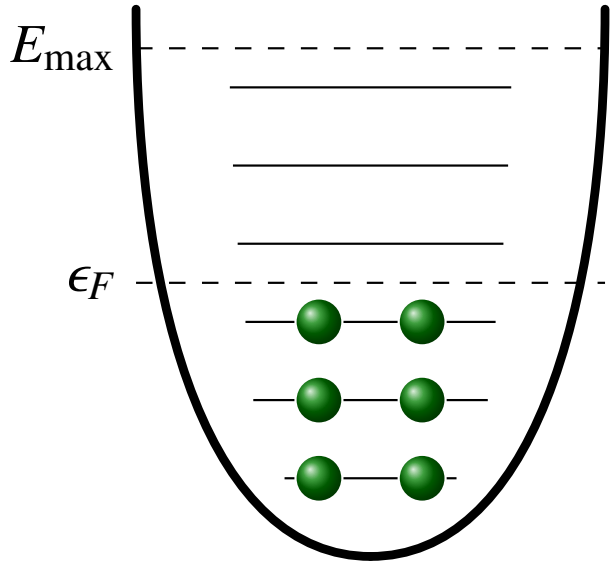
- Suppose $|\Phi_0\rangle$ is filled with states up to ϵ_F:

$$|\Phi_0\rangle = c^\dagger_{\alpha_1} \cdots c^\dagger_{\alpha_A} |-\rangle$$

- Let (a_i) be *below* and (b_i) *above* Fermi level. Define:

$$X^b_a = c^\dagger_{b_1} \cdots c^\dagger_{b_n} c_{a_n} \cdots c_{a_1}$$

- Moves particles from below ϵ_F to above ϵ_F
- Notice: $X^b_a |\Phi_0\rangle$ generates basis for $\mathscr{V}_{\mathrm{DP}}$.



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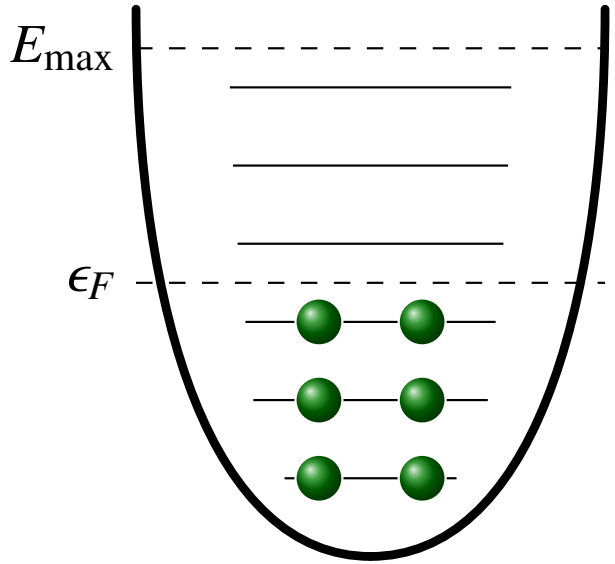

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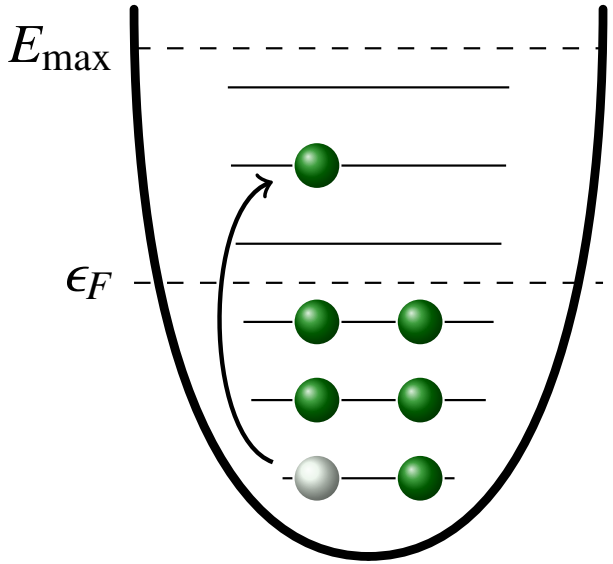

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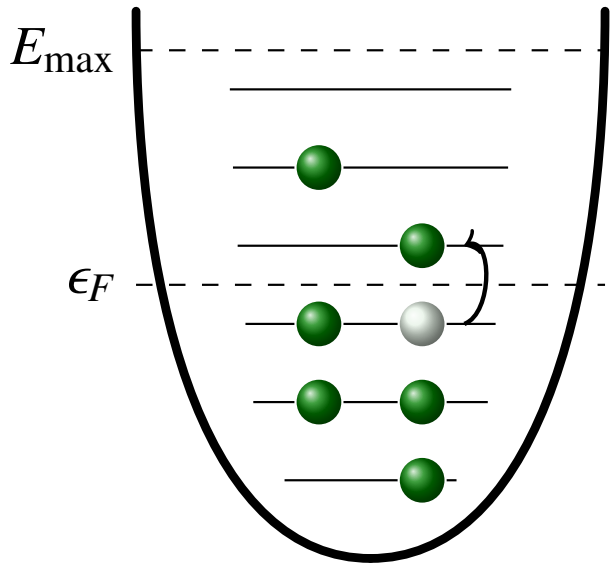

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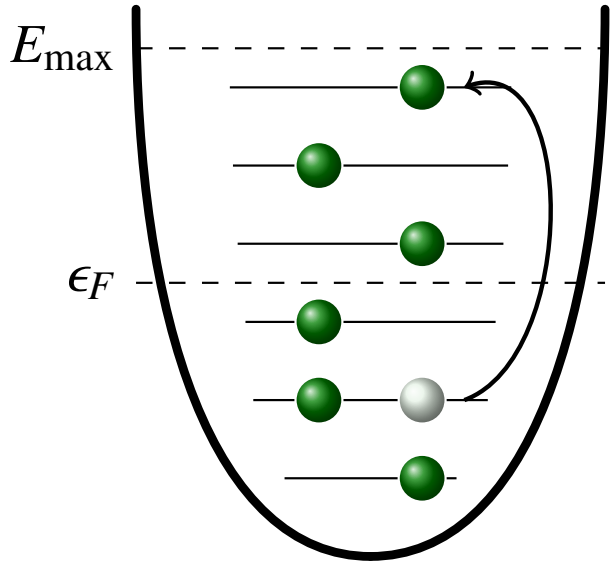

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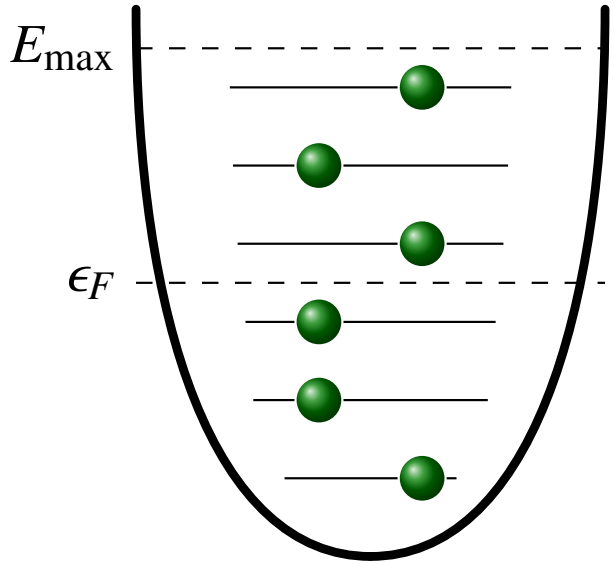

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The cluster operator T

- Recall the ansatz:

$$|\Psi\rangle = e^T |\Phi_0\rangle$$

- T is on the form

$$T = T_1 + T_2 + \cdots + T_K$$

where

$$T_n = \sum_{a,b} t_{a_1 a_2 \cdots a_n}^{b_1 b_2 \cdots b_n} X_{a_1 a_2 \cdots a_n}^{b_1 b_2 \cdots b_n}$$

- If $K = 1$, we get CCS ("singles"). $K = 2$ gives CCSD ("singles and doubles"), et.c. $K = A$ is exact!
- We set $\mathbf{t} = (\mathbf{t}^{(1)}, \cdots, \mathbf{t}^{(K)})$; a vector of all the amplitudes.

$$T = T(\mathbf{t}) \quad \longleftarrow \quad \text{a linear function of the amplitudes } \mathbf{t}^{(n)}$$

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$$T = T_1 + T_2 + \cdots + T_K$$
where
$$T_n = \sum_{a,b} t_{a_1 a_2 \cdots a_n}^{b_1 b_2 \cdots b_n} X_{a_1 a_2 \cdots a_n}^{b_1 b_2 \cdots b_n}$$
- If $K = 1$, we get CCS ("singles"). $K = 2$ gives CCSD ("singles and doubles"), et.c. $K = A$ is exact!
- We set $\mathbf{t} = (\mathbf{t}^{(1)}, \cdots, \mathbf{t}^{(K)})$; a vector of all the amplitudes.

$$T = T(\mathbf{t}) \quad \longleftarrow \quad \text{a linear function of the amplitudes } \mathbf{t}^{(n)}$$

The cluster operator T

- Recall the ansatz:
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CC equations

- Nonlinear search space $\mathscr{X}$ for CCSD$\cdots K$:

$$\mathscr{X} = \left\{ e^{T(\mathbf{t})} |\Phi_0\rangle \ : \ \mathbf{t} = (\mathbf{t}^{(1)}, \cdots, \mathbf{t}^{(K)}) \right\}$$

- *Could* attempt a variational search within $\mathscr{X}$, but this is too complicated.
- Instead, non-variational amplitude equations are used:

$$\mathbf{f}(\mathbf{t}) = 0, \quad f_i(\mathbf{t}) \equiv \langle \Phi_i | e^{-T(\mathbf{t})} H e^{T(\mathbf{t})} | \Phi_0 \rangle = 0 \qquad \forall i \neq 0$$

- Energy expression:

$$\begin{aligned} E_{\mathrm{CC}} = J(\mathbf{t}) &\equiv \langle \Phi_0 | e^{-T(\mathbf{t})} H e^{T(\mathbf{t})} | \Phi_0 \rangle \\ &= \langle \Phi_0 | H (1 + T_2 + \frac{1}{2} T_1^2) | \Phi_0 \rangle \end{aligned}$$

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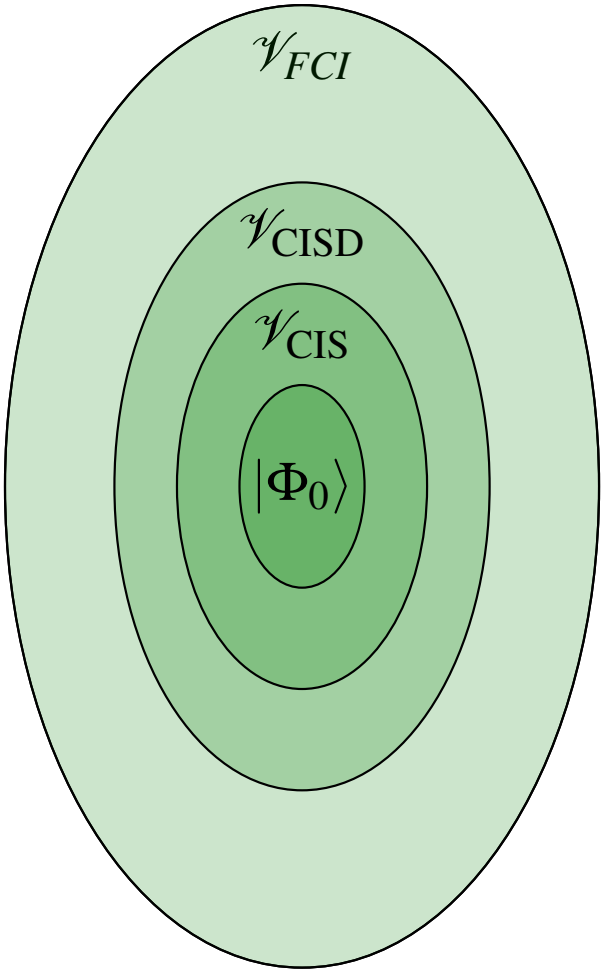
Basics of the coupled cluster method



- Left: Illustration of CI spaces formed by K-fold excitations of $|\Phi_0\rangle$.
- Illustration of CCS, truncating T at T_1. Notice: $e^T = 1 + T + T^2/2 + \cdots$ contains higher order excitations
- CISD; covering more of $\mathscr{V}_{\mathrm{DP}}$
- And so on ...
- CC works extremely well because of the "exponentiating"

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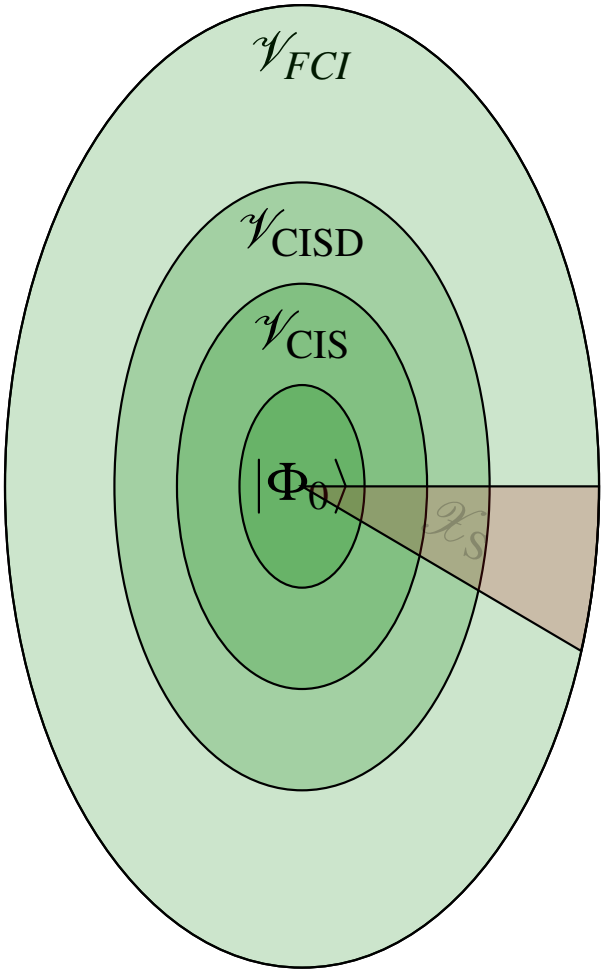

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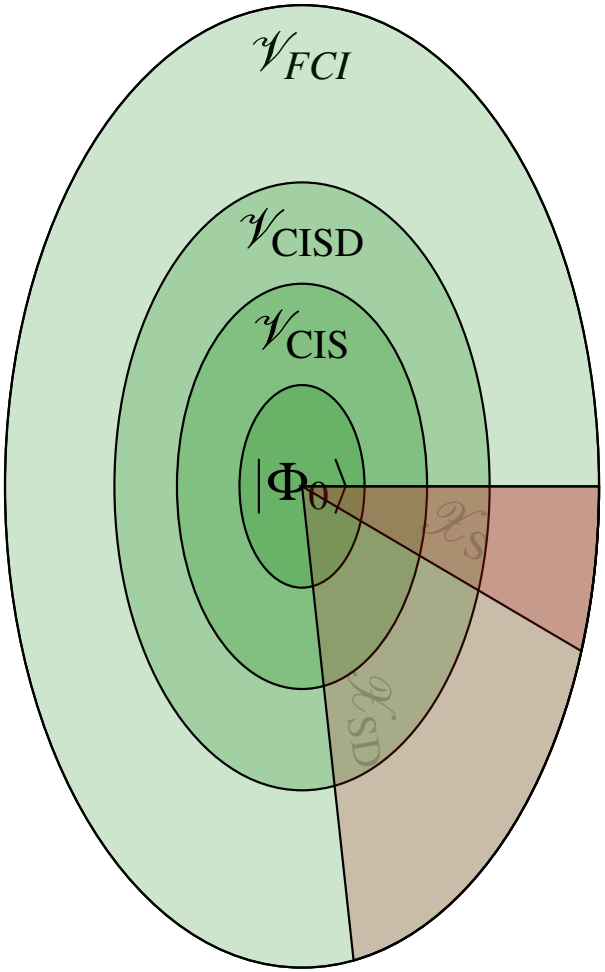

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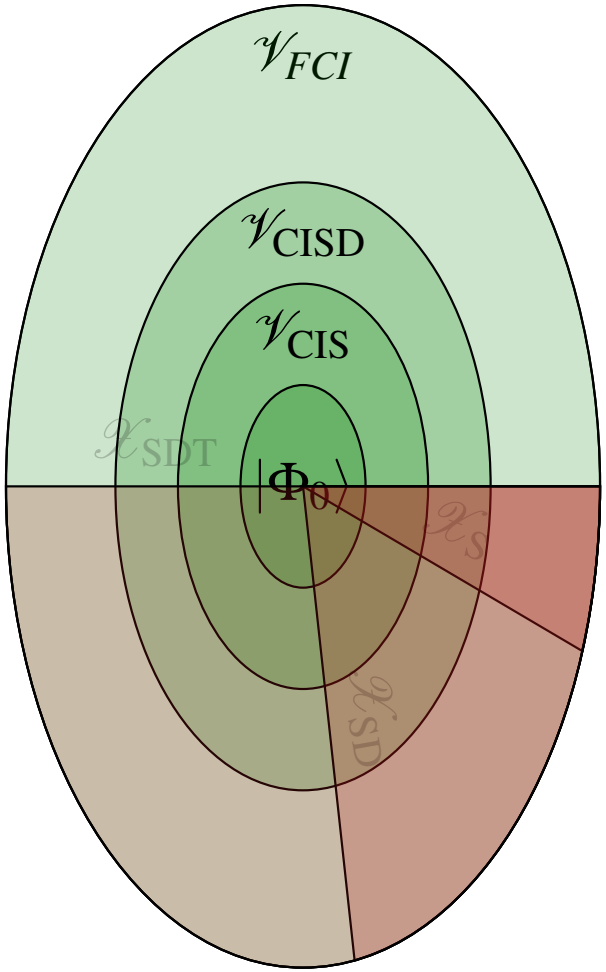

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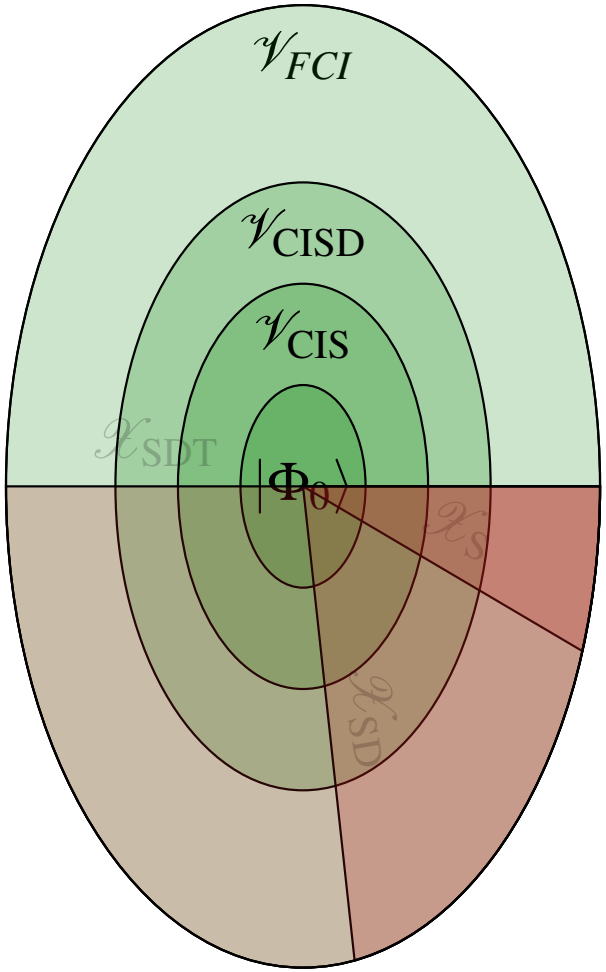

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Two axes of convergence/accuracy

Cluster operator truncation at $T = T_1 + \cdots T_K$

(At least) semi-empirically: For nuclei: CCS gives 90 % correlation energy, CCSD gives 99 %

$\Rightarrow$ Truncating T seems to give rise to a non-vanishing error in converged results, becoming smaller as we move from CCS to CCSD, and so on.

Model space size parameter $E_{\max}$

(At least) semi-empirically: Relevant quantities converge in the same way as FCI.

$\Rightarrow$ The FCI analysis should be useful for the CC analysis as well. The errors in CCS, CCSD, etc, could be understood from such analysis as well. Same types of estimates.

Goal

$$|E - E_{\mathrm{CC}}| \sim (E - E_{h,\mathrm{FCI}}) + \Delta E_{\mathrm{CCS}} + \Delta E_{\mathrm{CCSD}} + \cdots + \Delta E_{\mathrm{CCSD}\cdots K}$$

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Imagined route for quantum dots

1. Analysis of the Hartree-Fock method for quantum dots
   - Usually, HF orbitals are used instead of "bare" orbitals. We haven't discussed this. But ...
   - Luckily, we deal with the harmonic oscillator: simple analysis
   - Known abstract results (P-L. Lions and others) greatly simplify
2. Formulation of abstract results in terms of analytic properties of $|\Psi\rangle$, i.e., k in $|\Psi\rangle \in H^k(\mathbb{R}^{Ad})$
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Bibliography

Here is a list of relevant literature:

- Kvaal, S. *"Harmonic oscillator eigenfunction expansions, quantum dots, and effective interactions"*, `arXiv:0808.2145v2` (2009), to appear in PRB.
- Hoffmann–Ostenhof, M. *et al.*, *"Electronic wave functions near coalesce points"*, Phys. Rev. Lett. **68**, pp. 3857-3860 (1992)
- Lions, P.–L., *"Solutions of Hartree-Fock Equations for Coulomb Systems"*, Commun. Math. Phys. **109**, pp. 33–97 (1987)
- Babuska, I. & Osborn, J., *"Estimates for the Errors in Eigenvalue and Eigenvector Approximation by Galerkin Methods, with Particular Attention to the Case of Multiple Eigenvalues"*, SIAM J. Numer. Anal., **24**, pp. 1249 (1987)
- Schneider, R. *"Analysis of the projected CC method"*, Preprint (2009)
- Kutzelnigg, W. *"Error analysis and improvements of CC theory"*, Theor. Chim. Acta **80**, pp. 389–386 (1991)

Weak differentiability

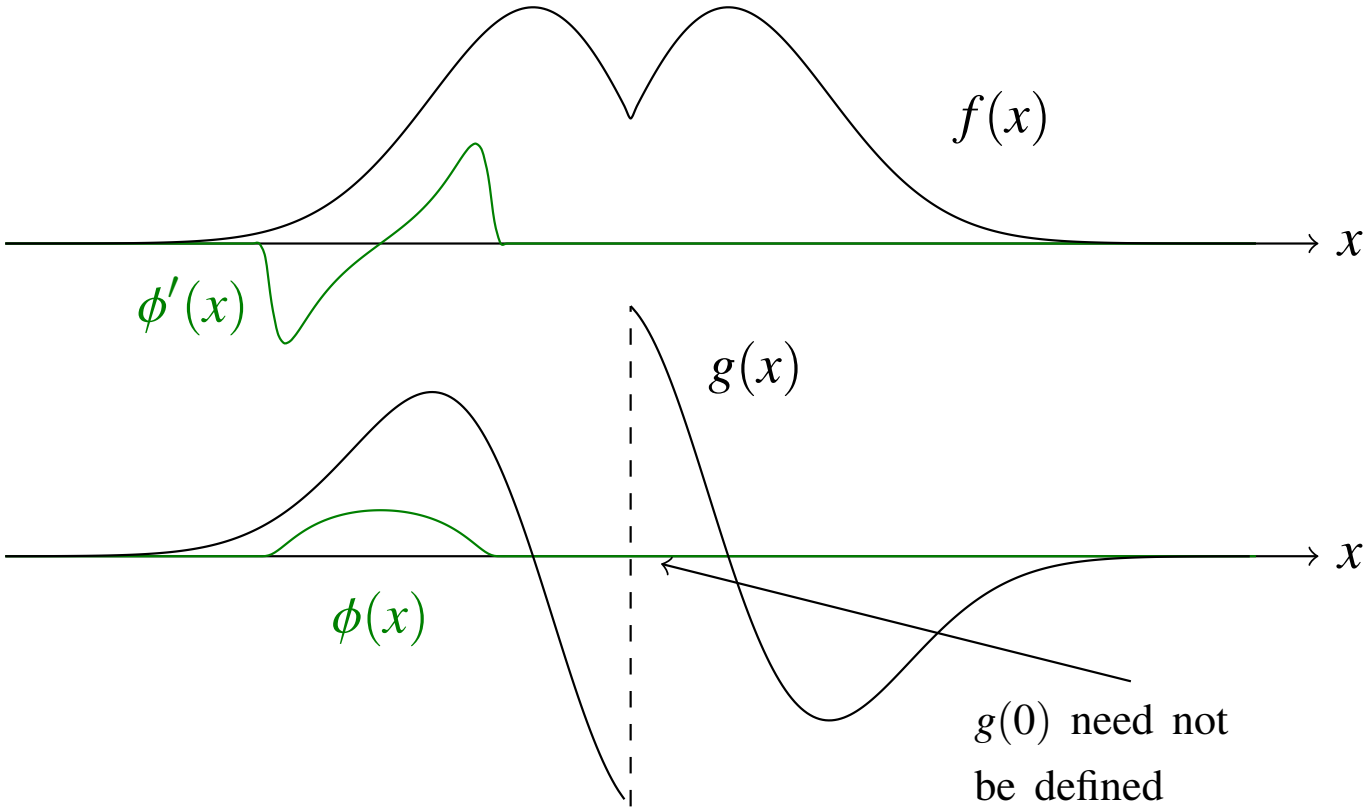
- Hilbert spaces of differentiable functions $\Rightarrow$ Weak differentiability concept
- Derivative in "average sense"; it "works" with respect to partial integration
- $f(x) \in L^2(\mathbb{R})$ is said to have a weak derivative if there exists $g(x) \in L^2$ if:

$$\int f(x)\phi'(x)\mathrm{d}x = -\int g(x)\phi(x)\mathrm{d}x \qquad \forall \phi \in C_0^\infty.$$

  Then $f'(x) = g(x)$ in the weak sense.
- Sobolev space $H^k(\mathbb{R}^n)$:

  k times weakly differentiable funcions in $L^2(\mathbb{R}^n)$

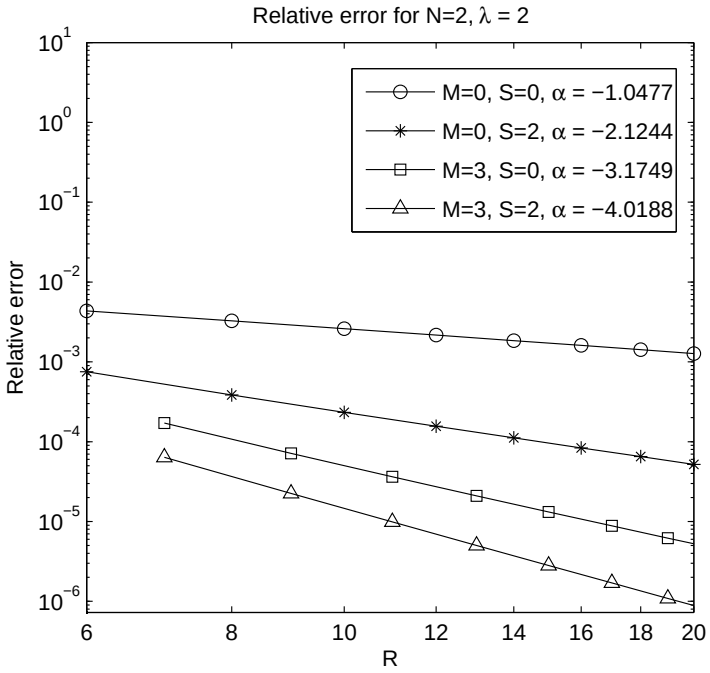
Weak differentiability *II*

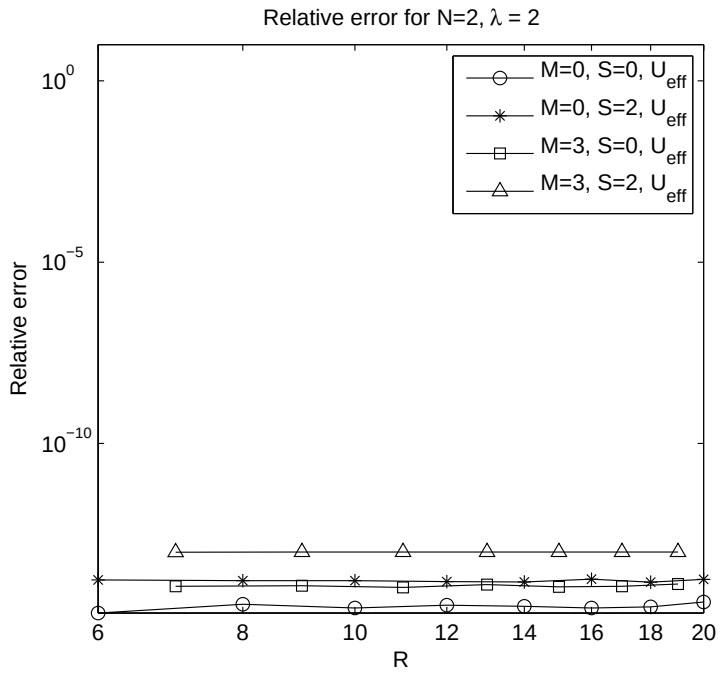


- $\phi(x)$ a smooth test function
- "Checks" a candidate for a weak derivative using i.b.p.
- Note: $f(x)$ is w. differentiable. $g(x)$ *not* w. differentiable due to jump.

FCI with renormalized interaction

Comparing with calculations using renormalized interaction of Lee-Suzukui type





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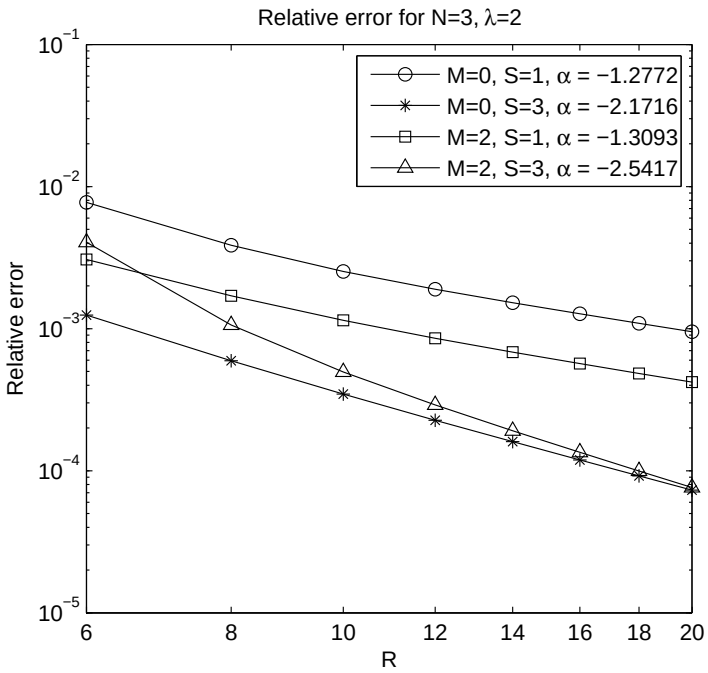

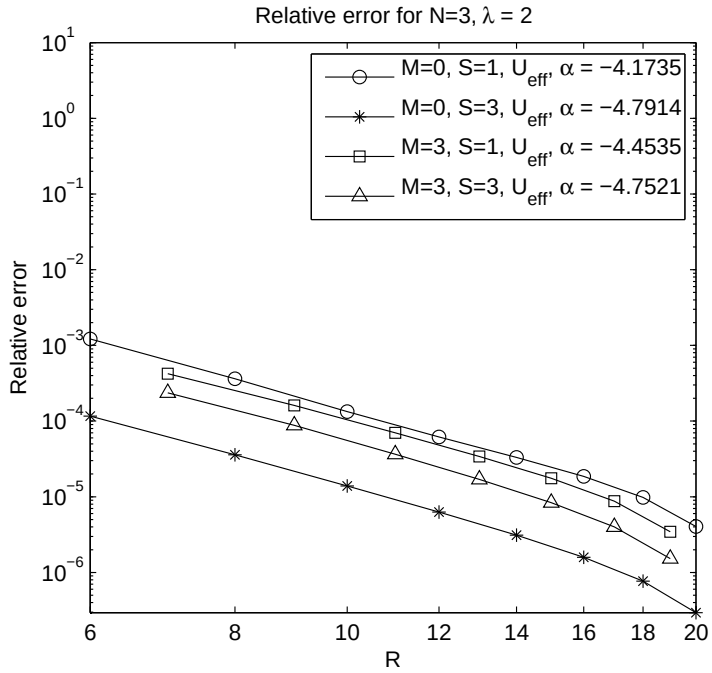

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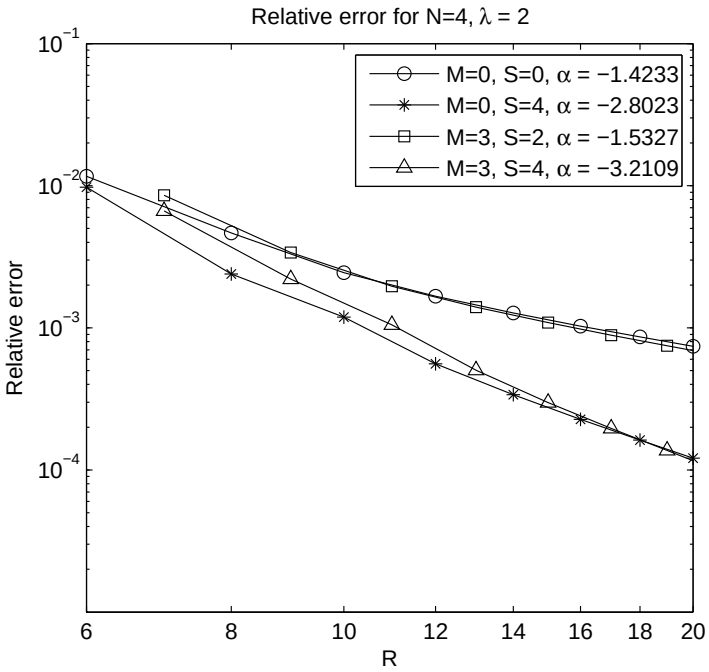

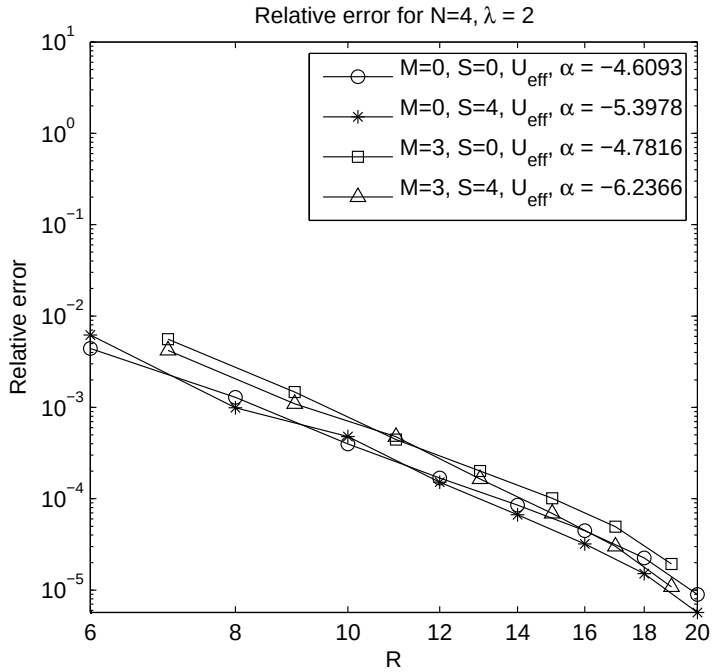

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