

# Introducción a la Física Nuclear 2023

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## Segunda Cuantización y Función de Onda de Dos Partícula

### Contenido:

Notación de braket. Espacio de Hilbert de una y muchas partículas. Bases, completitud y ortogonalidad. Espacio de Fock. Representación número de ocupación. Teorema de Wick. Ecuación de Hartree-Fock. Función de onda de dos partículas acopladas en segunda cuantificación. Representación de un operador de una y dos partículas en segunda cuantificación.

# **Espacio de Hilbert de una partícula**

# Representación bracket

## Representación coordenada

$$h(\bar{r})\phi_\alpha(\bar{r}) = \varepsilon_\alpha\phi_\alpha(\bar{r})$$

## Representación abstracta

$$h|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle$$

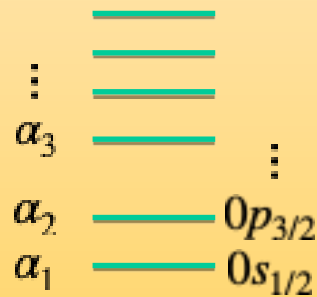
## Conexión

$$\langle\bar{r}|\alpha\rangle = \phi_\alpha(\bar{r})$$

$$\langle\bar{r}|h|\bar{r}\rangle = h(r)$$

$$h(\bar{r}) = \int d\bar{r}' \delta(\bar{r} - \bar{r}') \langle\bar{r}|h|\bar{r}'\rangle$$

$$h|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle \rightarrow h(\bar{r})\phi_\alpha(\bar{r}) = \varepsilon_\alpha\phi_\alpha(\bar{r})$$



Espectro(degenerado)

# Espacio abstracto

## Espacio de Hilbert de una partícula

 $\mathcal{H}$ 

## Base

 $\{ |\alpha\rangle \}$ 

$$h |\alpha\rangle = \varepsilon_\alpha |\alpha\rangle$$

## Completitud

$$\sum_{\alpha} \phi_{\alpha}^{*}(\bar{r}) \phi_{\alpha}(\bar{r}') = \delta(\bar{r} - \bar{r}') \rightarrow \sum_{\alpha} \langle \alpha | \bar{r} \rangle \langle \bar{r}' | \alpha \rangle = \delta(\bar{r} - \bar{r}') \rightarrow$$

$$\langle \bar{r} | \bar{r}' \rangle = \delta(\bar{r} - \bar{r}')$$

### Completitud

$$\sum_{\alpha} |\alpha\rangle \langle \alpha| = I$$

## Ortogonalidad


$$\int d\bar{r} \phi_{\alpha}^{*}(\bar{r}) \phi_{\alpha'}(\bar{r}) = \delta_{\alpha\alpha'} \rightarrow \int d\bar{r} \langle \alpha | \bar{r} \rangle \langle \bar{r} | \alpha' \rangle = \delta_{\alpha\alpha'} \rightarrow$$

### Ortogonalidad

$$\langle \alpha | \alpha' \rangle = \delta_{\alpha\alpha'}$$

# Espacio abstracto: representación bracket

**Ejemplo:**  $|\alpha\rangle = \{n, s, l, j, m\}$

$\vdots$   
 $\alpha_3$  
 $h|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle$

$\alpha_2$    
 $\alpha_1$    
 (no degenerado)

$$\langle r | nlj \rangle = R_{nlj}(r)$$

$$\langle \hat{r} | sljm \rangle = [Y_l(\hat{r})\chi_s]_{jm}$$

Representación coordenada

$$h(\vec{r})\phi_\alpha(\vec{r}) = \varepsilon_\alpha\phi_\alpha(\vec{r})$$

$$\phi_\alpha(\vec{r}) = R_{nlj}(r)[Y_l(\hat{r})\chi_s]_{jm}$$

$$\langle \vec{r} | \alpha \rangle = R_{nlj}(r)[Y_l(\hat{r})\chi_s]_{jm}$$

Completitud en el “espacio r”

$$\sum_n |nlj\rangle\langle nlj| = I_r$$

Idem ortogonalidad...

Completitud en el “espacio espín”

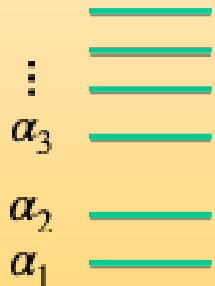
$$\sum_{sljm} |sljm\rangle\langle sljm| = I_{\hat{r}}$$

**Completitud**

$$I = I_r \otimes I_{\hat{r}}$$

# Espacio abstracto: representación bracket

Ejemplo:  $|\alpha\rangle = \{n, s, l, j, m\}$



$$h |\alpha\rangle = \varepsilon_\alpha |\alpha\rangle$$

Completitud en el “espacio r”

$$\sum_n |nlj\rangle\langle nlj| = I_r$$

Completitud en el “espacio espín”

$$\sum_{sljm} |sljm\rangle\langle sljm| = I_{\hat{r}}$$

Completitud  $I = I_r \otimes I_{\hat{r}}$

$$I = \sum_{nsljm} |nsljm\rangle\langle nsljm|$$

$$I = \sum_{\alpha} |\alpha\rangle\langle\alpha|$$

# **Espacio de Hilbert de muchas partículas**

# Espacio abstracto de N-partículas: completitud

## Espacio de Hilbert

$$\mathcal{H}_N = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)} \otimes \dots \otimes \mathcal{H}^{(N)}$$

Espacio  
Partícula 1

Espacio  
Partícula 2

Espacio  
Partícula N

$$|\alpha_1 \alpha_2 \dots \alpha_N\rangle = |\alpha_1\rangle |\alpha_2\rangle \dots |\alpha_N\rangle$$

Espacio de la  
Partícula  
I-ésima

Completitud

$$\sum_{\alpha_i} |\alpha_i\rangle \langle \alpha_i| = I_i$$

## Base

$$\{ |\alpha_1 \alpha_2 \dots \alpha_N\rangle \}$$

$$I = I^{(1)} \otimes I^{(2)} \dots \otimes I^{(N)}$$

Completitud

$$I = \sum_{\alpha_i} |\alpha_1 \alpha_2 \dots \alpha_N\rangle \langle \alpha_1 \alpha_2 \dots \alpha_N|$$



# Espacio abstracto de N-partículas: ortogonalidad

## Espacio de Hilbert

$$\mathcal{H}_N = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)} \otimes \dots \otimes \mathcal{H}^{(N)}$$

Espacio  
Partícula 1

Espacio  
Partícula 2

Espacio  
Partícula N

$$|\alpha_1 \alpha_2 \dots \alpha_N\rangle = |\alpha_1\rangle |\alpha_2\rangle \dots |\alpha_N\rangle$$

Espacio de la  
Partícula  
I-sima

Ortogonalidad

$$\langle \alpha_i | \alpha_{i'} \rangle = \delta_{\alpha_i \alpha_{i'}}$$

## Base

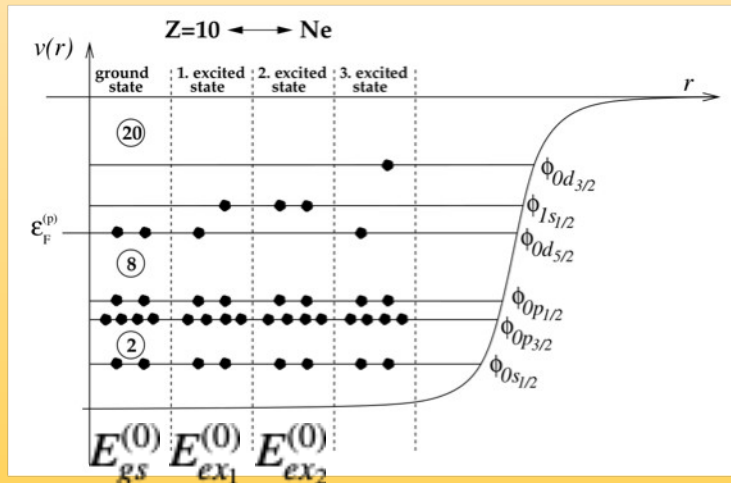
$$\{ |\alpha_1 \alpha_2 \dots \alpha_N\rangle \}$$

Ortogonalidad

$$\langle \alpha_1 \alpha_2 \dots \alpha_N | \alpha_1' \alpha_2' \dots \alpha_N' \rangle = \delta_{\alpha_1, \alpha_1'} \dots \delta_{\alpha_N, \alpha_N'}$$

# Función de onda de muchas partículas

$$\mathcal{H}_N = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)} \otimes \dots \otimes \mathcal{H}^{(N)}$$



$$\langle \bar{r}_1 \bar{r}_2 \dots \bar{r}_N | \alpha_1 \alpha_2 \dots \alpha_N \rangle = \Psi[\alpha_1 \alpha_2 \dots \alpha_N](\bar{r}_1 \bar{r}_2 \dots \bar{r}_N)$$

$$\Psi[\alpha_1 \alpha_2 \dots \alpha_N](\bar{r}_1 \bar{r}_2 \dots \bar{r}_N) \rightarrow |\alpha_1 \alpha_2 \dots \alpha_N\rangle$$

Vive en  $\mathcal{H}_N$

Función de onda de muchos cuerpos no antimetrizada

Está normalizada?

$$H_0 |\alpha_1 \alpha_2 \dots \alpha_N\rangle = E^{(0)} |\alpha_1 \alpha_2 \dots \alpha_N\rangle$$

Estado de muchas partículas sin interacción

$$E^{(0)} = \sum_{\alpha_i} \varepsilon_{\alpha_i} \rightarrow E_{gs}^{(0)}, E_{ex_1}^{(0)}, E_{ex_2}^{(0)}, \dots$$

# Antisimetrización y normalización

# Espacio abstracto de N-partículas antisimetrizadas

## Espacio de Hilbert

$$\mathcal{H}_N^{\mathcal{A}} = \text{sub} : \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)} \otimes \dots \otimes \mathcal{H}^{(N)}$$

$$|\alpha_1 \alpha_2 \dots \alpha_N\rangle_{\mathcal{A}} = \text{combinacion lineal} : |\alpha_1\rangle |\alpha_2\rangle \dots |\alpha_N\rangle$$

## Determinante de Slatter

$$|\alpha_1 \alpha_2 \dots \alpha_N\rangle_{\mathcal{A}} = \frac{1}{\sqrt{N!}} \sum_P (-)^P |\alpha_1 \alpha_2 \dots \alpha_N\rangle$$

## Base

$$\{ |\alpha_1 \alpha_2 \dots \alpha_N\rangle_{\mathcal{A}} \}$$

Función de onda de muchos  
cuerpos antisimétrica

# Espacio abstracto de N-partículas antisimetrizadas

## Espacio de Hilbert

$$\mathcal{H}_N^{\mathcal{A}} = \text{sub} : \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)} \otimes \dots \otimes \mathcal{H}^{(N)}$$

## Base

$$|\alpha_1 \alpha_2 \dots \alpha_N\rangle_{\mathcal{A}} = \frac{1}{\sqrt{N!}} \sum_P (-)^P |\alpha_1 \alpha_2 \dots \alpha_N\rangle$$

Completitud

$$I = \sum_{\alpha_i} |\alpha_1 \alpha_2 \dots \alpha_N\rangle_{\mathcal{A}} \langle \alpha_1 \alpha_2 \dots \alpha_N|$$

Ortogonalidad

$${}_{\mathcal{A}} \langle \alpha_1 \alpha_2 \dots \alpha_N | \alpha_1' \alpha_2' \dots \alpha_N' \rangle_{\mathcal{A}} = \delta_{\alpha_1, \alpha_1'} \dots \delta_{\alpha_N, \alpha_N'}$$

# Determinante de Slater

## Representación coordenada

Ket  $|\alpha_1\alpha_2\cdots\alpha_N\rangle_{\mathcal{A}}$

Bra  $\langle\bar{r}_1\bar{r}_2\cdots\bar{r}_N|$

## Función de onda

$$\langle\bar{r}_1\bar{r}_2\cdots\bar{r}_N|\alpha_1\alpha_2\cdots\alpha_N\rangle_{\mathcal{A}} = \tilde{\Psi}^{[\alpha_1\alpha_2\cdots\alpha_N]}(\bar{r}_1\bar{r}_2\cdots\bar{r}_N)$$

$$\tilde{\Psi}^{[\alpha_1\alpha_2\cdots\alpha_N]}(\bar{r}_1\bar{r}_2\cdots\bar{r}_N) \rightarrow |\alpha_1\alpha_2\cdots\alpha_N\rangle_{\mathcal{A}}$$

## Determinante de Slater

$$|\alpha_1\alpha_2\cdots\alpha_N\rangle_{\mathcal{A}} = \frac{1}{\sqrt{N!}} \sum_P (-)^P |\alpha_1\alpha_2\cdots\alpha_N\rangle$$

$$\langle\bar{r}_1\bar{r}_2\cdots\bar{r}_N|\alpha_1\alpha_2\cdots\alpha_N\rangle_{\mathcal{A}} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \langle\bar{r}_1|\alpha_1\rangle & \langle\bar{r}_2|\alpha_1\rangle & \cdots & \langle\bar{r}_N|\alpha_1\rangle \\ \vdots & \cdots & \vdots & \\ \langle\bar{r}_1|\alpha_N\rangle & \langle\bar{r}_2|\alpha_N\rangle & \cdots & \langle\bar{r}_N|\alpha_N\rangle \end{vmatrix}$$

**Antisimetrización y  
normalización con  
acople:  
Dos Partículas**

# Función de onda de dos partículas acopladas

## Función de onda no antisimetrizada

$$\Psi_{j_1 j_2}^{JM}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{m_1 m_2} \langle j_1 m_1 j_2 m_2 | JM \rangle \psi_{j_1 m_1}(\mathbf{r}_1) \psi_{j_2 m_2}(\mathbf{r}_2)$$

## Función de onda de partícula simple

$$\psi_{a m_a}(\mathbf{x}) = \phi_a(r) [\chi_s Y_{l_a}(\hat{r})]_{j_a m_a} \quad \phi_a(r) = \frac{u_a(r)}{r}.$$

$a = \{nlj\}$

## Propiedad

$$\Psi_{j_1 j_2}^{JM}(\mathbf{r}_2, \mathbf{r}_1) = (-)^{j_1 + j_2 - J} \Psi_{j_2 j_1}^{JM}(\mathbf{r}_1, \mathbf{r}_2)$$

## Ortogonalidad

$$\int d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 [\Psi_{j_1 j_2}^{JM}(\mathbf{r}_1, \mathbf{r}_2)]^\dagger \Psi_{j'_1 j'_2}^{JM}(\mathbf{r}_1, \mathbf{r}_2) = \delta_{j_1 j'_1} \delta_{j_2 j'_2}$$



# Función de onda de dos partículas acopladas y antisimetrizadas

## Función de onda antisimetrizada

$$\tilde{\Psi}_{j_1 j_2}^{JM}(\mathbf{r}_1, \mathbf{r}_2) = N_{j_1 j_2} [\Psi_{j_1 j_2}^{JM}(\mathbf{r}_1, \mathbf{r}_2) - \Psi_{j_1 j_2}^{JM}(\mathbf{r}_2, \mathbf{r}_1)]$$

$$N_{j_1 j_2} = \frac{1}{\sqrt{2(1+\delta_{j_1 j_2})}}$$

Considerar  
comparar con  
segunda  
cuantización

$$\Psi_{j_1 j_2}^{JM}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{m_1 m_2} \langle j_1 m_1 j_2 m_2 | JM \rangle \psi_{j_1 m_1}(\mathbf{r}_1) \psi_{j_2 m_2}(\mathbf{r}_2)$$

## Ortogonalidad

$$\int d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 [\tilde{\Psi}_{j_1 j_2}^{JM}(\mathbf{r}_1, \mathbf{r}_2)]^\dagger \tilde{\Psi}_{j'_1 j'_2}^{JM}(\mathbf{r}_1, \mathbf{r}_2) = \delta_{j_1 j'_1} \delta_{j_2 j'_2}$$

## Propiedad

$$J=0 \rightarrow j_1 = j_2$$

$$\int d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 N_{j_1 j_2} N_{j'_1 j'_2} [\Psi_{j_1 j_2}^{JM}(\mathbf{r}_1, \mathbf{r}_2) - (-)^{j_1+j_2-J} \Psi_{j_2 j_1}^{JM}(\mathbf{r}_1, \mathbf{r}_2)]^\dagger$$

$$[\Psi_{j'_1 j'_2}^{JM}(\mathbf{r}_1, \mathbf{r}_2) - (-)^{j'_1+j'_2-J} \Psi_{j'_2 j'_1}^{JM}(\mathbf{r}_1, \mathbf{r}_2)] = \delta_{j_1 j'_1} \delta_{j_2 j'_2}$$

$$N_{j_1 j_2} N_{j'_1 j'_2} [2\delta_{j_1 j'_1} \delta_{j_2 j'_2} - 2(-)^{j_2+j_1-J} \delta_{j_1 j'_2} \delta_{j_2 j'_1}] = \delta_{j_1 j'_1} \delta_{j_2 j'_2} \rightarrow N_{j_1 j_2} = \frac{1}{\sqrt{2(1+\delta_{j_1 j_2})}}$$

# Función de onda de dos partículas acopladas y antisimetrizadas: propiedades

## Función de onda antisimetrizada

$$\tilde{\Psi}_{j_1 j_2}^{JM}(\mathbf{r}_1, \mathbf{r}_2) = N_{j_1 j_2} [\Psi_{j_1 j_2}^{JM}(\mathbf{r}_1, \mathbf{r}_2) - \Psi_{j_1 j_2}^{JM}(\mathbf{r}_2, \mathbf{r}_1)]$$

$$N_{j_1 j_2} = \frac{1}{\sqrt{2(1+\delta_{j_1 j_2})}}$$

$$\Psi_{j_1 j_2}^{JM}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{m_1 m_2} \langle j_1 m_1 j_2 m_2 | JM \rangle \psi_{j_1 m_1}(\mathbf{r}_1) \psi_{j_2 m_2}(\mathbf{r}_2)$$

## Propiedades

$$\tilde{\Psi}_{ab}^{JM}(\mathbf{x}_2, \mathbf{x}_1) = (-)^{j_a + j_b - J} \tilde{\Psi}_{ba}^{JM}(\mathbf{x}_1, \mathbf{x}_2)$$

$$\tilde{\Psi}_{ba}^{JM}(\mathbf{x}_1, \mathbf{x}_2) = -(-)^{j_a + j_b - J} \tilde{\Psi}_{ab}^{JM}(\mathbf{x}_1, \mathbf{x}_2)$$

$$\tilde{\Psi}_{ab}^{JM}(\mathbf{x}_2, \mathbf{x}_1) = -\tilde{\Psi}_{ab}^{JM}(\mathbf{x}_1, \mathbf{x}_2)$$

# Función de onda de dos partículas acopladas y antisimetrizadas

## EN SEGUNDA CUANTIZACION

$$\{c_\alpha^\dagger, c_\beta^\dagger\} = c_\alpha^\dagger c_\beta^\dagger + c_\beta^\dagger c_\alpha^\dagger = 0$$

$$|\alpha\rangle = c_\alpha^\dagger |0\rangle \quad |nljm\rangle = c_{nljm}^\dagger |0\rangle$$

$$\{c_\alpha, c_\beta\} = c_\alpha c_\beta + c_\beta c_\alpha = 0$$

$$h(\vec{r})\phi_\alpha(\vec{r}) = \varepsilon_\alpha \phi_\alpha(\vec{r})$$

$$\{c_\alpha, c_\beta^\dagger\} = c_\alpha c_\beta^\dagger + c_\beta^\dagger c_\alpha = \delta_{\alpha\beta}$$

$$\phi_\alpha(\vec{r}) = \langle \vec{r} | c_\alpha^\dagger | 0 \rangle$$

$$|\alpha\beta\rangle = c_\alpha^\dagger c_\beta^\dagger |0\rangle$$

Hacer desarrollo...

$$N_{ab} = \frac{1}{\sqrt{1+\delta_{ab}}}$$

$$\alpha = (a, m_a)$$

Luego, repetimos con Wick

$$A_{JM}^\dagger(ab) = \frac{1}{\sqrt{1+\delta_{ab}}} \sum_{m_a m_b} \langle j_a m_a j_b m_b | JM \rangle a_{a m_a}^\dagger a_{b m_b}$$

$$\begin{aligned} A_{JM}(cd) &= [A_{JM}^\dagger(cd)]^\dagger = A_{JM}(cd) \\ &= \frac{1}{\sqrt{1+\delta_{cd}}} \sum_{m_c m_d} \langle j_c m_c j_d m_d | JM \rangle a_{d m_d} a_{c m_c} \end{aligned}$$

**Sistemas con número de  
partículas  
NO CONSTANTE**

# Definiciones

# Operadores de creación/destrucción

Vacío

Operador de creación

Operador de destrucción

$$|0\rangle$$

$$c_{\alpha}^{\dagger}$$

$$c_{\alpha} = (c_{\alpha}^{\dagger})^{\dagger}$$

$$c_{\alpha}|0\rangle = 0$$

Estados de uno, dos, ... partículas

$$|\alpha\rangle = c_{\alpha}^{\dagger}|0\rangle \rightarrow \mathcal{H}_1 = \mathcal{H}^{(1)}$$

$$|\alpha_1\alpha_2\rangle = c_{\alpha_1}^{\dagger}c_{\alpha_2}^{\dagger}|0\rangle \rightarrow \mathcal{H}_2 = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)}$$

$\vdots$

$$|\alpha_1\alpha_2\cdots\alpha_N\rangle = c_{\alpha_1}^{\dagger}c_{\alpha_2}^{\dagger}\cdots c_{\alpha_N}^{\dagger}|0\rangle \rightarrow \mathcal{H}_N = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)} \otimes \cdots \otimes \mathcal{H}^{(N)}$$

Espacio de  $N$  partículas

# Espacio de Fock

# Espacio de Fock

Motivación...

Espacio usual  $\mathcal{H}_N = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)} \otimes \dots \otimes \mathcal{H}^{(N)}$

Espacio para N=0, 1, ... partículas = Espacio de Fock

$$\mathcal{F} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \dots \mathcal{H}_N \oplus \dots$$

$$\mathcal{H}_1 = \mathcal{H}^{(1)}$$

$$\mathcal{H}_2 = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)} \otimes$$



# Representación número de partícula

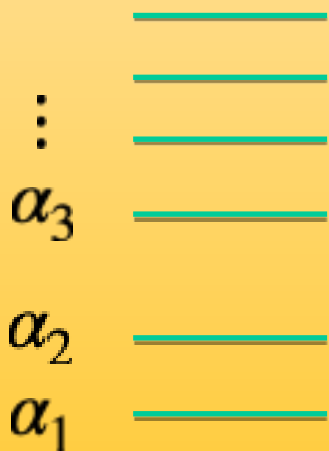
# Estado número de partículas

## Vacío de Fock

$$\mathcal{F} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \dots \mathcal{H}_N \oplus \dots$$

$$|0\rangle = |000\dots\rangle$$

En cada estado  $i$  hay 0 partículas



**Espectro de una partícula**

(no degenerado)

## Estado número de ocupación

$$|\alpha_1\alpha_2\dots\alpha_N\rangle = |n_1n_2n_3\dots\rangle$$

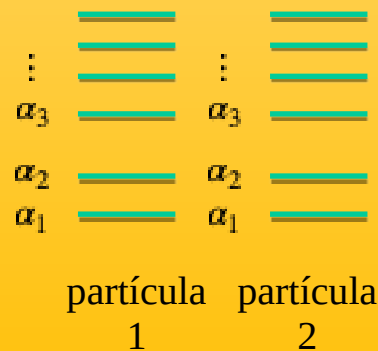
La partícula está en un estado  $\alpha_i$

En cada estado  $i$  hay  $n_i$  partículas

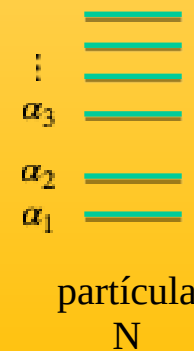
$$n_i = \begin{cases} 1 & i \in \{\alpha_1\alpha_2\dots\alpha_N\} \\ 0 & i \notin \{\alpha_1\alpha_2\dots\alpha_N\} \end{cases}$$

$$\sum_{i=1}^{\infty} n_i = N$$

Ejemplificar



...



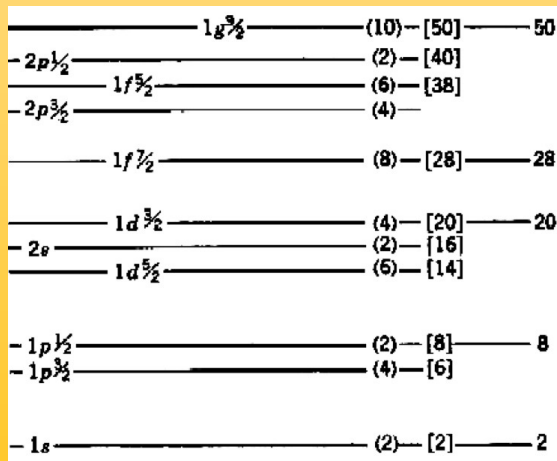
# Estado número de partículas

## Vacío de Fock

$$\mathcal{F} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \dots \mathcal{H}_N \oplus \dots$$

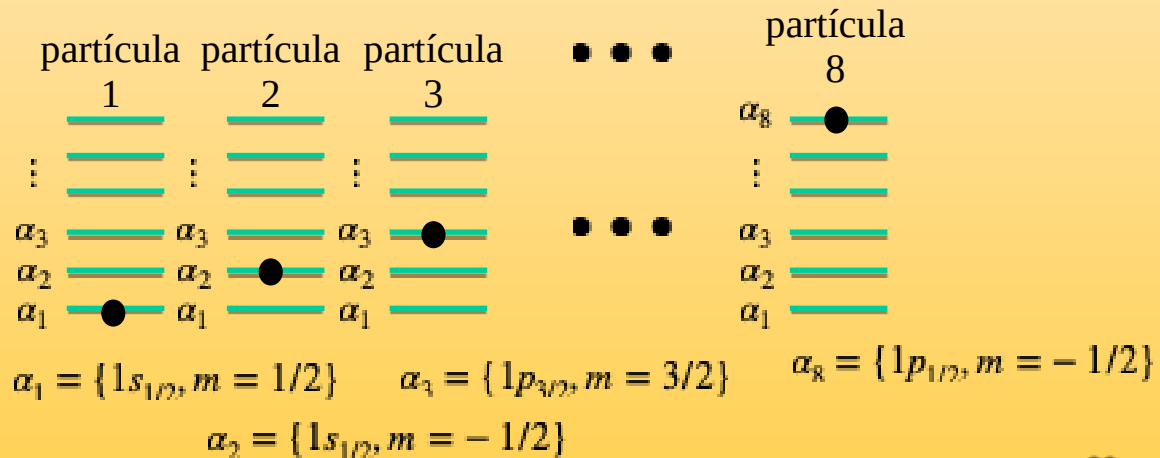
$$|0\rangle = |000\dots\rangle$$

## Espectro de una partícula



## Estado número de ocupación

$$|\alpha_1 \alpha_2 \dots \alpha_N\rangle = |n_1 n_2 n_3 \dots\rangle$$



$$|g.s.\rangle = |\alpha_1 \alpha_2 \dots \alpha_N\rangle = |1 1 \dots 1 0 0 \dots\rangle$$

$$|Ex_1\rangle = |\alpha_1 \alpha_2 \dots \alpha_N\rangle = |0 1 \dots 1 1 0 \dots\rangle$$

$$\sum_{i=1}^{\infty} n_i = 8$$

# Operadores de creación/destrucción revisados

## Operador creación

$$c_{\alpha}^{\dagger}|n_1 n_2 n_3 \cdots\rangle = \begin{cases} \eta_{\alpha}|n_1 \cdots n_{\alpha} + 1 \cdots\rangle & n_{\alpha} = 0 \\ 0 & n_{\alpha} = 1 \end{cases}$$

Fase

$$\eta_{\alpha} = (-)^{\sum_{\beta < \alpha} n_{\beta}} = \pm 1$$

## Operador destrucción

$$c_{\alpha}|n_1 n_2 n_3 \cdots\rangle = \begin{cases} \eta_{\alpha}|n_1 \cdots n_{\alpha} - 1 \cdots\rangle & n_{\alpha} = 1 \\ 0 & n_{\alpha} = 0 \end{cases}$$

# Deducción del operador de un cuerpo

# Ecuación de Schroedinger

## Ecuación de Schroedinger

$$H = \sum_{i=1}^A t(\mathbf{r}_i) + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i, \mathbf{r}_j)$$

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}_1, \dots, \mathbf{r}_A, t) = H \Psi(\mathbf{r}_1, \dots, \mathbf{r}_A, t) \quad \Psi(\mathbf{r}_1, \dots, \mathbf{r}_A, t) = \sum_{\alpha'_1, \dots, \alpha'_A} C(\alpha'_1, \dots, \alpha'_A, t) \phi_{\alpha'_1}(\mathbf{r}_1) \dots \phi_{\alpha'_A}(\mathbf{r}_A)$$

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = H |\Psi\rangle$$

$$|\Psi\rangle = \sum_{\alpha'_1, \dots, \alpha'_A} C(\alpha'_1, \dots, \alpha'_A, t) |\alpha'_1 \dots \alpha'_A\rangle$$

$$\langle \alpha_1 \dots \alpha_A | i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \langle \alpha_1 \dots \alpha_A | H |\Psi\rangle$$

$$\langle \alpha_1 \dots \alpha_A | i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \langle \alpha_1 \dots \alpha_A | \sum_{i=1}^A t(\mathbf{r}_i) + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i, \mathbf{r}_j) |\Psi\rangle$$

$$\langle \alpha_1 \dots \alpha_A | i\hbar \frac{\partial}{\partial t} \sum_{\alpha'_1, \dots, \alpha'_A} C(\alpha'_1, \dots, \alpha'_A, t) |\alpha'_1 \dots \alpha'_A\rangle = \langle \alpha_1 \dots \alpha_A | \sum_{i=1}^A t(\mathbf{r}_i) + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i, \mathbf{r}_j) |\Psi\rangle$$

# Ecuación de Schroedinger

$$\langle \alpha_1 \cdots \alpha_A | i\hbar \frac{\partial}{\partial t} | \Psi \rangle = \langle \alpha_1 \cdots \alpha_A | \sum_{i=1}^A t(\mathbf{r}_i) + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i, \mathbf{r}_j) | \Psi \rangle$$

$$\langle \alpha_1 \cdots \alpha_A | i\hbar \frac{\partial}{\partial t} \sum_{\alpha'_1, \dots, \alpha'_A} C(\alpha'_1, \dots, \alpha'_A, t) | \alpha'_1 \cdots \alpha'_A \rangle = \langle \alpha_1 \cdots \alpha_A | \sum_{i=1}^A t(\mathbf{r}_i) + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i, \mathbf{r}_j) | \Psi \rangle$$

$$i\hbar \frac{\partial}{\partial t} C(\alpha_1, \dots, \alpha_A, t) = \langle \alpha_1 \cdots \alpha_A | \sum_{i=1}^A t(\mathbf{r}_i) + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i, \mathbf{r}_j) | \Psi \rangle$$

$$i\hbar \frac{\partial}{\partial t} C(\alpha_1, \dots, \alpha_A, t) = \sum_{i=1}^A \langle \alpha_1 \cdots \alpha_A | t(\mathbf{r}_i) | \Psi \rangle + \frac{1}{2} \sum_{i \neq j} \langle \alpha_1 \cdots \alpha_A | V(\mathbf{r}_i, \mathbf{r}_j) | \Psi \rangle$$

$$| \Psi \rangle = \sum_{\alpha'_1, \dots, \alpha'_A} C(\alpha'_1, \dots, \alpha'_A, t) | \alpha'_1 \cdots \alpha'_A \rangle$$

$$i\hbar \frac{\partial}{\partial t} C(\alpha_1, \dots, \alpha_A, t) = \sum_{i=1}^A \langle \alpha_1 \cdots \alpha_A | t(\mathbf{r}_i) \sum_{\alpha'_1, \dots, \alpha'_A} C(\alpha'_1, \dots, \alpha'_A, t) | \alpha'_1 \cdots \alpha'_A \rangle + \frac{1}{2} \sum_{i \neq j} \langle \alpha_1 \cdots \alpha_A | V(\mathbf{r}_i, \mathbf{r}_j) | \Psi \rangle$$

# Ecuación de Schroedinger

$$\langle \alpha_1 \cdots \alpha_A | i\hbar \frac{\partial}{\partial t} | \Psi \rangle = \langle \alpha_1 \cdots \alpha_A | \sum_{i=1}^A t(\mathbf{r}_i) + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i, \mathbf{r}_j) | \Psi \rangle$$

$$i\hbar \frac{\partial}{\partial t} C(\alpha_1, \dots, \alpha_A, t) = \sum_{i=1}^A \langle \alpha_1 \cdots \alpha_A | t(\mathbf{r}_i) | \Psi \rangle + \frac{1}{2} \sum_{i \neq j} \langle \alpha_1 \cdots \alpha_A | V(\mathbf{r}_i, \mathbf{r}_j) | \Psi \rangle$$

$$i\hbar \frac{\partial}{\partial t} C(\alpha_1, \dots, \alpha_A, t) = \sum_{i=1}^A \langle \alpha_1 \cdots \alpha_A | t(\mathbf{r}_i) \sum_{\alpha'_1, \dots, \alpha'_A} C(\alpha'_1, \dots, \alpha'_A, t) | \alpha'_1 \cdots \alpha'_A \rangle + \frac{1}{2} \sum_{i \neq j} \langle \alpha_1 \cdots \alpha_A | V(\mathbf{r}_i, \mathbf{r}_j) | \Psi \rangle$$

$$i\hbar \frac{\partial}{\partial t} C(\alpha_1, \dots, \alpha_A, t) = \sum_{i=1}^A \sum_{\alpha'_1, \dots, \alpha'_A} C(\alpha'_1, \dots, \alpha'_A, t) \langle \alpha_1 \cdots \alpha_A | t(\mathbf{r}_i) | \alpha'_1 \cdots \alpha'_A \rangle + \frac{1}{2} \sum_{i \neq j} \langle \alpha_1 \cdots \alpha_A | V(\mathbf{r}_i, \mathbf{r}_j) | \Psi \rangle$$

El operador  $t(\mathbf{r}_i)$  actúa solo en la partícula  $\beta'$ , llamemos al estado de la partícula  $i$ -ésima

$$i\hbar \frac{\partial}{\partial t} C(\alpha_1, \dots, \alpha_A, t) = \sum_{i=1}^A \sum_{\alpha'_1, \dots, \beta', \dots, \alpha'_A} C(\alpha'_1, \dots, \beta', \dots, \alpha'_A, t) \delta_{\alpha_1 \alpha'_1} \cdots \delta_{\alpha_{i-1} \alpha'_{i-1}} \delta_{\alpha_{i+1} \alpha'_{i+1}} \cdots \delta_{\alpha_A \alpha'_A} \langle \alpha_i | t(\mathbf{r}_i) | \beta' \rangle + \frac{1}{2} \cdots$$



# Ecuación de Schroedinger

$$\langle \alpha_1 \cdots \alpha_A | i\hbar \frac{\partial}{\partial t} | \Psi \rangle = \langle \alpha_1 \cdots \alpha_A | \sum_{i=1}^A t(\mathbf{r}_i) + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i, \mathbf{r}_j) | \Psi \rangle$$

$$i\hbar \frac{\partial}{\partial t} C(\alpha_1, \dots, \alpha_A, t) = \sum_{i=1}^A \langle \alpha_1 \cdots \alpha_A | t(\mathbf{r}_i) | \Psi \rangle + \frac{1}{2} \sum_{i \neq j} \langle \alpha_1 \cdots \alpha_A | V(\mathbf{r}_i, \mathbf{r}_j) | \Psi \rangle$$

$$i\hbar \frac{\partial}{\partial t} C(\alpha_1, \dots, \alpha_A, t) = \sum_{i=1}^A \sum_{\alpha'_1, \dots, \beta', \dots, \alpha'_A} C(\alpha'_1, \dots, \beta', \dots, \alpha'_A, t) \delta_{\alpha_1 \alpha'_1} \cdots \delta_{\alpha_{i-1} \alpha'_{i-1}} \delta_{\alpha_{i+1} \alpha'_{i+1}} \cdots \delta_{\alpha_A \alpha'_A} \langle \alpha_i | t(\mathbf{r}_i) | \beta' \rangle + \frac{1}{2} \cdots$$

$$i\hbar \frac{\partial}{\partial t} C(\alpha_1, \dots, \alpha_A, t) = \sum_{i=1}^A \sum_{\beta'} C(\alpha_1, \dots, \alpha_{i-1}, \beta', \alpha_{i+1}, \dots, \alpha_A, t) \langle \alpha_i | t(\mathbf{r}_i) | \beta' \rangle + \frac{1}{2} \cdots$$

Todas las integral  $t(\mathbf{r}_i)$  son iguales para cualquier partícula,

$$i\hbar \frac{\partial}{\partial t} C(\alpha_1, \dots, \alpha_A, t) = \sum_{i=1}^A \sum_{\beta'} C(\alpha_1, \dots, \alpha_{i-1}, \beta', \alpha_{i+1}, \dots, \alpha_A, t) \langle \alpha_i | t(\mathbf{r}_i) | \beta' \rangle + \frac{1}{2} \cdots$$

# Redefinición de coeficientes

$$\tilde{C}(n_1, n_2, \dots, n_\infty, t) \equiv C(\alpha_1, \alpha_2, \dots, \alpha_1, \alpha_A, t) \quad |\Psi\rangle = \sum_{\alpha_1, \dots, \alpha_A} C(\alpha_1, \dots, \alpha_A, t) |\alpha_1 \dots \alpha_A\rangle$$

$$\sum_{\alpha_1, \dots, \alpha_A} |C(\alpha_1, \dots, \alpha_A, t)|^2 = 1$$

$$\sum_{\alpha_1, \dots, \alpha_A} |C(\alpha_1, \dots, \alpha_A, t)|^2 = \sum_{n_1, n_2, \dots, n_\infty} |\tilde{C}(n_1, n_2, \dots, n_\infty, t)|^2 \sum_{\alpha_1, \dots, \alpha_A(n_1, \dots, n_\infty)} 1 = 1$$

$$\sum_{n_1, n_2, \dots, n_\infty} |\tilde{C}(n_1, n_2, \dots, n_\infty, t)|^2 \frac{A!}{n_1! n_2! \dots n_\infty!} = 1 \quad \sum_{i=1}^{\infty} n_i = A$$

$$|\Psi\rangle = \sum_{\alpha_1, \dots, \alpha_A} C(\alpha_1, \dots, \alpha_A, t) |\alpha_1 \dots \alpha_A\rangle = \sum_{\alpha_1, \dots, \alpha_A} \tilde{C}(n_1, n_2, \dots, n_\infty, t) |\alpha_1 \dots \alpha_A\rangle$$

# Redefinición de coeficientes

$$\tilde{C}(n_1, n_2, \dots, n_\infty, t) \equiv C(\alpha_1, \alpha_2, \dots, \alpha_1, \alpha_A, t) \quad |\Psi\rangle = \sum_{\alpha_1, \dots, \alpha_A} C(\alpha_1, \dots, \alpha_A, t) |\alpha_1 \dots \alpha_A\rangle$$

$$\sum_{n_1, n_2, \dots, n_\infty} |\tilde{C}(n_1, n_2, \dots, n_\infty, t)|^2 \frac{A!}{n_1! n_2! \dots n_\infty!} = 1 \quad \sum_{i=1}^{\infty} n_i = A$$

$$f(n_1, n_2, \dots, n_\infty) = \left( \frac{A!}{n_1! n_2! \dots n_\infty!} \right)^{1/2} \tilde{C}(n_1, n_2, \dots, n_\infty, t) \quad \sum_{n_1, n_2, \dots, n_\infty} |f(n_1, n_2, \dots, n_\infty)|^2 = 1$$

$$|\Psi\rangle = \sum_{\alpha_1, \dots, \alpha_A} C(\alpha_1, \dots, \alpha_A, t) |\alpha_1 \dots \alpha_A\rangle = \sum_{\alpha_1, \dots, \alpha_A} \tilde{C}(n_1, n_2, \dots, n_\infty, t) |\alpha_1 \dots \alpha_A\rangle$$

$$= \sum_{n_1, \dots, n_\infty} f(n_1, n_2, \dots, n_\infty, t) \left( \frac{n_1! n_2! \dots n_\infty!}{A!} \right)^{1/2} \sum_{\alpha_1, \dots, \alpha_A(n_1, \dots, n_\infty)} |\alpha_1 \dots \alpha_A\rangle$$

# Redefinición de coeficientes

$$|\Psi\rangle = \sum_{\alpha_1, \dots, \alpha_A} C(\alpha_1, \dots, \alpha_A, t) |\alpha_1 \dots \alpha_A\rangle$$

$$|\Psi\rangle = \sum_{n_1, \dots, n_\infty} f(n_1, n_2, \dots, n_\infty, t) \left( \frac{n_1! n_2! \dots n_\infty!}{A!} \right)^{1/2} \sum_{\alpha_1, \dots, \alpha_A(n_1, \dots, n_\infty)} |\alpha_1 \dots \alpha_A\rangle$$

$$\sum_{n_1, n_2, \dots, n_\infty} |f(n_1, n_2, \dots, n_\infty)|^2 = 1$$

$$\sum_{i=1}^{\infty} n_i = A$$

$$|\Psi\rangle = \sum_{n_1, \dots, n_\infty} f(n_1, n_2, \dots, n_\infty, t) \left( \frac{n_1! n_2! \dots n_\infty!}{A!} \right)^{1/2} |\alpha_1 \dots \alpha_A\rangle_{\mathcal{A}}$$

Lo vamos a usar más adelante...

$$|\Psi\rangle = \sum_{n_1, \dots, n_\infty} f(n_1, n_2, \dots, n_\infty, t) |n_1, n_2, \dots, n_\infty\rangle$$

$$\sum_{i=1}^{\infty} n_i = A$$

# Volviendo a la Ecuación de Schroedinger

$$\langle \alpha_1 \cdots \alpha_A | i\hbar \frac{\partial}{\partial t} | \Psi \rangle = \langle \alpha_1 \cdots \alpha_A | \sum_{i=1}^A t(\mathbf{r}_i) + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i, \mathbf{r}_j) | \Psi \rangle$$

$$i\hbar \frac{\partial}{\partial t} C(\alpha_1, \dots, \alpha_A, t) = \sum_{i=1}^A \langle \alpha_1 \cdots \alpha_A | t(\mathbf{r}_i) | \Psi \rangle + \frac{1}{2} \sum_{i \neq j} \langle \alpha_1 \cdots \alpha_A | V(\mathbf{r}_i, \mathbf{r}_j) | \Psi \rangle$$

Todas las integral  $t(\mathbf{r}_i)$  son iguales para cualquier partícula,

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} C(\alpha_1, \dots, \alpha_A, t) &= \sum_{i=1}^A \sum_{\beta'} C(\alpha_1, \dots, \alpha_{i-1}, \beta', \alpha_{i+1}, \dots, \alpha_A, t) \langle \alpha_i | t(\mathbf{r}) | \beta' \rangle + \frac{1}{2} \cdots \\ &= \sum_{i=1}^A \sum_{\beta'} \tilde{C}(n_1, \dots, n_{\alpha_i} - 1, \dots, n_{\beta'} + 1, \dots, n_{\infty}, t) \langle \alpha_i | t(\mathbf{r}) | \beta' \rangle + \frac{1}{2} \cdots \end{aligned}$$

Esto expone el hecho que el estado  $\alpha_i$  aparece una vez menos, mientras el estado  $\beta'$  una vez más

La suma sobre  $i$  resulta equivalente a suma sobre estados en la forma  $\sum_{\beta} n_{\beta}$

$$i\hbar \frac{\partial}{\partial t} C(\alpha_1, \dots, \alpha_A, t) = \sum_{\beta} \sum_{\beta'} n_{\beta} \tilde{C}(n_1, \dots, n_{\beta} - 1, \dots, n_{\beta'} + 1, \dots, n_{\infty}, t) \langle \beta | t(\mathbf{r}) | \beta' \rangle + \frac{1}{2} \cdots$$

# Volviendo a la Ecuación de Schroedinger

$$\langle \alpha_1 \cdots \alpha_A | i\hbar \frac{\partial}{\partial t} | \Psi \rangle = \langle \alpha_1 \cdots \alpha_A | \sum_{i=1}^A t(\mathbf{r}_i) + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i, \mathbf{r}_j) | \Psi \rangle$$

$$i\hbar \frac{\partial}{\partial t} C(\alpha_1, \dots, \alpha_A, t) = \sum_{i=1}^A \langle \alpha_1 \cdots \alpha_A | t(\mathbf{r}_i) | \Psi \rangle + \frac{1}{2} \sum_{i \neq j} \langle \alpha_1 \cdots \alpha_A | V(\mathbf{r}_i, \mathbf{r}_j) | \Psi \rangle$$

$$i\hbar \frac{\partial}{\partial t} C(\alpha_1, \dots, \alpha_A, t) = \sum_{\beta} \sum_{\beta'} n_{\beta} \tilde{C}(n_1, \dots, n_{\beta} - 1, \dots, n_{\beta'} + 1, \dots, n_{\infty}, t) \langle \beta | t(\mathbf{r}) | \beta' \rangle + \frac{1}{2} \dots$$

$$i\hbar \frac{\partial}{\partial t} \left( \frac{n_1! \cdots n_{\infty}!}{A!} \right)^{1/2} f(n_1, \dots, n_{\infty}, t) = \sum_{\beta} n_{\beta} \left( \frac{\dots n_{\beta}! \dots}{A!} \right)^{1/2} f(n_1, \dots, n_{\beta} \dots n_{\infty}, t) \langle \beta | t(\mathbf{r}) | \beta' \rangle$$

$$+ \sum_{\beta \neq \beta'} n_{\beta} \left( \frac{\dots (n_{\beta} - 1)! \dots (n_{\beta'} + 1)! \dots}{A!} \right)^{1/2} f(n_1, \dots, n_{\beta} - 1 \dots n_{\beta'} + 1 \dots n_{\infty}, t) \langle \beta | t(\mathbf{r}) | \beta' \rangle + \frac{1}{2} \dots$$

# Volviendo a la Ecuación de Schroedinger

$$\langle \alpha_1 \cdots \alpha_A | i\hbar \frac{\partial}{\partial t} | \Psi \rangle = \langle \alpha_1 \cdots \alpha_A | \sum_{i=1}^A t(\mathbf{r}_i) + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i, \mathbf{r}_j) | \Psi \rangle$$

$$i\hbar \frac{\partial}{\partial t} \left( \frac{n_1! \cdots n_\infty!}{A!} \right)^{1/2} f(n_1, \dots, n_\infty, t) = \sum_{\beta} n_{\beta} \left( \frac{\cdots n_{\beta}! \cdots}{A!} \right)^{1/2} f(n_1, \dots, n_{\beta} \cdots n_\infty, t) \langle \beta | t(\mathbf{r}) | \beta' \rangle$$

$$+ \sum_{\beta \neq \beta'} n_{\beta} \left( \frac{\cdots (n_{\beta} - 1)! \cdots (n_{\beta'} + 1)! \cdots}{A!} \right)^{1/2} f(n_1, \dots, n_{\beta} - 1 \cdots n_{\beta'} + 1 \cdots n_\infty, t) \langle \beta | t(\mathbf{r}) | \beta' \rangle + \frac{1}{2} \cdots$$

$$i\hbar \frac{\partial}{\partial t} f(n_1, \dots, n_\infty, t) = \sum_{\beta} n_{\beta} f(n_1, \dots, n_{\beta} \cdots n_\infty, t) \langle \beta | t(\mathbf{r}) | \beta' \rangle$$

$$+ \sum_{\beta \neq \beta'} (n_{\beta})^{1/2} (n_{\beta'+1})^{1/2} f(n_1, \dots, n_{\beta} - 1 \cdots n_{\beta'} + 1 \cdots n_\infty, t) \langle \beta | t(\mathbf{r}) | \beta' \rangle + \frac{1}{2} \cdots$$

$$| \Psi \rangle = \sum_{\alpha_1, \dots, \alpha_A} C(\alpha_1, \dots, \alpha_A, t) | \alpha_1 \cdots \alpha_A \rangle$$

$$| \Psi \rangle = \sum_{n_1, \dots, n_\infty} f(n_1, n_2, \dots, n_\infty, t) \left( \frac{n_1! n_2! \cdots n_\infty!}{A!} \right)^{1/2} | \alpha_1 \cdots \alpha_A \rangle_{\mathcal{A}} = \sum_{n_1, \dots, n_\infty} f(n_1, n_2, \dots, n_\infty, t) | n_1, n_2, \dots, n_\infty \rangle$$

# Volviendo a la Ecuación de Schroedinger

$$\langle \alpha_1 \cdots \alpha_A | i\hbar \frac{\partial}{\partial t} | \Psi \rangle = \langle \alpha_1 \cdots \alpha_A | \sum_{i=1}^A t(\mathbf{r}_i) + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i, \mathbf{r}_j) | \Psi \rangle$$

$$i\hbar \frac{\partial}{\partial t} f(n_1, \dots, n_\infty, t) = \sum_{\beta} n_{\beta} f(n_1, \dots, n_{\beta} \cdots n_{\infty}, t) \langle \beta | t(\mathbf{r}) | \beta' \rangle + \sum_{\beta \neq \beta'} (n_{\beta})^{1/2} (n_{\beta'+1})^{1/2} f(n_1, \dots, n_{\beta} - 1 \cdots n_{\beta'} + 1 \cdots n_{\infty}, t) \langle \beta | t(\mathbf{r}) | \beta' \rangle + \frac{1}{2} \cdots$$

$$| \Psi \rangle = \sum_{n_1, \dots, n_{\infty}} f(n_1, n_2, \dots, n_{\infty}, t) | n_1, n_2, \dots, n_{\infty} \rangle$$

$$i\hbar \frac{\partial}{\partial t} | \Psi \rangle = \cdots + \sum_{n'_1 \cdots n'_{\infty}} \sum_{\beta \neq \beta'} \langle \beta | t(\mathbf{r}) | \beta' \rangle f(\cdots, n'_{\beta} \cdots n'_{\beta'} \cdots, t) (n'_{\beta} + 1)^{1/2} (n'_{\beta'})^{1/2} | \cdots n'_{\beta} + 1 \cdots n'_{\beta'} - 1 \cdots \rangle + \cdots$$

$$(n'_{\beta} + 1)^{1/2} (n'_{\beta'})^{1/2} | n'_1 \cdots n'_{\beta} + 1 \cdots n'_{\beta'} - 1 \cdots n_{\infty} \rangle = c_{\beta}^{\dagger} c_{\beta'} | n'_1 n'_2 \cdots n_{\infty} \rangle$$

$$i\hbar \frac{\partial}{\partial t} | \Psi \rangle = \cdots + \sum_{\beta \neq \beta'} \langle \beta | t(\mathbf{r}) | \beta' \rangle c_{\beta}^{\dagger} c_{\beta'} | \Psi \rangle + \cdots$$



# Operador de una partícula

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \sum_{\alpha, \beta} \langle \alpha | t(\mathbf{r}) | \beta \rangle c_{\alpha}^{\dagger} c_{\beta} |\Psi\rangle + \frac{1}{2} \dots$$

$$T = \sum_{i=1}^A t(\mathbf{r}_i)$$

$$T = \sum_{\alpha, \beta} \langle \alpha | t | \beta \rangle c_{\alpha}^{\dagger} c_{\beta}$$

Aplicarlo al Hamiltoniano de campo medio

$$t_{\alpha\beta} = \langle \alpha | t | \beta \rangle = \int \phi_{\alpha}^{\dagger}(\mathbf{r}) t(\mathbf{r}) \phi_{\beta}(\mathbf{r}) d^3\mathbf{r}$$

**Ejemplo:**

$$J_z = \hbar \sum_{\alpha} m_{\alpha} c_{\alpha}^{\dagger} c_{\alpha}$$

# Operadores en segunda cuantización

## Ejemplo operador de una partícula

$$J_z = \sum_{\alpha\beta} |\alpha\rangle\langle\alpha| J_z |\beta\rangle\langle\beta|$$

Proyección Momento angular

$J_z$

$$J_z = \sum_{\alpha\beta} |\alpha\rangle\langle\alpha| \hbar m_\beta |\beta\rangle\langle\beta| = \sum_{\alpha\beta} \hbar m_\beta |\alpha\rangle\langle\alpha|\beta\rangle\langle\beta|$$

$$J_z = \sum_{\alpha\beta} \hbar m_\beta \delta_{\alpha\beta} |\alpha\rangle\langle\beta|$$

$$J_z = \hbar \sum_{\alpha} m_\alpha |\alpha\rangle\langle\alpha|$$

# Operadores en segunda cuantización

## Operador de dos partículas

$$V = \sum_{i < j} v(\mathbf{r}_i, \mathbf{r}_j) = \frac{1}{2} \sum_{i \neq j} v(\mathbf{r}_i, \mathbf{r}_j)$$

$$V = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma}$$

$$v_{\alpha\beta\gamma\delta} = \int \phi_{\alpha}^{\dagger}(\mathbf{r}_1) \phi_{\beta}^{\dagger}(\mathbf{r}_2) v(\mathbf{r}_1, \mathbf{r}_2) \phi_{\gamma}(\mathbf{r}_1) \phi_{\delta}(\mathbf{r}_2) d^3\mathbf{r}_1 d^3\mathbf{r}_2$$

# Operadores en segunda cuantización

## Interacción de dos partículas

$$V = \sum_{i < j} v(\mathbf{r}_i, \mathbf{r}_j) = \frac{1}{2} \sum_{i \neq j} v(\mathbf{r}_i, \mathbf{r}_j)$$

$$V = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma}$$

$$V = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma}$$

$$\bar{v}_{\alpha\beta\gamma\delta} \equiv v_{\alpha\beta\gamma\delta} - v_{\alpha\beta\delta\gamma}$$

$$\bar{v}_{\alpha\beta\gamma\delta} = \text{n.as.} \langle \alpha\beta | V | \gamma\delta \rangle \text{n.as.}$$

Tomando elementos de matriz con la función de onda antisimetrizada y normalizada

$$v_{\alpha\beta\gamma\delta} = \int \phi_{\alpha}^{\dagger}(\mathbf{r}_1) \phi_{\beta}^{\dagger}(\mathbf{r}_2) v(\mathbf{r}_1, \mathbf{r}_2) \phi_{\gamma}(\mathbf{r}_1) \phi_{\delta}(\mathbf{r}_2) d^3\mathbf{r}_1 d^3\mathbf{r}_2$$

## Propiedades

$$\bar{v}_{\alpha\beta\gamma\delta} = -\bar{v}_{\beta\alpha\gamma\delta} = -\bar{v}_{\alpha\beta\delta\gamma} = \bar{v}_{\beta\alpha\delta\gamma} = \bar{v}_{\gamma\delta\alpha\beta}^*$$

# Teorema de Wick

# Definiciones

## Motivación

$$\langle 0 | AB \dots | 0 \rangle = ?$$

Ejemplo: elemento de matriz de un observable o interacción de dos cuerpos

## Orden normal:

$$\mathcal{N}[ABB^\dagger] = (-1)^{(\# \text{ de perm.})} B^\dagger AB$$

## Ejemplo:

$$\mathcal{N}[c_\alpha^\dagger c_\beta c_\gamma^\dagger c_\delta] = \dots$$

$$\mathcal{N} = -c_\alpha^\dagger c_\gamma^\dagger c_\beta c_\delta$$

## Contracción

$$\overline{AB} = AB - \mathcal{N}[AB] = \langle \Psi_0 | AB | \Psi_0 \rangle$$

$$:AB: = AB - \mathcal{N}[AB] = \langle \Psi_0 | AB | \Psi_0 \rangle$$

## Ejemplos:

$$\overline{c_k c_l^\dagger} = \langle 0 | c_k c_l^\dagger | 0 \rangle = \delta_{kl}$$

$$\overline{c_k^\dagger c_l^\dagger} = 0$$

$$AB =: AB : + \mathcal{N}[AB]$$

$$\{c_\alpha, c_\beta^\dagger\} = c_\alpha c_\beta^\dagger + c_\beta^\dagger c_\alpha = \delta_{\alpha\beta}$$

# Teorema de Wick

**Contracción:**  $\overline{AB} = AB - \mathcal{N}[AB] = \langle \Psi_0 | AB | \Psi_0 \rangle$

**Orden normal:**  $\mathcal{N}[ABB^\dagger] = (-1)^{(\# \text{ de perm.})} B^\dagger AB$

## **Teorema de Wick:**

$$\begin{aligned} ABCDEF\dots &= \mathcal{N}[ABCDEF\dots] \\ &+ \mathcal{N}[\overline{AB}CDEF\dots] + \mathcal{N}[\overline{AC}BDEF\dots] + \dots \\ &+ \mathcal{N}[\overline{AB}\overline{CD}EF\dots] + \mathcal{N}[\overline{AC}\overline{BD}EF\dots] + \dots \\ &\vdots \\ &+ \text{ todos los pares contraídos} \end{aligned}$$

## **Aplicación: valor medio vacío**

$$\langle 0 | ABCDEF\dots | 0 \rangle = \langle 0 | \text{ todos los pares contraídos } | 0 \rangle$$

# Aplicación de Wick en las ecuaciones de Hartree-Fock



# Campo Medio: Hartree-Fock

**Hamiltoniano de muchos cuerpos:**  $H = T + V$

$$T = \sum_{i=1}^A t(\mathbf{r}_i)$$

**Interacción:**  $V = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma}$      $\bar{v}_{\alpha\beta\gamma\delta} = v_{\alpha\beta\gamma\delta} - v_{\alpha\beta\delta\gamma}$

$$V = \sum_{i<j}^{i=1} v(\mathbf{r}_i, \mathbf{r}_j) = \frac{1}{2} \sum_{i \neq j} v(\mathbf{r}_i, \mathbf{r}_j)$$

Única contracción  
no nula

$$4V = \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} \mathcal{N}[c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma}]$$

$$\langle HF | c_a^{\dagger} c_b | HF \rangle = \delta_{ab}$$

$$- \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} \langle HF | c_{\alpha}^{\dagger} c_{\delta} | HF \rangle \mathcal{N}[c_{\beta}^{\dagger} c_{\gamma}]$$

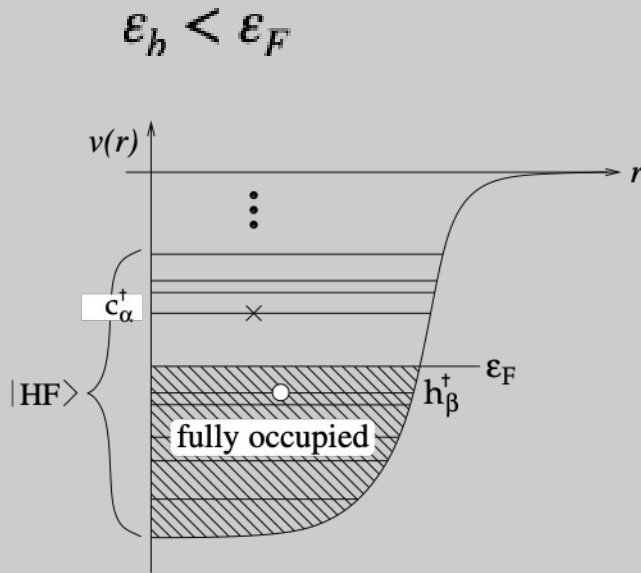
$$+ \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} \langle HF | c_{\alpha}^{\dagger} c_{\gamma} | HF \rangle \mathcal{N}[c_{\beta}^{\dagger} c_{\delta}]$$

$$+ \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} \langle HF | c_{\beta}^{\dagger} c_{\delta} | HF \rangle \mathcal{N}[c_{\alpha}^{\dagger} c_{\gamma}]$$

$$- \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} \langle HF | c_{\beta}^{\dagger} c_{\gamma} | HF \rangle \mathcal{N}[c_{\alpha}^{\dagger} c_{\delta}]$$

$$- \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} \langle HF | c_{\alpha}^{\dagger} c_{\delta} | HF \rangle \langle HF | c_{\beta}^{\dagger} c_{\gamma} | HF \rangle$$

$$+ \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} \langle HF | c_{\alpha}^{\dagger} c_{\gamma} | HF \rangle \langle HF | c_{\beta}^{\dagger} c_{\delta} | HF \rangle$$



Crédito: Suhonen

# Campo Medio: Hartree-Fock

**Hamiltoniano de muchos cuerpos:**  $H = T + V$

$$T = \sum_{i=1}^A t(\mathbf{r}_i)$$

**Interacción:**  $V = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma}$       $\bar{v}_{\alpha\beta\gamma\delta} = v_{\alpha\beta\gamma\delta} - v_{\alpha\beta\delta\gamma}$

$$V = \sum_{i<j}^{i=1} v(\mathbf{r}_i, \mathbf{r}_j) = \frac{1}{2} \sum_{i \neq j} v(\mathbf{r}_i, \mathbf{r}_j)$$

$$4V = \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} \mathcal{N}[c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma}]$$

$$\langle HF | c_a^{\dagger} c_b | HF \rangle = \delta_{ab}$$

$$- \sum_{\substack{\alpha\beta\gamma \\ \varepsilon_{\alpha} \leq \varepsilon_F}} \bar{v}_{\alpha\beta\gamma\alpha} \mathcal{N}[c_{\beta}^{\dagger} c_{\gamma}] + \sum_{\substack{\alpha\beta\delta \\ \varepsilon_{\alpha} \leq \varepsilon_F}} \bar{v}_{\alpha\beta\alpha\delta} \mathcal{N}[c_{\beta}^{\dagger} c_{\delta}]$$

$$+ \sum_{\substack{\alpha\beta\gamma \\ \varepsilon_{\beta} \leq \varepsilon_F}} \bar{v}_{\alpha\beta\gamma\beta} \mathcal{N}[c_{\alpha}^{\dagger} c_{\gamma}] - \sum_{\substack{\alpha\beta\delta \\ \varepsilon_{\beta} \leq \varepsilon_F}} \bar{v}_{\alpha\beta\beta\delta} \mathcal{N}[c_{\alpha}^{\dagger} c_{\delta}]$$

$$- \sum_{\substack{\alpha\beta \\ \varepsilon_{\alpha} \leq \varepsilon_F \\ \varepsilon_{\beta} \leq \varepsilon_F}} \bar{v}_{\alpha\beta\beta\alpha} + \sum_{\substack{\alpha\beta \\ \varepsilon_{\alpha} \leq \varepsilon_F \\ \varepsilon_{\beta} \leq \varepsilon_F}} \bar{v}_{\alpha\beta\alpha\beta}$$

$$\bar{v}_{\alpha\beta\gamma\delta} = -\bar{v}_{\beta\alpha\gamma\delta}$$

$$= -\bar{v}_{\alpha\beta\delta\gamma}$$

$$= \bar{v}_{\beta\alpha\delta\gamma}$$

# Campo Medio: Hartree-Fock

**Hamiltoniano de muchos cuerpos:**  $H = T + V$

$$T = \sum_{i=1}^A t(\mathbf{r}_i)$$

**Interacción:**  $V = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma}$      $\bar{v}_{\alpha\beta\gamma\delta} = v_{\alpha\beta\gamma\delta} - v_{\alpha\beta\delta\gamma}$

$$V = \sum_{i<j}^{i=1} v(\mathbf{r}_i, \mathbf{r}_j) = \frac{1}{2} \sum_{i \neq j} v(\mathbf{r}_i, \mathbf{r}_j)$$

## Propiedades

$$\begin{aligned} \bar{v}_{\alpha\beta\gamma\delta} &= -\bar{v}_{\beta\alpha\gamma\delta} \\ &= -\bar{v}_{\alpha\beta\delta\gamma} \\ &= \bar{v}_{\beta\alpha\delta\gamma} \end{aligned}$$

$$\begin{aligned} V &= \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} \mathcal{N}[c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma}] \\ &+ \sum_{\substack{\alpha\beta\gamma \\ \varepsilon_{\alpha} \leq \varepsilon_F}} \bar{v}_{\alpha\beta\alpha\gamma} \mathcal{N}[c_{\beta}^{\dagger} c_{\gamma}] \\ &+ \frac{1}{2} \sum_{\substack{\alpha\beta \\ \varepsilon_{\alpha} \leq \varepsilon_F \\ \varepsilon_{\beta} \leq \varepsilon_F}} \bar{v}_{\alpha\beta\alpha\beta} \end{aligned}$$

$$\mathcal{N}[c_{\beta}^{\dagger} c_{\gamma}] = c_{\beta}^{\dagger} c_{\gamma} - \langle HF | c_{\beta}^{\dagger} c_{\gamma} | HF \rangle = c_{\beta}^{\dagger} c_{\gamma} - \delta_{\beta\gamma}$$

# Campo Medio: Hartree-Fock

**Hamiltoniano de muchos cuerpos:**  $H = T + V$

**Interacción:**  $V = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma}$      $\bar{v}_{\alpha\beta\gamma\delta} = v_{\alpha\beta\gamma\delta} - v_{\alpha\beta\delta\gamma}$

$T = \sum_{i=1}^A t(\mathbf{r}_i)$

$V = \sum_{i<j}^{i=1} v(\mathbf{r}_i, \mathbf{r}_j) = \frac{1}{2} \sum_{i \neq j} v(\mathbf{r}_i, \mathbf{r}_j)$

$$\mathcal{N}[c_{\beta}^{\dagger} c_{\gamma}] = c_{\beta}^{\dagger} c_{\gamma} - \langle HF | c_{\beta}^{\dagger} c_{\gamma} | HF \rangle = c_{\beta}^{\dagger} c_{\gamma} - \delta_{\beta\gamma}$$

$$V = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} \mathcal{N}[c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma}]$$

**Operador de una partícula**  $\longrightarrow + \sum_{\alpha\beta} \left( \sum_{\substack{\gamma \\ \epsilon_{\gamma} \leq \epsilon_F}} \bar{v}_{\gamma\alpha\gamma\beta} \right) c_{\alpha}^{\dagger} c_{\beta}$

**Escalar**  $\longrightarrow - \frac{1}{2} \sum_{\substack{\alpha\beta \\ \epsilon_{\alpha} \leq \epsilon_F \\ \epsilon_{\beta} \leq \epsilon_F}} \bar{v}_{\alpha\beta\alpha\beta}$

# Campo Medio: Hartree-Fock

**Hamiltoniano de muchos cuerpos:**

$$\begin{aligned}
 H &= T + V \\
 &= + \sum_{\alpha\beta} \left( t_{\alpha\beta} + \sum_{\substack{\gamma \\ \epsilon_\gamma \leq \epsilon_F}} \bar{V}_{\gamma\alpha\gamma\beta} \right) c_\alpha^\dagger c_\beta \\
 &\quad + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \bar{V}_{\alpha\beta\gamma\delta} \mathcal{N}[c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma] \\
 &\quad - \frac{1}{2} \sum_{\substack{\alpha\beta \\ \epsilon_\alpha \leq \epsilon_F \\ \epsilon_\beta \leq \epsilon_F}} \bar{V}_{\alpha\beta\alpha\beta}
 \end{aligned}$$

$$T = \sum_{i=1}^A t(\mathbf{r}_i)$$

$$V = \sum_{i<j} v(\mathbf{r}_i, \mathbf{r}_j) = \frac{1}{2} \sum_{i \neq j} v(\mathbf{r}_i, \mathbf{r}_j)$$

**Ecuación de autovalores de HF:**

$$t_{\alpha\beta} + \sum_{\substack{\gamma \\ \epsilon_\gamma \leq \epsilon_F}} \bar{v}_{\gamma\alpha\gamma\beta} = \epsilon_{\alpha\beta} \delta_{\alpha\beta}$$

**Hamiltoniano campo medio:**

$$H = H_{HF} + V_{Res}$$

$$\begin{aligned}
 H_{HF} &= \sum_{\alpha} \epsilon_{\alpha} c_{\alpha}^{\dagger} c_{\alpha} & V_{Res} &= \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \bar{V}_{\alpha\beta\gamma\delta} \mathcal{N}[c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma}] - \frac{1}{2} \sum_{\substack{\alpha\beta \\ \epsilon_{\alpha} \leq \epsilon_F \\ \epsilon_{\beta} \leq \epsilon_F}} \bar{V}_{\alpha\beta\alpha\beta}
 \end{aligned}$$

# Ecuación de Hartree-Fock en coordenadas

**Ecuación de autovalores de HF:**

$$t_{\alpha\beta} + \sum_{\substack{\gamma \\ \varepsilon_\gamma \leq \varepsilon_F}} \bar{v}_{\gamma\alpha\gamma\beta} = \varepsilon_{\alpha\beta} \delta_{\alpha\beta} \quad \bar{v}_{\alpha\beta\gamma\delta} = v_{\alpha\beta\gamma\delta} - v_{\alpha\beta\delta\gamma}$$

**Representación coordenada:**

$$-\frac{\hbar^2}{2m} \nabla^2 \phi_\alpha(\mathbf{x}) + V_H(\mathbf{x}) \phi_\alpha(\mathbf{x}) - \int d^3\mathbf{r}' V_F(\mathbf{x}', \mathbf{x}) \phi_\alpha(\mathbf{x}') = \varepsilon_\alpha \phi_\alpha(\mathbf{x})$$

$$V_H(\mathbf{x}) = \sum_{\substack{\beta \\ \varepsilon_\beta \leq \varepsilon_F}} \int d^3\mathbf{r}' \phi_\beta^\dagger(\mathbf{x}') V(\mathbf{x}', \mathbf{x}) \phi_\beta(\mathbf{x}')$$

$$V_F(\mathbf{x}', \mathbf{x}) = \sum_{\substack{\beta \\ \varepsilon_\beta \leq \varepsilon_F}} \phi_\beta^\dagger(\mathbf{x}') V(\mathbf{x}', \mathbf{x}) \phi_\beta(\mathbf{x})$$

# **Hamiltoniano en segunda cuantización acoplado**

# (recordemos) Función de onda de dos partículas acopladas

## Función de onda antisimetrizada

$$\Phi_{ab}^{JM}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2(1 + \delta_{ab})}} \sum_{m_a, m_b} \langle j_a m_a j_b m_b | JM \rangle \left[ \psi_{am_a}(\mathbf{r}_1) \psi_{bm_b}(\mathbf{r}_2) - \psi_{am_a}(\mathbf{r}_2) \psi_{bm_b}(\mathbf{r}_1) \right]$$

## Función de onda de partícula simple

$$\psi_{am_a}(\mathbf{r}) = \frac{u_a(r)}{r} \mathcal{Y}_{l j m}$$

$$a = \{n, l, j\}$$

## Representación coordenada

$$\Phi_{ab}^{JM}(\mathbf{r}_1, \mathbf{r}_2) = \langle \mathbf{r}_1 \mathbf{r}_2 | \Phi_{ab}^{JM} \rangle$$

## Segunda cuantización

$$|\Phi_{ab}^{JM}\rangle = A_{JM}^\dagger(ab) |0\rangle$$



# Operador de dos partículas acopladas

## Estado de dos partículas

$$|\Phi_{ab}^{JM}\rangle = A_{JM}^\dagger(ab) |0\rangle$$

## Operador creación de dos partículas acopladas

$$A_{JM}^\dagger(ab) = \frac{1}{\sqrt{1 + \delta_{ab}}} \sum_{m_a m_b} \langle j_a m_a j_b m_b | JM \rangle c_{a m_a}^\dagger c_{b m_b}^\dagger$$

## Propiedad

$$A_{JM}^\dagger(ab) = - (-)^{j_a + j_b - J} A_{JM}^\dagger(ba)$$

# Operador de dos partículas acopladas

## Estado de dos partículas

$$|\Phi_{ab}^{JM}\rangle = A_{JM}^\dagger(ab) |0\rangle$$

$$A_{JM}^\dagger(ab) = \frac{1}{\sqrt{1 + \delta_{ab}}} \sum_{m_a m_b} \langle j_a m_a j_b m_b | JM \rangle c_{a m_a}^\dagger c_{b m_b}^\dagger$$

## Operador destrucción de dos partículas acopladas

$$A_{JM}(cd) = [A_{JM}^\dagger(cd)]^\dagger$$

$$A_{JM}(ab) |0\rangle = 0$$

# Hamiltoniano en 2da cuantización acoplado(informativo)

## Hamiltoniano coordenadas

$$H = \sum_{i=1}^A h(\mathbf{r}_i) + \sum_{i<j=1}^A V(\mathbf{r}_i, \mathbf{r}_j)$$

## Hamiltoniano 2da cuantización

$$H = \sum_{am_a} \epsilon_a c_{am_a}^\dagger c_{am_a} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma$$

## Hamiltoniano acoplado

$$H = \sum_{am_a} \epsilon_a c_{am_a}^\dagger c_{am_a} + \sum_{JM} \sum_{b \leq a} \sum_{d \leq c} E_J(ab, cd) A_{JM}^\dagger(ab) A_{JM}(cd)$$

# Hamiltoniano en 2da cuantización acoplado

## Hamiltoniano coordenadas

$$H = \sum_{i=1}^A h(\mathbf{r}_i) + \sum_{i<j=1}^A V(\mathbf{r}_i, \mathbf{r}_j)$$

## Hamiltoniano acoplado

$$H = \sum_{am_a} \epsilon_a c_{am_a}^\dagger c_{am_a} + \sum_{JM} \sum_{b \leq a} \sum_{d \leq c} E_J(ab, cd) A_{JM}^\dagger(ab) A_{JM}(cd)$$

## Propiedades

$$E_J(ab, cd) = E_J(cd, ab)$$

$$E_J(ab, cd) = -(-)^{j_a+j_b-J} E_J(ba, cd)$$

$$E_J(ab, cd) = -(-)^{j_a+j_b+j_c+j_d} E_J(ba, dc)$$

## Elementos de matriz

$$E_J(ab, cd) = \langle \Phi_{ab}^{JM} | V | \Phi_{cd}^{JM} \rangle$$

# **Ejemplo: Hamiltoniano con interacción delta de Dirac**

# Función correlacionada(informativo)

**Base:**  $|\Phi_{ab}^{JM}\rangle = A_{JM}^\dagger(ab)|0\rangle$

**Función de onda correlacionada:**

$$\Psi_{EJM}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{d \leq c} X_{cd, EJ} \Phi_{cd}^{JM}(\mathbf{r}_1, \mathbf{r}_2)$$

$$|\Psi_{EJM}\rangle = \sum_{d \leq c} X_{cd, EJ} A_{JM}^\dagger(cd)|0\rangle$$

**Normalización:**

$$\sum_{d \leq c} X_{cd, EJ}^2 = 1$$

**Ecuación de Schroedinger:**  $H|\Psi_{EJM}\rangle = E|\Psi_{EJM}\rangle$

**Ecuación de autovalores:**

$$\langle \Phi_{ab}^{JM} | H | \Psi_{EJM} \rangle = E \langle \tilde{\Phi}_{ab}^{JM} | \Psi_{EJM} \rangle$$

$$\sum_{d \leq c} X_{cd, EJ} \{ (\varepsilon_a + \varepsilon_b - E) \delta_{ac} \delta_{bd} + \langle \Phi_{ab}^{JM} | V_{nn} | \Phi_{cd}^{JM} \rangle \} = E X_{ab, EJ}$$

# Interacción delta de Dirac

**Función de onda correlacionada:**

$$\Psi_{EJM}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{d \leq c} X_{cd,EJ} \Phi_{cd}^{JM}(\mathbf{r}_1, \mathbf{r}_2)$$

**Ecuación de autovalores:**

$$\sum_{d \leq c} X_{cd,EJ} \left\{ (\varepsilon_a + \varepsilon_b - E) \delta_{ac} \delta_{bd} + \langle \Phi_{ab}^{JM} | V_{nn} | \Phi_{cd}^{JM} \rangle \right\} = E X_{ab,EJ}$$

**Interacción delta:**

$$V = -4\pi V_0 \delta(\mathbf{r}_2 - \mathbf{r}_1) V(r_1)$$

$$V_k(r_1, r_2) = -4\pi V_0 \frac{\delta(r_2 - r_1)}{r_1 r_2}$$

**Expansión en ondas parciales:**

$$V(\mathbf{r}_1 - \mathbf{r}_2) = \sum_k V_k(r_1, r_2) P_k(\cos(\theta))$$

$$V_k(r_1, r_2) = \frac{2k+1}{2} \int_{-1}^1 P_k(x) V(\mathbf{r}_1 - \mathbf{r}_2)$$

**Elementos de matriz:**

$$E_J(ab, cd) = V_0 I_{abcd} M_{ang}^J$$

$$M_{ang}^J = (-)^{j_a + j_c + l_b + l_d} \left\{ 1 + (-)^{l_a + l_b + l_c + l_d} \right\} \left\{ \frac{1 + (-)^{l_c + l_d + J}}{2} \right\} \\ \times \frac{1}{2(2J+1)} \left\{ \frac{(2j_a + 1)(2j_b + 1)(2j_c + 1)(2j_d + 1)}{(1 + \delta_{ab})(1 + \delta_{cd})} \right\}^{1/2} \\ \times \langle j_a \ 1/2 \ j_b \ -1/2 | J0 \rangle \langle j_c \ 1/2 \ j_d \ -1/2 | J0 \rangle$$

**Recordar R0**

$$I_{abcd} = \int \phi_a(r) \phi_b(r) \phi_c(r) \phi_d(r) V(r) r^2 dr \quad V(r) = 1$$

# Comparación con experimento

**Función de onda correlacionada:**

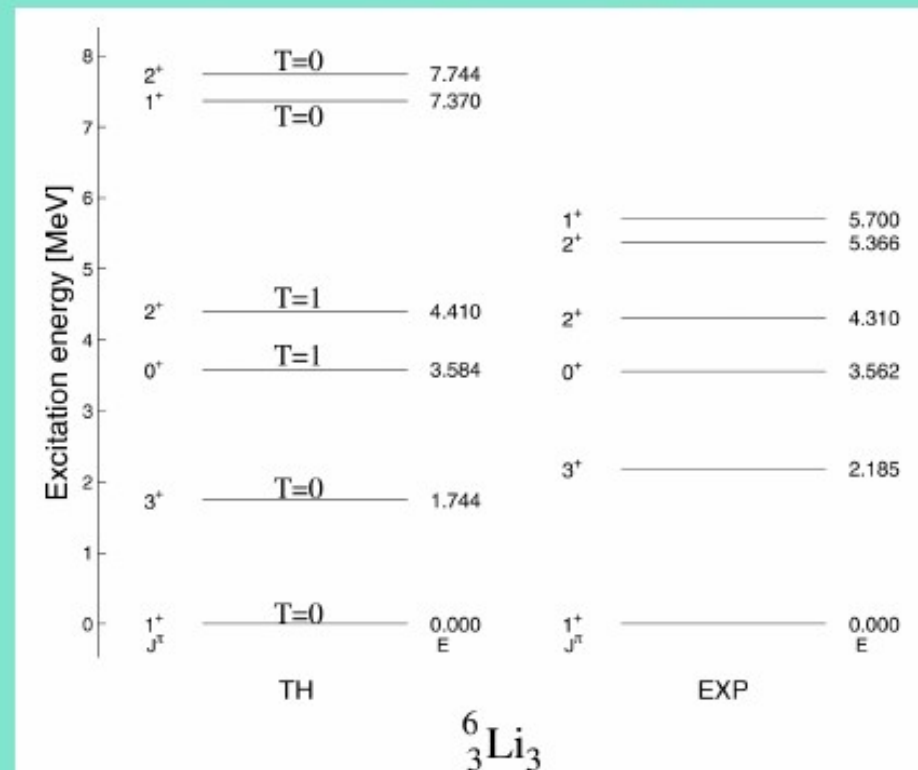
$$\Psi_{EJM}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{d \leq c} X_{cd, EJ} \Phi_{cd}^{JM}(\mathbf{r}_1, \mathbf{r}_2)$$

**Ecuación de autovalores:**

$$\sum_{d \leq c} X_{cd, EJ} \{ (\varepsilon_a + \varepsilon_b - E) \delta_{ac} \delta_{bd} + \langle \Phi_{ab}^{JM} | V_{nn} | \Phi_{cd}^{JM} \rangle \} = E X_{ab, EJ}$$

**Elementos de matriz:**

$$E_J(ab, cd) = V_0 I_{abcd} M_{ang}^J$$



Crédito: Fig. 8.1 J. Suhonen. From nucleons to Nucleus. 2007



# **Ejemplo: Hamiltoniano de apareamiento**

# Volviendo a la Interacción Separable

## Hamiltoniano

$$H = \sum_{am_a} \varepsilon_a c_{am_a}^\dagger c_{am_a} + \sum_{JM} \sum_{b \leq a} \sum_{d \leq c} E_J(ab, cd) A_{JM}^\dagger(ab) A_{JM}(cd)$$

## Elementos de matriz

$$E_J(ab, cd) = \langle \Phi_{ab}^{JM} | V | \Phi_{cd}^{JM} \rangle = -G_J M_J(ab) M_J(cd)$$

## Ground state $J = 0$

$$H = \sum_{am_a} \varepsilon_a c_{am_a}^\dagger c_{am_a} + \sum_{b \leq a} \sum_{d \leq c} E_0(ab, cd) A_{00}^\dagger(ab) A_{00}(cd)$$

$$A_{JM}^\dagger(ab) = \frac{1}{\sqrt{1 + \delta_{ab}}} \sum_{m_a m_b} \langle j_a m_a j_b m_b | JM \rangle c_{am_a}^\dagger c_{bm_b}^\dagger \rightarrow A_{00}^\dagger(ab)$$

# Solución Exacta de Many-Body: Hamiltoniano de apareamiento

$$H = \sum_{am_a} \epsilon_a c_{am_a}^\dagger c_{am_a} + \sum_{a,c} E_0(aa, cc) A_{00}^\dagger(aa) A_{00}(cc)$$

$$H = \sum_{am_a} \epsilon_a c_{am_a}^\dagger c_{am_a} - G_0 \left[ \sum_a M_0(aa) A_{00}^\dagger(aa) \right] \left[ \sum_c M_0(cc) A_{00}(cc) \right]$$

$$H = \sum_{am_a} \epsilon_a c_{am_a}^\dagger c_{am_a} - GP^\dagger P$$

Time reverse

$$\tilde{c}_{a,m_a}^\dagger = (-)^{j_a - m_a} \tilde{c}_{a,-m_a}^\dagger$$

Operador de pairing

$$P^\dagger = \sum_{am_a} M_0(aa) c_{am_a}^\dagger \tilde{c}_{a,m_a}^\dagger$$

# Forma escalar del Hamiltoniano y tensor

# Sobre tensores

## Definición

$$[J_z, T_{kq}] = qT_{kq}$$

$$[J_{\pm}, T_{kq}] = \sqrt{(k \pm q - 1)(k \mp q)} T_{kq \pm 1}$$

## Tensor

$$A_{JM}^{\dagger}$$

$$A_{JM}^{\dagger}(ab) = \frac{1}{\sqrt{1 + \delta_{ab}}} \sum_{m_a m_b} \langle j_a m_a j_b m_b | JM \rangle c_{a m_a}^{\dagger} c_{b m_b}^{\dagger}$$

$$|\Phi_{ab}^{JM}\rangle = A_{JM}^{\dagger}(ab) |0\rangle$$

## No tensor

$$A_{JM}(cd) = [A_{JM}^{\dagger}(cd)]^{\dagger}$$

## Tensor

$$\tilde{A}_{JM}(ab) = (-)^{J-M} A_{JM}(ab)$$

# Producto escalar

## Acople de tensores

$$A_{JM}^\dagger$$

$$\tilde{A}_{JM}(ab) = (-)^{J-M} A_{JM}(ab)$$

$$\sum_M A_{JM}^\dagger A_{JM} = \sqrt{2J+1} \left[ A_{JM}^\dagger \tilde{A}_{JM} \right]_{00}$$

# Hamiltoniano en forma escalar

## Hamiltoniano coordenadas

$$H = \sum_{i=1}^A h(\mathbf{r}_i) + \sum_{i<j=1}^A V(\mathbf{r}_i, \mathbf{r}_j)$$

## Hamiltoniano acoplado

$$H = \sum_{am_a} \varepsilon_a c_{am_a}^\dagger c_{am_a} + \sum_{JM} \sum_{b \leq a} \sum_{d \leq c} E_J(ab, cd) A_{JM}^\dagger(ab) A_{JM}(cd)$$

## Hamiltoniano manifiestamente escalar

$$H = \sum_{am_a} \varepsilon_a a_{am_a}^\dagger a_{am_a} + \sum_J \sum_{b \leq a} \sum_{d \leq c} \sqrt{2J+1} E_J(ab, cd) \left[ A_J^\dagger(ab) \tilde{A}_J(cd) \right]_{00}$$

**Fin**