# FYS4480 Oral exam, midterm one and two

## Helium and Beryllium using CIS and Hartree-Fock, pairing model

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# Setup

Represent states using creation $a_p^\dagger$ and annihilation $a_q$ operators (occupation representation/second quantization), obeying

$$\{a_p^\dagger, a_q\} = \delta_{pq}, \qquad \{a_p^\dagger, a_q^\dagger\} = \{a_p, a_q\} = 0$$

$p$ and $q$ are sets of relevant quantum numbers. We need to pick a single particle (SP) computational basis, having $n$ possible single particle states.

$$\text{3D HO:} \qquad p = \{n_r, l, m_l, s, m_s\}, \qquad a_p^\dagger |0\rangle = |p\rangle \longrightarrow \psi_p(\mathbf{x}) = \psi_{n_r l m}(r, \theta, \phi) = \dots$$

Need a Hamiltonian to solve $\hat{H} = \hat{H}_0 + \hat{V}$, with $\hat{H}_0$ representing single particle energy contributions, and $\hat{V}$ interactions.

Often start with an $N$-particle ground state ansatz $|\Phi_0\rangle = a_1^\dagger, \dots a_N^\dagger |0\rangle$.

And consider excitations of this

$$\begin{aligned}
\text{1p1h} \qquad & |\Phi_i^a\rangle = a_a^\dagger a_i |\Phi_0\rangle \\
\text{2p2h} \qquad & |\Phi_{ij}^{ab}\rangle = a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle \\
\text{NpNh} \qquad & |\Phi_{ij\dots}^{ab\dots}\rangle = a_a^\dagger a_b^\dagger \dots a_j a_i |\Phi_0\rangle
\end{aligned}$$

# Full configuration interaction (FCI)

Start with $N$ particle ground state ansatz $|\Phi_0\rangle$.

Not an eigenstate of $\hat{V}$ and therefor not the true ground state of the system.

By considering every possible $N$ particle state in our system (using $\{a_1^\dagger, \ldots, a_N^\dagger, \ldots, a_n^\dagger\}$), we can construct our ground state $|\Psi_0\rangle$ as a linear combination of excited states.

$$|\Psi_0\rangle = C_0 + \sum_{ai} C_i^a |\Phi_i^a\rangle + \sum_{ai} C_{ij}^{ab} |\Phi_{ij}^{ab}\rangle + \ldots$$

Normally solved by considering the Hamiltonian in matrix representation, with elements $H_{XY} = \langle\Phi_X| \hat{H} |\Phi_Y\rangle$, with $X, Y \in \{\text{0p0h}, \text{1p1h} \ldots \text{NpNh}\}$, giving the eigenvalue problem

$$H\mathbf{c} = E\mathbf{c}$$

When solved, the smallest eigenvalue $E^{(0)}$ will yield the ground state energy, and $|\Psi_0\rangle$ can be found by considering the eigenvectors $\mathbf{c}^{(0)} = (C_0, C_i^a \ldots C_{ij}^{ab} \ldots\ldots C_{ij\ldots}^{ab\ldots})$. Excited states can also be found by considering the other eigenvalues and vectors $E^{(i)}, \mathbf{c}^{(i)}$.

FCI

Example, pairing interaction: $\hat{V}$ only works between spin-paired states at the same energy level. We let $p = 1, 2, 3, 4$ denote energy levels, with SP states also having a spin $\sigma = \pm$, a total of $n = 8$ SP states.

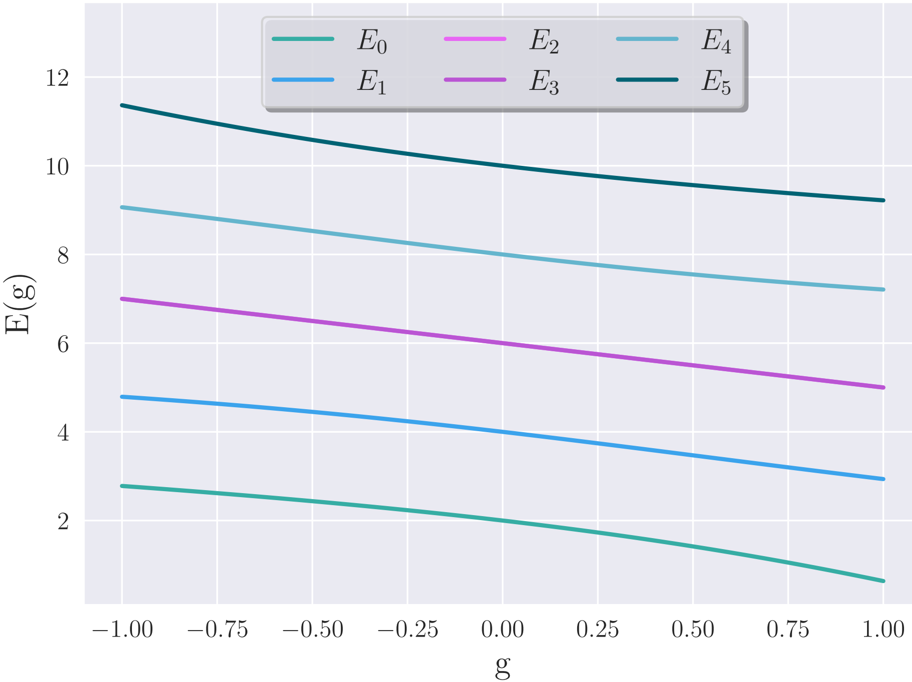
$$\hat{H} = \hat{H}_0 + \hat{V}, \qquad \hat{H}_0 = \sum_{p\sigma}(p-1)a^{\dagger}_{p\sigma}a_{p\sigma}, \qquad \hat{V} = -\frac{1}{2}g\sum_{pq}a^{\dagger}_{p+}a^{\dagger}_{p-}a_{q-}a_{q+}$$

Diagonal SP Hamiltonian $\hat{H}_0$ and two body interaction $\hat{V}$. Consider $N = 4$ particles with total spin $S = 0$, writing $|PQ\rangle = |p+p-q+q-\rangle$ we have a total of six different many body states.

| | |
|---|---|
| 0p0h | $\|12\rangle$ |
| 2p2h | $\|13\rangle, \|14\rangle, \|23\rangle, \|24\rangle$ |
| 4p4h | $\|34\rangle$ |

By setting up the matrix $\langle KL|\hat{H}|RS\rangle$, we get a small eigenvalue problem of a $6\times 6$ matrix.

## FCI




But there is a problem...

In all but very simple problems, this approach is unfeasible. In general, we have to consider

$$\binom{n}{N} = \frac{n!}{N!(n-N)!}$$

many body states. Taking our pairing model example, lifting the $S = 0$ restriction yields 70 different states. This is still possible, but increasing both $n$ and $N$ results in disaster

| $N \downarrow / n \rightarrow$ | 8 | 32 | 64 | 128 |
|---|---|---|---|---|
| 4 | 70 | $10^4$ | $10^5$ | $10^7$ |
| 8 | | $10^7$ | $10^9$ | $10^{12}$ |
| 16 | | $10^8$ | $10^{14}$ | $10^{19}$ |
| 32 | | | $10^{18}$ | $10^{30}$ |

**Table.** NB: Order of magnitude values

## Pros:

- Provides exact solutions within a truncated basis set
- Understandable and relatively easy to set up
- Excited states thrown into the bargain

## Cons:

- Computational complexity, bad scaling
- Only possible for tiny systems, with few states and particles.
- Practically only a benchmarking tool

## Custom Subsection

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# Custom Title

## Custom Subsection with Footnote

This frame has a custom title and a custom subtitle.[1]

[1] This is a footnote. See also Author (2022).

## Typographics

These examples follow the Metropolis Theme

- Regular
- Alert
- *Italic*
- **Bold**

**Items**

- Cats
  - British Shorthair
- Dogs
- Birds

**Enumerations**

1. First
   1.1 First subpoint
2. Second
3. Last

**Descriptions**

Apples Yes

Oranges No

Grappes No

**Table.** Largest cities in the world (source: Wikipedia)

| City | Population |
|---|---|
| Mexico City | 20,116,842 |
| Shanghai | 19,210,000 |
| Peking | 15,796,450 |
| Istanbul | 14,160,467 |

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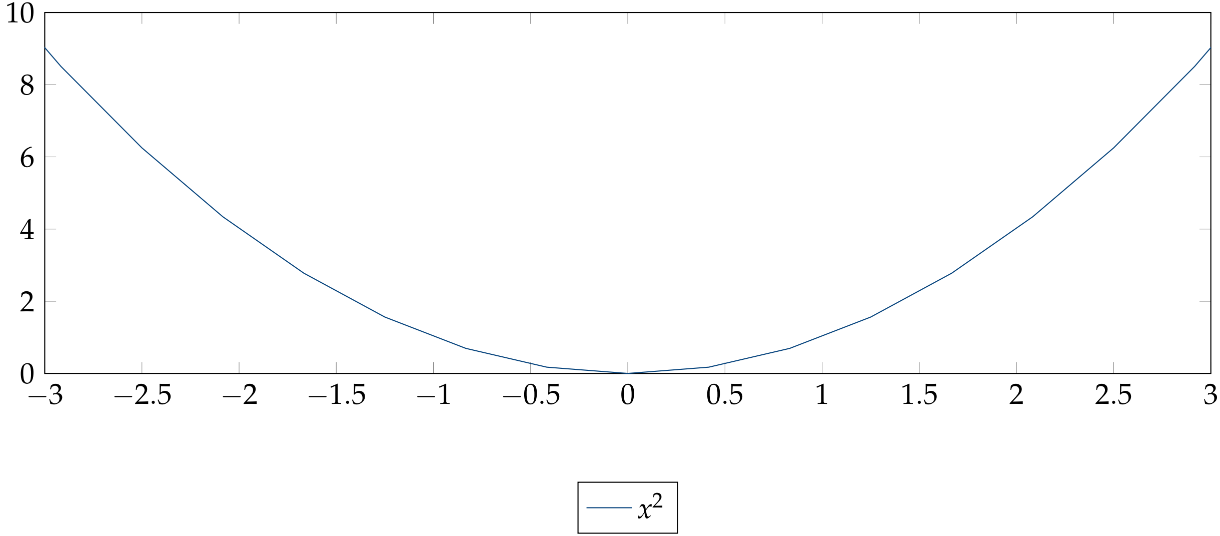
**Figure.** Plot of $y = x^2$



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**Example**

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# Maths

## Equations

- A numbered equation:

$$y_t = \beta x_t + \varepsilon_t \tag{1}$$

- Another equation:

$$\mathbf{Y} = \boldsymbol{\beta}\mathbf{X} + \boldsymbol{\varepsilon}_t$$

- Theorems are numbered consecutively.

**Theorem 1 (Example Theorem)**

*Given a discrete random variable X, which takes values in the alphabet $\mathcal{X}$ and is distributed according to $p : \mathcal{X} \to [0, 1]$:*

$$\mathrm{H}(X) := -\sum_{x \in \mathcal{X}} p(x) \log p(x) = \mathbb{E}[-\log p(X)] \tag{2}$$

- Definition numbers are prefixed by the section number in the respective part.

### Definition 1.1 (Example Definition)

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$$\mathrm{H}(X) := -\sum_{x \in \mathcal{X}} p(x) \log p(x) = \mathbb{E}[-\log p(X)] \tag{3}$$

- Examples are numbered as definitions.

**Example 1.1 (Example Theorem)**

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$$\mathrm{H}(X) := -\sum_{x \in \mathcal{X}} p(x) \log p(x) = \mathbb{E}[-\log p(X)] \tag{4}$$

# Part I

## Demo Presentation Part 2

# References I

Author, Example (2022). "Reference Title". In: *Journal of Examples* 0.0, pp. 1–10.