

# PY4T01 Condensed Matter Theory: Lecture 15

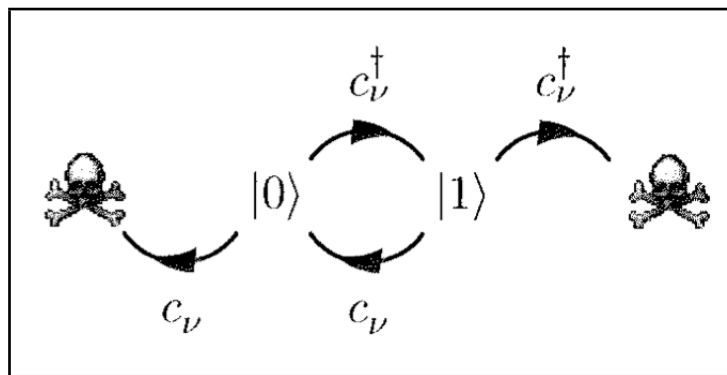
## Introducing electron-electron interaction

Let us go back to the  $H_2$  molecule and re-write  $H$  as (second quantization formalism)

$$H = \epsilon_0 \sum_{\nu=1}^2 c_{\nu}^{\dagger} c_{\nu} + \gamma [c_1^{\dagger} c_2 + c_2^{\dagger} c_1]$$

The operators  $c_{\nu}$  and  $c_{\mu}^{\dagger}$  are defined as

$$\begin{aligned} c_{\nu} |0_{\nu}\rangle &= 0 & c_{\nu}^{\dagger} |0_{\nu}\rangle &= |1_{\nu}\rangle \\ c_{\nu} |1_{\nu}\rangle &= |0_{\nu}\rangle & c_{\nu}^{\dagger} |1_{\nu}\rangle &= 0 \end{aligned}$$



A particular electronic configuration of the  $H_2$  molecule is written in terms of the vectors

$$|\alpha_1, \alpha_2\rangle \quad \text{where} \quad \alpha_{\nu} = 0, 1$$

$H$  acts as following:

1. The first term “counts” electrons

$$c_1^\dagger c_1 |\alpha_1, \alpha_2\rangle = \hat{n}_1 |\alpha_1, \alpha_2\rangle = \alpha_1 |\alpha_1, \alpha_2\rangle$$

2. The second term “transfers” electrons

$$c_1^\dagger c_2 |0_1, 1_2\rangle = |1_1, 0_2\rangle$$

The problem can be then solved as usual.

1. Take a generic wave-function written on this “new” basis

$$|\psi\rangle = \psi_1 |1_1, 0_2\rangle + \psi_2 |0_1, 1_2\rangle$$

2. Expand the Schrödinger equation

$$H|\psi\rangle = \epsilon_0 \sum_{\nu=1}^2 c_\nu^\dagger c_\nu |\psi\rangle + \gamma [c_1^\dagger c_2 + c_2^\dagger c_1] |\psi\rangle = E|\psi\rangle$$

$$\epsilon_0 \sum_{\nu=1}^2 c_\nu^\dagger c_\nu |\psi\rangle = \epsilon_0 |\psi\rangle$$

$$\begin{aligned} \gamma \left[ c_1^\dagger c_2 + c_2^\dagger c_1 \right] (\psi_1 |1_1, 0_2\rangle + \psi_2 |0_1, 1_2\rangle) &= \\ &= \gamma (\psi_1 |0_1, 1_2\rangle + \psi_2 |1_1, 0_2\rangle) \end{aligned}$$

3. Project over  $\langle \alpha_1, \alpha_2 |$  by using

$$\langle \alpha_1, \alpha_2 | \beta_1, \beta_2 \rangle = \delta_{\alpha_1, \beta_1} \delta_{\alpha_2, \beta_2}$$

to obtain

$$\begin{cases} \epsilon_0 \psi_1 + \gamma \psi_2 = E \psi_1 \\ \gamma \psi_1 + \epsilon_0 \psi_2 = E \psi_2 \end{cases}$$

4. Solve

$$\begin{pmatrix} \epsilon_0 & \gamma \\ \gamma & \epsilon_0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

5. We obtain the known solutions

$$E_{\text{bond}} = \epsilon_0 + \gamma, \quad |\psi_{\text{bond}}\rangle = \frac{1}{\sqrt{2}} [|1_1, 0_2\rangle + |0_1, 1_2\rangle]$$

$$E_{\text{anti}} = \epsilon_0 - \gamma, \quad |\psi_{\text{anti}}\rangle = \frac{1}{\sqrt{2}} [|1_1, 0_2\rangle - |0_1, 1_2\rangle]$$

**Note:**

The action of the operators  $c_\nu$  and  $c_\mu^\dagger$  is defined by their *algebra* given by the anti-commutation rules:

$$\{c_\mu^\dagger, c_\nu^\dagger\} = \{c_\mu, c_\nu\} = 0 \quad \{c_\mu, c_\nu^\dagger\} = \delta_{\mu,\nu}$$

with

$$\{A, B\} = AB + BA$$

It then follows

1. The eigenvalues of  $c_\nu^\dagger c_\nu$  are 0 or 1

$$(c_\nu^\dagger c_\nu)^2 = c_\nu^\dagger (c_\nu c_\nu^\dagger) c_\nu = c_\nu^\dagger (1 - c_\nu^\dagger c_\nu) c_\nu = c_\nu^\dagger c_\nu$$

$$\left. \begin{array}{l} c_\nu^\dagger c_\nu |n_\nu\rangle = n_\nu |n_\nu\rangle \\ (c_\nu^\dagger c_\nu)^2 |n_\nu\rangle = n_\nu^2 |n_\nu\rangle \end{array} \right\} \rightarrow n_\nu = 0, 1$$

2.  $c_\nu^\dagger c_\nu |n_\nu\rangle = n_\nu |n_\nu\rangle \rightarrow c_\nu^\dagger c_\nu (c_\nu |n_\nu\rangle) = (1 - n_\nu) c_\nu |n_\nu\rangle$   
with  $n_\nu = 1$

3.  $c_\nu^\dagger c_\nu |n_\nu\rangle = n_\nu |n_\nu\rangle \rightarrow c_\nu^\dagger c_\nu (c_\nu^\dagger |n_\nu\rangle) = (1 - n_\nu) c_\nu^\dagger |n_\nu\rangle$   
with  $n_\nu = 0$

## Second Quantization (very quick)

Let us go back to the time-dependent Schrödinger equation

$$i\hbar\dot{\Psi}(\mathbf{r}) = \left[ -\frac{\hbar^2\nabla^2}{2m} + U(\mathbf{r}) \right] \Psi(\mathbf{r})$$

This is an “equation of motion”, which can be derived from the Lagrangian density

$$L = i\hbar\Psi^\dagger\dot{\Psi} - \frac{\hbar^2}{2m}\nabla\Psi^\dagger \cdot \nabla\Psi - U(\mathbf{r})\Psi^\dagger\Psi$$

If  $\Psi$  is the *dynamical variable* the conjugate momentum is

$$\pi = \frac{\partial L}{\partial\dot{\Psi}} = i\hbar\Psi^\dagger$$

The Hamiltonian density is given by

$$\mathcal{H} = \pi\dot{\Psi} - L = \frac{\hbar^2}{2m}\nabla\Psi^\dagger \cdot \nabla\Psi + U\Psi^\dagger\Psi$$

and the Hamiltonian is obtained by integrating

$$H = \int \mathcal{H} d^3\mathbf{r} = \int \Psi^\dagger \left( -\frac{\hbar^2\nabla^2}{2m} + U \right) \Psi d^3\mathbf{r}$$

**Second quantization** consists in making  $\Psi$  and  $\Psi^\dagger$  operators (quantum fields) satisfying the following anti-commutation relations (for fermions)

$$\begin{aligned}\{\Psi(\mathbf{r}), \Psi^\dagger(\mathbf{r}')\} &= \delta(\mathbf{r} - \mathbf{r}') \\ \{\Psi^\dagger(\mathbf{r}), \Psi^\dagger(\mathbf{r}')\} &= \{\Psi(\mathbf{r}), \Psi(\mathbf{r}')\} = 0\end{aligned}$$

This is due to Jordan and Wigner (1928). Particles satisfying the anticommutation rules are Fermions.

Now the operators  $c_\nu^\dagger$  and  $c_\nu$  can be introduced. Expand the wave function over a convenient basis. For a chain of H atom if  $\phi_\nu(\mathbf{r})$  is the  $1s$  orbital located at  $\mathbf{r} - \mathbf{R}_\nu$

$$\Psi(\mathbf{r}) = \sum_{\nu} c_{\nu} \phi_{\nu}(\mathbf{r})$$

$$\Psi^\dagger(\mathbf{r}) = \sum_{\nu} c_{\nu}^\dagger \phi_{\nu}(\mathbf{r})$$

Finally from the anticommutation relations for the fields (integrating in  $\mathbf{r}$ ):

$$\{c_{\mu}^\dagger, c_{\nu}^\dagger\} = \{c_{\mu}, c_{\nu}\} = 0 \quad \{c_{\mu}, c_{\nu}^\dagger\} = \delta_{\mu, \nu}$$

What about the Hamiltonian?

$$H = \int \Psi^\dagger \left( -\frac{\hbar^2 \nabla^2}{2m} + U \right) \Psi d^3 \mathbf{r}$$

$$H = \sum_{\mu, \nu} \left[ \int \phi_\mu(\mathbf{r}) \left( -\frac{\hbar^2 \nabla^2}{2m} + U \right) \phi_\nu(\mathbf{r}) d^3 \mathbf{r} \right] c_\mu^\dagger c_\nu$$

$$H = \sum_{\mu, \nu} H_{\mu\nu} c_\mu^\dagger c_\nu$$

where  $H_{\mu\nu}$  is the Hamiltonian matrix (as derived from the tight-binding method)

(For more details see: G.D. Mahan, *Many-Particle Physics*, Kluwer Academic)

## Many-particle operators

The Coulomb electron-electron interaction depends on the position of two electrons

$$\frac{1}{2} \sum_i \sum_{j \neq i} V(\mathbf{r}_i - \mathbf{r}_j) = \frac{1}{2} \sum_i \sum_{j \neq i} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

In second quantization this leads to the operator

$$H_{e-e} = \frac{1}{2} \sum_{\nu_i \nu_j \nu_k \nu_l} V_{\nu_i \nu_j \nu_k \nu_l} c_{\nu_i}^\dagger c_{\nu_k}^\dagger c_{\nu_l} c_{\nu_j}$$

with

$$V_{\nu_i \nu_j \nu_k \nu_l} = \int d^3 \mathbf{r}_i \int d^3 \mathbf{r}_j \phi_{\nu_i}(\mathbf{r}_i) \phi_{\nu_j}(\mathbf{r}_i) \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \phi_{\nu_k}(\mathbf{r}_j) \phi_{\nu_l}(\mathbf{r}_j)$$





## The Hubbard model for H<sub>2</sub>

Consider the Hubbard Hamiltonian for H<sub>2</sub>

$$H_U = \epsilon_0 \sum_{\mu\sigma} \hat{n}_{\mu\sigma} + \gamma \sum_{\sigma} (c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}) + U \sum_{\mu} \hat{n}_{\mu\uparrow} \hat{n}_{\mu\downarrow}$$

where

1.  $c_{\mu\sigma}^\dagger$

creates an electron on the H atom at  $\mathbf{R}_\mu$  with spin  $\sigma = \uparrow, \downarrow$

2.  $c_{\mu\sigma}$

destroys an electron on the H atom at  $\mathbf{R}_\mu$  with spin  $\sigma = \uparrow, \downarrow$

3.  $\epsilon_0 \sum_{\mu\sigma} \hat{n}_{\mu\sigma} + \gamma \sum_{\sigma} (c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma})$

is the standard (non-interacting tight-binding Hamiltonian for H<sub>2</sub>)

4.  $U \sum_{\mu} \hat{n}_{\mu\uparrow} \hat{n}_{\mu\downarrow}$

is the on-site Coulomb repulsion

Consider the case of the H atom. Then

$$H_U = \epsilon_0 \sum_{\sigma} \hat{n}_{\sigma} + U \hat{n}_{\uparrow} \hat{n}_{\downarrow}$$

		$U=0$	$U \neq 0$
No. $e^-$	$ \Psi\rangle^-$		
0	$ 0\rangle^-$	0	0
1	$ \uparrow\rangle^-$ $ \downarrow\rangle^-$	$\epsilon_0$	$\epsilon_0$
2	$ \uparrow\downarrow\rangle^-$	$2\epsilon_0$	$2\epsilon_0 + U$

For interacting system the **spectrum depends on the number of electrons**

## Solving the Hubbard model for $H_2$

Solve for different  $N = n_{\uparrow} + n_{\downarrow}$

### $N=0$

Only the trivial solution

$$E = 0, \quad |\psi\rangle = 0$$

### $N=1$

The wave-function can be written as

$$|\psi\rangle = \psi_1 |\uparrow, 0\rangle + \psi_2 |0, \uparrow\rangle$$

or

$$|\psi\rangle = \psi_1 |\downarrow, 0\rangle + \psi_2 |0, \downarrow\rangle$$

where

$$|\sigma, 0\rangle = c_{1\sigma}^{\dagger} |0, 0\rangle$$

$$|0, \sigma\rangle = c_{2\sigma}^{\dagger} |0, 0\rangle$$

this is completely equivalent to the case done at the very beginning (note that  $U \sum_{\mu} \hat{n}_{\mu\uparrow} \hat{n}_{\mu\downarrow} |\sigma, 0\rangle = U \sum_{\mu} \hat{n}_{\mu\uparrow} \hat{n}_{\mu\downarrow} |0, \sigma\rangle = 0$ )

The Hamiltonian matrix then is

$$\begin{pmatrix} \epsilon_0 & \gamma \\ \gamma & \epsilon_0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

with solutions

$$E_{\text{bond}} = \epsilon_0 + \gamma, \quad |\psi_{\text{bond}}\rangle = \frac{1}{\sqrt{2}} [|\sigma, 0\rangle + |0, \sigma\rangle]$$

$$E_{\text{anti}} = \epsilon_0 - \gamma, \quad |\psi_{\text{anti}}\rangle = \frac{1}{\sqrt{2}} [|\sigma, 0\rangle - |0, \sigma\rangle]$$

and total energy

$$E_{\text{total}} = \epsilon_0 + \gamma$$

Note that the solution has spin  $\sigma$  ( $1/2$ ), but it is doubly degenerate.

## N=2

There are six possible electronic configurations (states)

$$1. |1\rangle = |\uparrow, \downarrow\rangle = c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger |0, 0\rangle$$

$$2. |2\rangle = |\downarrow, \uparrow\rangle = c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger |0, 0\rangle$$

$$3. |3\rangle = |\downarrow\uparrow, 0\rangle = c_{1\downarrow}^\dagger c_{1\uparrow}^\dagger |0, 0\rangle$$

$$4. |4\rangle = |0, \downarrow\uparrow\rangle = c_{2\downarrow}^\dagger c_{2\uparrow}^\dagger |0, 0\rangle$$

$$5. |5\rangle = |\uparrow, \uparrow\rangle = c_{1\uparrow}^\dagger c_{2\uparrow}^\dagger |0, 0\rangle$$

$$6. |6\rangle = |\downarrow, \downarrow\rangle = c_{1\downarrow}^\dagger c_{2\downarrow}^\dagger |0, 0\rangle$$

Note that for  $|1\rangle, |2\rangle, |3\rangle, |4\rangle$ ,  $n_\uparrow = n_\downarrow = 1$ , i.e. they are spin singlet. Instead  $|5\rangle, |6\rangle$  are spin triplet, i.e.  $n_\sigma = 2$ . Since there is no term in the Hamiltonian which flips the spin there are no matrix element between  $\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}$  and either  $|5\rangle$  or  $|6\rangle$ . Now calculate the energy.

## Triplets

$$|\psi\rangle = |5\rangle \quad \text{or} \quad |\psi\rangle = |6\rangle$$

and

$$E_{\text{total}} = 2\epsilon_0$$

## Singlets

The wave-function is then written on the  $\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}$  basis set

$$|\psi\rangle = \psi_1|1\rangle + \psi_2|2\rangle + \psi_3|3\rangle + \psi_4|4\rangle$$

again one writes

$$H_U|\psi\rangle = E|\psi\rangle$$

and project over  $|j\rangle$  ( $j = 1, 2, 3, 4$ )

This finally gives the matrix equation

$$\begin{pmatrix} 2\epsilon_0 & 0 & \gamma & \gamma \\ 0 & 2\epsilon_0 & \gamma & \gamma \\ \gamma & \gamma & 2\epsilon_0 + U & 0 \\ \gamma & \gamma & 0 & 2\epsilon_0 + U \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$$

The solutions are (eigenvalues and eigenvectors)

$$\epsilon_1 = 2\epsilon_0 + \frac{U}{2} - \frac{\sqrt{U^2 + 16\gamma^2}}{2}$$

$$|\psi_1\rangle = \frac{1}{\sqrt{2}} [\{|1\rangle + |2\rangle\} \cos \theta + \{|3\rangle + |4\rangle\} \sin \theta]$$

$$\varepsilon_2 = 2\varepsilon_0 + \frac{U}{2} + \frac{\sqrt{U^2 + 16\gamma^2}}{2}$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}} [-\{|1\rangle + |2\rangle\} \sin \theta + \{|3\rangle + |4\rangle\} \cos \theta]$$

$$\varepsilon_3 = 2\varepsilon_0$$

$$|\psi_3\rangle = \frac{1}{\sqrt{2}} (|1\rangle - |2\rangle)$$

$$\varepsilon_4 = 2\varepsilon_0 + U$$

$$|\psi_4\rangle = \frac{1}{\sqrt{2}} (|3\rangle - |4\rangle),$$

where

$$\tan \theta = \frac{-4\gamma}{U + \sqrt{U^2 + 16\gamma^2}}.$$

The ground state energy is therefore the one given by  $E_{\text{total}} = \varepsilon_1$ .

Note that:

1. For  $\gamma = 0$  (two isolated H atoms)

$$\varepsilon_1 = 2\varepsilon_0, \quad |\psi_1\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$$

$$\varepsilon_2 = 2\varepsilon_0 + U, \quad |\psi_2\rangle = \frac{1}{\sqrt{2}}(|3\rangle + |4\rangle)$$

$$\varepsilon_3 = 2\varepsilon_0, \quad |\psi_3\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)$$

$$\varepsilon_4 = 2\varepsilon_0 + U, \quad |\psi_4\rangle = \frac{1}{\sqrt{2}}(|3\rangle - |4\rangle),$$

2. For  $U = 0$  (non-interacting)

$$\varepsilon_1 = 2(\varepsilon_0 - \gamma), \quad |\psi_1\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle - |3\rangle - |4\rangle)$$

$$\varepsilon_2 = 2(\varepsilon_0 + \gamma), \quad |\psi_2\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle + |3\rangle + |4\rangle)$$

$$\varepsilon_3 = 2\varepsilon_0, \quad |\psi_3\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)$$

$$\varepsilon_4 = 2\varepsilon_0, \quad |\psi_4\rangle = \frac{1}{\sqrt{2}}(|3\rangle - |4\rangle),$$



Note also that: One does not necessarily need to separate singlet and triplet. The full basis can be used:

$$|\psi\rangle = \psi_1|1\rangle + \psi_2|2\rangle + \psi_3|3\rangle + \psi_4|4\rangle + \psi_5|5\rangle + \psi_6|6\rangle$$

and the Hamiltonian matrix becomes

$$\begin{pmatrix} 2\epsilon_0 & 0 & \gamma & \gamma & 0 & 0 \\ 0 & 2\epsilon_0 & \gamma & \gamma & 0 & 0 \\ \gamma & \gamma & 2\epsilon_0 + U & 0 & 0 & 0 \\ \gamma & \gamma & 0 & 2\epsilon_0 + U & 0 & 0 \\ 0 & 0 & 0 & 0 & 2\epsilon_0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2\epsilon_0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \psi_5 \\ \psi_6 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \psi_5 \\ \psi_6 \end{pmatrix}$$

### N=3

The wave-function can be written as

$$|\psi\rangle = \psi_1|\uparrow, \uparrow\downarrow\rangle + \psi_2|\uparrow\downarrow, \uparrow\rangle$$

or

$$|\psi\rangle = \psi_1|\downarrow, \uparrow\downarrow\rangle + \psi_2|\uparrow\downarrow, \downarrow\rangle$$

where

$$|\sigma, \uparrow\downarrow\rangle = c_{1\sigma}^\dagger c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger |0, 0\rangle$$

$$|\uparrow\downarrow, \sigma\rangle = c_{2\sigma}^\dagger c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger |0, 0\rangle$$

this is similar to the  $N = 1$  case ( $U \sum_\mu \hat{n}_{\mu\uparrow} \hat{n}_{\mu\downarrow} |\sigma, \uparrow\downarrow\rangle = U |\sigma, \uparrow\downarrow\rangle$ )

The Hamiltonian matrix then is

$$\begin{pmatrix} 3\epsilon_0 + U & \gamma \\ \gamma & 3\epsilon_0 + U \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

with solutions

$$E_{\text{bond}} = 3\epsilon_0 + U + \gamma, \quad |\psi_{\text{bond}}\rangle = \frac{1}{\sqrt{2}} [|\sigma, \uparrow\downarrow\rangle + |\uparrow\downarrow, \sigma\rangle]$$

$$E_{\text{anti}} = 3\epsilon_0 + U - \gamma, \quad |\psi_{\text{anti}}\rangle = \frac{1}{\sqrt{2}} [|\sigma, \uparrow\downarrow\rangle - |\uparrow\downarrow, \sigma\rangle]$$

and total energy

$$E_{\text{total}} = 3\epsilon_0 + U + \gamma$$

Note that the solution has spin  $\sigma$  ( $1/2$ ), but it is doubly degenerate.

**N=4**

Only the trivial solution

$$E_{\text{total}} = 4\epsilon_0 + 2U, \quad |\psi\rangle = |\uparrow\downarrow, \uparrow\downarrow\rangle$$

Let us summarize the spectrum found

$N$	spectrum
0	0
1	$\epsilon_0 + \gamma \quad \times 2$ $\epsilon_0 - \gamma \quad \times 2$
2	$2\epsilon_0 + \frac{U}{2} - \frac{\sqrt{U^2 + 16\gamma^2}}{2}$ $2\epsilon_0 + \frac{U}{2} + \frac{\sqrt{U^2 + 16\gamma^2}}{2}$ $2\epsilon_0$ $2\epsilon_0 + U$ $2\epsilon_0$ $2\epsilon_0$
3	$3\epsilon_0 + U + \gamma \quad \times 2$ $3\epsilon_0 + U - \gamma \quad \times 2$
4	$4\epsilon_0 + 2U$

## How complicate can it get?

In general the wave-function need to be constructed over the basis defined by

$$|\Psi_\kappa\rangle = (\prod_i^N \hat{c}_{i\sigma}^\dagger) |0\rangle, \quad (1)$$

The matrix elements of  $H_U$  are

$$H_{ij} = \langle \Psi_i | H_U | \Psi_j \rangle. \quad (2)$$

For a  $L$ -sites and  $n_\uparrow$  and  $n_\downarrow$  electrons the number of basis function is

$$\kappa = \binom{L}{n_\uparrow} \cdot \binom{L}{n_\downarrow}, \quad \text{where,} \quad \binom{m}{n} = \frac{m!}{n!(m-n)!}. \quad (3)$$

The scaling is terrible!!

$L$	$n_{\uparrow}$	$n_{\downarrow}$	Hilbert Space dimension
2	1	1	4
4	2	2	36
6	3	3	400
8	4	4	4,900
10	5	5	63,504
12	6	6	853,776
14	7	7	11,778,624
16	8	8	165,636,900
18	9	9	2,363,904,400
20	10	10	34,134,779,536

System	$L$	$N$	Hilbert Space	Time	Memory
Na <sub>2</sub>	2	2	4	1 $\mu$ sec	128b
Na <sub>6</sub>	6	6	400	1 sec	1.2Mb
Na <sub>10</sub>	10	10	63,504	46 days	3.2Gb
Na <sub>12</sub>	12	12	853,776	308 years	43Gb