Computational Many-Body Methods in Physics

Anton N. Torgersen

University of Oslo
FYS4480

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Outline

Introduction: The Many-Body Problem

Goal: Solve the Schrödinger equation for N interacting particles.

$$\hat{H}\,|\Psi\rangle = E\,|\Psi\rangle$$

The Challenge: The Hilbert space grows factorially with N-particles and K-orbitals. A change in one particle creates a corresponding change in the entire many-body state.

$\Longrightarrow$ Exact diagonalization (FCI) is impossible for large systems.

The Independent Particle Basis

The Pauli Principle Fermionic wavefunctions must be anti-symmetric. The simplest ansatz satisfying this is the **Slater Determinant**:

$$|\Phi_0\rangle \leftrightarrow \Psi_{SD}(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \frac{1}{\sqrt{N!}} \det |\phi_p(\mathbf{r}_q)|$$

Second Quantization To handle this efficiently, we work in Fock space using creation ($a^\dagger$) and annihilation (a) operators.

- **correspondence:** A Slater Determinant is represented as a string of operators acting on the vacuum:
$$|\Phi_0\rangle = \prod_{i \leq F} a_i^\dagger |0\rangle = a_1^\dagger a_2^\dagger \ldots a_N^\dagger |0\rangle$$
- **Anti-commutation:** $\{a_p, a_q^\dagger\} = \delta_{pq}$ enforces the Pauli principle.

The Model System: Pairing Model

To compare methods, we use the **Pairing Hamiltonian** as a test case:

$$\hat{H} = \hat{H}_0 + \hat{H}_I$$

- **Single Particle ($\hat{H}_0$):** simple energy levels with equal spacing.

$$\hat{H}_0 = \sum_{p,\sigma} (p-1) \hat{a}^\dagger_{p\sigma} \hat{a}_{p\sigma}$$

- **Interaction ($\hat{H}_I$):** Constant pairing strength g. Moves pairs $(p+, p-)$ to $(q+, q-)$.

$$\hat{H}_I = -\frac{1}{2} g \sum_{pq} \hat{a}^\dagger_{p+} \hat{a}^\dagger_{p-} \hat{a}_{q-} \hat{a}_{q+}$$

Pairing model representation

We will truncate the Hilbert space to only have 4 particles and 4 levels.

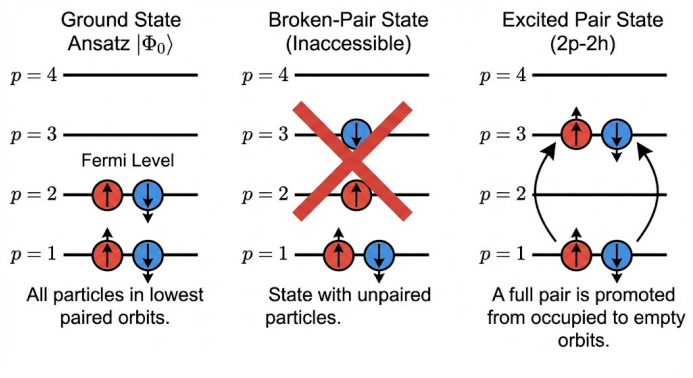

Figure 1: Schematic of the pairing model

Full Configuration Interaction (FCI)

The Exact Solution

- Expands the wavefunction Ψ in the complete basis of all possible Slater Determinants generated from the reference $|\Phi_0\rangle$.
- **The Expansion:**

$$|\Psi_{FCI}\rangle = \left(1 + \sum_{ia} \hat{C}_i^a + \sum_{ijab} \hat{C}_{ij}^{ab} + \dots\right) |\Phi_0\rangle$$

$$|\Psi_{FCI}\rangle = c_0 |\Phi_0\rangle + \sum_{ia} c_i^a |\Phi_i^a\rangle + \sum_{ijab} c_{ij}^{ab} \left|\Phi_{ij}^{ab}\right\rangle + \dots$$

The Method: Exact Diagonalization

- Construct the full Hamiltonian matrix in this many-body basis.
- Solve the eigenvalue problem $\hat{H}\mathbf{c} = E\mathbf{c}$ to find exact energies and coefficients.

FCI Scaling

The Curse of Dimensionality The dimension of the Hilbert space (D_{FCI}) is the number of ways to distribute N particles in K orbitals:

$$D_{FCI} = \binom{K}{N} = \frac{K!}{N!(K-N)!}$$

- Scales factorially with system size.
- FCI is only feasible for very small systems

Pairing Matrix Elements

The Hamiltonian Matrix for $N = 4$ particles in $K = 4$ levels:

$$H = \begin{pmatrix} 2-g & -g/2 & -g/2 & -g/2 & -g/2 & 0 \\ -g/2 & 4-g & -g/2 & -g/2 & 0 & -g/2 \\ -g/2 & -g/2 & 6-g & 0 & -g/2 & -g/2 \\ -g/2 & -g/2 & 0 & 6-g & -g/2 & -g/2 \\ -g/2 & 0 & -g/2 & -g/2 & 8-g & -g/2 \\ 0 & -g/2 & -g/2 & -g/2 & -g/2 & 10-g \end{pmatrix}$$

FCI Results

Results from Midterm (Pairing Model) Exact diagonalization of the Hamiltonian matrix for $N = 4$ particles.

Coupling g	E_{FCI} (Ground State)	Character
-1.0	2.7799	Repulsive
0.0	2.0000	Non-interacting
0.5	1.4168	Attractive
1.0	0.6355	Strong Coupling

Table 1: Exact eigenvalues computed via `numpy.linalg.eigh` (from Calculations.ipynb).

The Mean-Field

The Physical Intuition We simplify the many-body problem by assuming each particle moves independently in an average potential (mean field) created by all other particles.

The Ansatz We assume the ground state is accurately described by a **single** Slater Determinant (the reference state defined earlier):

$$|\Psi\rangle \approx |\Phi_{HF}\rangle$$

The goal of Hartree-Fock is to find the specific set of orthonormal orbitals $\{\phi_p\}$ that minimize the energy of this determinant.

The Energy Functional

The Quantity to Minimize Before finding the orbitals, we must define the energy of our ansatz. Using the Slater-Condon rules, the expectation value of the Hamiltonian for a single determinant is:

$$E[\Phi_{HF}] = \langle \Phi_{HF} | \hat{H} | \Phi_{HF} \rangle$$

The Explicit Functional:

$$E_{HF} = \sum_{i=1}^{N} \langle i | \hat{h}_0 | i \rangle + \frac{1}{2} \sum_{i,j=1}^{N} \langle ij | \hat{v} | ij \rangle_{AS}$$

We must find the expansion coefficients $C_{i\alpha}$ (where $\psi_i = \sum C_{i\alpha}\phi_\alpha$) that minimize this scalar E_{HF}, subject to the orthonormality constraint $\langle \psi_i | \psi_j \rangle = \delta_{ij}$.

The Hartree-Fock Equations

The Minimization By introducing Lagrange multipliers ϵ_i to enforce the constraints and setting the derivative $\frac{\delta \mathcal{L}}{\delta C_{i\alpha}} = 0$, we convert the minimization problem into a Generalized Eigenvalue Problem:

$$\epsilon_i^{HF} C_{i\alpha} = \sum_{\beta} \hat{h}_{\alpha\beta}^{HF} C_{i\beta} \tag{1}$$

The Fock Matrix Elements $\hat{h}_{\alpha\beta}^{HF}$: This matrix effectively "absorbs" the two-body interaction into a one-body mean field:

$$\hat{h}_{\alpha\beta}^{HF} = \langle \alpha | \, \hat{h}_0 \, | \beta \rangle + \sum_{j \leq F} \sum_{\gamma\delta} C_{j\gamma}^* C_{j\delta} \, \langle \alpha\gamma | \, \hat{v} \, | \beta\delta \rangle_{AS}$$

Hartree-Fock Results (Pairing Model)

Application to the Pairing Hamiltonian For the Pairing Model, we found that the standard canonical basis is already the optimal HF basis.

- **Why?** The Pairing Hamiltonian $\hat{V}$ moves pairs ($p \leftrightarrow q$) but does not mix the single-particle levels (p).
- **Result:** The Hartree-Fock energy is simply the expectation value of the reference state:

$$E_{HF} = \langle \Phi_0 | \hat{H} | \Phi_0 \rangle = 2 - g \tag{2}$$

The Normal-Ordered Hamiltonian

Calculating Corrections Since Hartree-Fock provides the optimal reference $|\Phi_0\rangle$, it is convenient to measure all energies relative to the HF energy (E_{HF}).
We utilize Normal Ordering (Wick's Theorem) to redefine our Hamiltonian:

$$\hat{H} = E_{HF} + \hat{H}_N$$

The Normal-Ordered Hamiltonian $\hat{H}_N$: This operator handles the remaining electron correlation. It has a zero vacuum expectation value ($\langle\Phi_0|\,\hat{H}_N\,|\Phi_0\rangle = 0$).

$$\hat{H}_N = \hat{F}_N + \hat{V}_N$$

- $\hat{F}_N = \sum \epsilon_p \{a_p^\dagger a_p\}$: The one-body Fock operator.
- $\hat{V}_N = \frac{1}{4}\sum \langle pq|\,v\,|rs\rangle_{AS}\,\{a_p^\dagger a_q^\dagger a_s a_r\}$: The two-body interaction.

MBPT: Formalism and Partitioning

Partitioning the Hamiltonian We use the Normal-Ordered form we just defined:

$$\hat{H}_N = \hat{F}_N + \hat{V}_N$$

We identify the parts for perturbation theory:

- **Reference ($\hat{H}_0$):** The Fock operator $\hat{F}_N$.
- **Perturbation:** The fluctuation potential $\hat{V}_N$.

The Eigenvalue Problems We seek to estimate the correlation energy ΔE, where:

$$\hat{F}_N |\Phi_0\rangle = W_0 |\Phi_0\rangle \quad \text{(in normal ordering } W_0 = 0\text{)}$$
$$(E_{HF} + \hat{H}_N) |\Psi\rangle = (E_{HF} + \Delta E) |\Psi\rangle$$

The Projection Operator $\hat{Q}$ We define a projector onto the excited determinants (orthogonal to $|\Phi_0\rangle$):

$$\hat{Q} = 1 - |\Phi_0\rangle \langle\Phi_0| = \sum_{j,a} \left|\Phi_j^a\right\rangle \left\langle\Phi_j^a\right| + \dots$$

Formalism of MBPT (Rayleigh-Schrödinger)

The Energy Expansion Starting from the Schrödinger equation, we derive the iterative expansion for the correlation energy ΔE:

$$\Delta E = \sum_{i=0}^{\infty} \langle \Phi_0 | \hat{V}_N \left\{ \frac{\hat{Q}}{W_0 - \hat{F}_N} (\hat{V}_N - \Delta E) \right\}^i | \Phi_0 \rangle \tag{3}$$

From Here to Rayleigh-Schrödinger (RS): This equation contains ΔE on the right-hand side, which generates "unlinked" terms.

- **The Linked Diagram Theorem:** Proves that the terms containing ΔE exactly cancel the unlinked diagrams.
- **Final RS Result:** We are left with a series containing only *linked* diagrams, with no ΔE on the right-hand side.

The Linked Diagram Theorem

Theorem: The exact energy shift ΔE is determined **only** by the sum of all **linked** diagrams:

$$\Delta E = \sum_{n=1}^{\infty} \langle \Phi_0 | \, \hat{V}_N \left(\frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{V}_N \right)^{n-1} | \Phi_0 \rangle_{linked}$$

Allows us to ignore disconnected graphs.

Diagrammatic Representation

Visualizing Interactions (Goldstone Diagrams) Instead of writing out long strings of operators, we use diagrams to represent contributions to the energy.

- **Time:** Runs upwards.
- **Lines:**
  - Up arrow ($\uparrow$): Particle (state above Fermi level).
  - Down arrow ($\downarrow$): Hole (state below Fermi level).
- **Vertices:** Dashed horizontal lines represent the interaction $\langle pq| \hat{v} |rs\rangle$.

Example: The Second Order Energy $E^{(2)}$ corresponds to a diagram where two particles are excited (2p-2h), interact, and then de-excite back to the ground state.

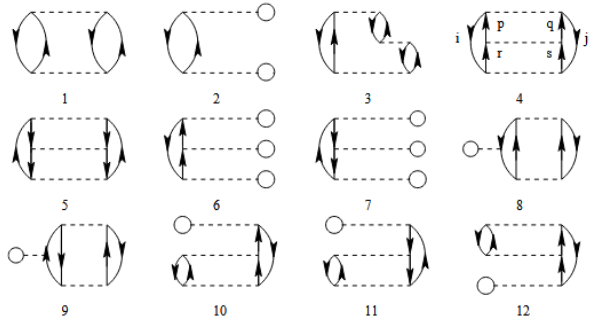

Figure 2: Examples of different Diagrams representing perturbative contributions.

MBPT vs FCI Results

Convergence Analysis Pairing Model

Method	$g = -1.0$	$g = 0.5$	$g = 1.0$
E_{FCI} (Exact)	**2.7799**	**1.4168**	**0.6355**
$E^{(0+1)}$ (HF)	3.0000	1.5000	1.0000
$E^{(2)}$	-0.4667	-0.0624	-0.2190
$E^{(3)}$	+0.5156	-0.0165	-0.1005
$E^{(4)}$	-0.7527	-0.0056	-0.0588
E_{Total} (order 4)	2.2962	**1.4155**	**0.6217**

Table 2: Comparison of Perturbation theory orders vs Exact result.

Observation:

- Excellent agreement for $g = 0.5$ (weak coupling).
- Divergence/oscillations start appearing at strong coupling ($g = -1.0$).

Coupled Cluster Theory

The Exponential Wavefunction We define the wavefunction using an exponential operator acting on the reference:

$$|\Psi_{CC}\rangle = e^{\hat{T}}|\Phi_0\rangle = \left(1 + \hat{T} + \frac{1}{2!}\hat{T}^2 + \dots\right)|\Phi_0\rangle$$

This ensures size-extensivity (energy additivity) for non-interacting systems.

The Cluster Operator The operator $\hat{T}$ generates particle-hole excitations: $\hat{T} = \hat{T}_1 + \hat{T}_2 + \dots$
Truncation Exact CC is too expensive, so we truncate $\hat{T}$.

- **CCSD:** $\hat{T} \approx \hat{T}_1 + \hat{T}_2$. The "gold standard" ($O(N^6)$).
- *Pairing Model:* The Hamiltonian conserves electron pairs. Single excitations ($\hat{T}_1$) break pairs and are forbidden. I.e. we use **CCD** ($\hat{T} \approx \hat{T}_2$) without loss of accuracy.

$$\hat{T}_{CCD} = \frac{1}{4}\sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i$$

CC Equations (Normal Ordered)

Calculation To calculate the Normal-Ordered Hamiltonian (H_N) we use the BCH expansion:

$$\bar{H}_N = e^{-\hat{T}} \hat{H}_N e^{\hat{T}} = \hat{H}_N + [\hat{H}_N, \hat{T}] + \frac{1}{2}[[\hat{H}_N, \hat{T}], \hat{T}] + \dots$$

Equations (General CCSD) We project $\bar{H}_N |\Phi_0\rangle$ onto the reference and excited determinants, and solve for the equations:

$$\begin{aligned} \Delta E_{CC} &= \langle \Phi_0 | \bar{H}_N | \Phi_0 \rangle \\ 0 &= \langle \Phi_i^a | \bar{H}_N | \Phi_0 \rangle \\ 0 &= \left\langle \Phi_{ij}^{ab} \right| \bar{H}_N | \Phi_0 \rangle \end{aligned}$$

One Iteration of CCD (Pairing Model)

The Iterative Process In CCD, we solve for the amplitudes t_{ij}^{ab} iteratively. We start with the MBPT(2) guess and update using the non-linear equations.

Numerical Example ($N = 4$, $g = 1.0$)

- **Initialization (MBPT2):** The calculation starts with the perturbative result:

$$E_{corr}^{(0)} = -0.2190$$

- **Iteration 1:** Solving the amplitude equations once drastically improves the energy:

$$E_{corr}^{(1)} = -0.3128$$

- **Convergence (Iter 60):** The non-linear terms stabilize the solution to the fully correlated limit:

$$E_{corr}^{final} = -0.3696$$

Comparison: Pairing Model Results

CCD vs MBPT vs Exact (FCI) Comparing the correlation energies ($\Delta E = E_{total} - E_{HF}$) across interaction regimes.

Method	$g = -1$ (Strong Repulsion)	$g = 0.5$ (Weak)	$g = 1$ (Strong Attraction)
MBPT(2)	-0.4667	-0.0624	-0.2190
CCD (Iter 60)	**-0.2189**	**-0.0834**	**-0.3696**
FCI (Exact)	**-0.2201**	**-0.0832**	**-0.3645**

Table 3: Correlation energies calculated for N=4 particles.

Conclusions:

- **Weak Coupling ($g = 0.5$):** All methods agree well.
- **Strong Coupling ($g = 1.0$):** MBPT2 underestimates correlation by $\approx 40\%$. CCD captures the infinite order effects, matching Exact FCI almost perfectly.
- **Robustness:** CCD remains stable and accurate even where simple perturbation theory begins to break down.

Motivation

The Problem Solving the Schrödinger equation for $\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ is exponentially expensive.

Solution Replace the wavefunction with the electron density $n(\mathbf{r})$:

$$n(\mathbf{r}) = N \int |\Psi(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N)|^2 d^3 r_2 \ldots d^3 r_N$$

This reduces the problem from $3N$ variables to just 3 (x, y, z).

The Hohenberg-Kohn Theorems

Theorem I: Existence The external potential v_{ext} is uniquely determined by the ground state density $n_0(\mathbf{r})$.

$$n_0(\mathbf{r}) \leftrightarrow v_{ext}(\mathbf{r}) \leftrightarrow \Psi_0$$

Theorem II: The Universal Functional The total energy is a functional of the density:

$$E[n] = \int v_{ext}(\mathbf{r}) n(\mathbf{r}) d^3r + F_{HK}[n]$$

Where $F_{HK}[n]$ is a **universal functional** (independent of the specific system) containing all internal electron operators:

$$F_{HK}[n] = \langle \Psi | \, \hat{T} + \hat{V}_{ee} \, | \Psi \rangle$$

The Kohn-Sham Method

The Ansatz To make the problem solvable, Kohn and Sham mapped the real interacting system to a fictitious system of non-interacting electrons (helps with T) that yields the exact same ground state density:

$$n(\mathbf{r}) = \sum_{i=1}^{N} |\phi_i(\mathbf{r})|^2$$

Partitioning the Functional We rewrite the universal functional F_{HK} by separating the known parts from the unknown many-body effects:

$$F_{HK}[n] = T_s[n] + E_H[n] + E_{XC}[n]$$

The Exchange-Correlation Energy (E_{XC}) This term is defined as the "garbage bin" for all the complex physics we cannot calculate exactly (quantum exchange and correlation):

$$E_{XC}[n] = (T_{true} - T_s) + (V_{ee} - E_H)$$

Implementation: Equations and Approximations

Deriving the Equations Minimizing the total energy $E[n]$ with respect to the orbitals ϕ_i (variational principle) yields a set of single-particle eigenvalue equations:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + v_{ext} + v_{Hartree} + \frac{\delta E_{XC}}{\delta n}\right)\phi_i = \epsilon_i \phi_i$$

The Unknown Term The equation above is exact, but useless without knowing the functional derivative $\frac{\delta E_{XC}}{\delta n}$. We must approximate it.

The Solution: Local Density Approximation (LDA) LDA assumes that at any point $\mathbf{r}$, the exchange-correlation energy depends only on the density at that specific point, using the known values from a Homogeneous Electron Gas (ϵ_{HEG}):

$$E_{XC}^{LDA}[n] = \int n(\mathbf{r})\epsilon_{HEG}(n(\mathbf{r}))d^3r$$

Comparison: DFT vs Hartree-Fock

Similarities: Both are Mean-Field theories solving single-particle equations ($O(N^3)$ to $O(N^4)$).

Feature	**Hartree-Fock (HF)**	**DFT (Kohn-Sham)**
Exchange	Exact.	Approximate (in E_{XC}).
Correlation	None (by definition).	Included (approx. in E_{XC}).
Main Error	Always overestimates Energy.	Depends on functional choice.

Table 4: Key differences between the two mean-field approaches.

Final Summary

Method	Strengths	Weaknesses
FCI	**Exact solution.** The benchmark for all other methods.	Exponential scaling ($N!$). Limited to tiny systems.
Hartree-Fock	Computationally cheap ($O(N^4)$). Provides the orbital basis.	Zero correlation energy.
MBPT	Systematically improvable. Simple to implement.	Diverges for strong interactions (e.g., $g = -1$). More computationally expensive for every term.
Coupled Cluster	The Gold Standard. High accuracy and size-extensive.	Expensive ($O(N^6)$). Mathematical complexity.
DFT	Efficient ($O(N^3)$) with electron correlation included.	Exact functional is unknown. No systematic improvement.

- **Weak Coupling ($g = 0.5$):** Perturbation theory (MBPT) is sufficient and efficient.
- **Strong Coupling ($g = -1.0$):** Perturbation theory breaks down. Non-perturbative

Thank You!

The Lipkin-Meshkov-Glick (LMG) Model

System Definition

- $N = 4$ fermions distributed in two energy levels with degeneracy $d = 4$.
- States characterized by spin $\sigma = \pm 1$ and quantum number p.

Quasi-Spin Formalism The Hamiltonian is expressed using quasi-spin operators $\hat{J}_z, \hat{J}_\pm$:

$$\hat{H} = \hat{H}_0 + \hat{H}_1 + \hat{H}_2 \tag{4}$$

Using the commutation relations derived in Midterm 1, these terms are:

$$\hat{H}_0 = \epsilon \hat{J}_z$$

$$\hat{H}_1 = \frac{1}{2} V(\hat{J}_+^2 + \hat{J}_-^2) \quad \text{(Moves pairs of particles)}$$

$$\hat{H}_2 = \frac{1}{2} W(\hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+ - \hat{N}) \quad \text{(Spin exchange term)}$$

Hartree-Fock Stability in the Lipkin Model

Variational Analysis We introduced a mixing coefficient x ($C_{\alpha+}^2 = x$) between the levels. The stability of the non-interacting ground state ($x = 0$) depends on the interaction strength.

Stability Condition

The trivial HF solution is a stable minimum if and only if:

$$\frac{\epsilon}{3} > -(V + W)$$

Phase Transition Example

- **Case 1 - Weak:** $\frac{\epsilon}{3} > -(V + W) \implies$ Standard HF is stable.
- **Case 2 - Strong:** With $V = -4/3, W = -1$, the condition fails ($0.67 < 2.33$).
- **Result:** The system undergoes a phase transition to a "mixed" state with lower energy ($E_{mixed} \approx -7.57$ vs $E_{HF} = -4.0$) which is much closer to the FCI result of -7.75.

Second Order MBPT Energy Pairing model

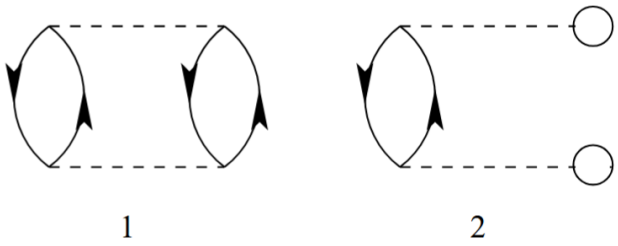

Figure 3: The two diagrams for second order energy in MBPT

In our case we have:

$$E^{(2)} = \sum_{a>F} \sum_{i \leq F} \frac{\left\langle i\bar{i} \right| V_N \left| a\bar{a} \right\rangle \left| \left\langle a\bar{a} \right| V_N \left| i\bar{i} \right\rangle \right.}{2(\epsilon_i - \epsilon_a)}$$

Where $E^{(2)}$ scales as $O(N^4)$.