Introducción a la Física Nuclear 2024

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Segunda Cuantización

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

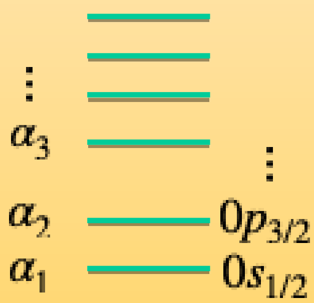
Representación bracket

Representación coordenada

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

Representación abstracta

$$\boxed{h\,|\,\alpha\rangle = \varepsilon_\alpha\,|\,\alpha\rangle}$$



Espectro(degenerado)

Conexión

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

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

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

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

Espacio abstracto

Espacio de Hilbert de una partícula

$$\mathscr{H}$$

Base

$$\{\,|\alpha\rangle\}$$

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

Completitud

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

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

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

(no degenerado)

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

Representación coordenada

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

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

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

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

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

Completitud en el “espacio r”

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

Completitud en el “espacio espín”

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

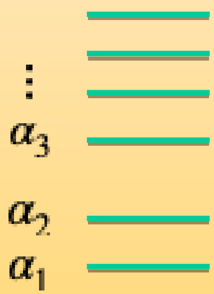
Completitud

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

Idem ortogonalidad…

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

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

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

Espacio de Hilbert de muchas partículas

Espacio abstracto de N-partículas: completitud

<u>Espacio de Hilbert</u>

$$\mathscr{H}_N = \mathscr{H}^{(1)} \otimes \mathscr{H}^{(2)} \otimes \cdots \otimes \mathscr{H}^{(N)}$$

Espacio Partícula 1

Espacio Partícula 2

Espacio Partícula N

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

Espacio de la Partícula I-ésima

Completitud

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

<u>Base</u>

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

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

Completitud

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

Espacio abstracto de N-partículas: ortogonalidad

Espacio de Hilbert

$$\mathscr{H}_N = \mathscr{H}^{(1)} \otimes \mathscr{H}^{(2)} \otimes \cdots \otimes \mathscr{H}^{(N)}$$

Espacio Partícula 1

Espacio Partícula 2

Espacio Partícula N

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

Espacio de la Partícula I-sima

Ortogonalidad

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

Base

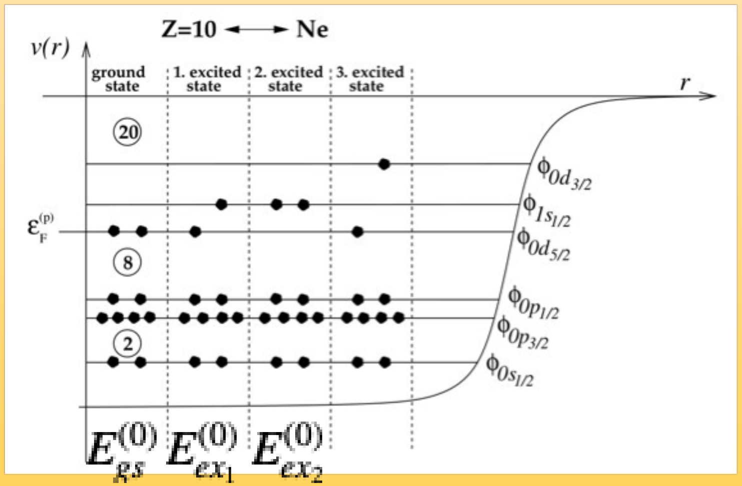
$$\{ |\alpha_1 \alpha_2 \cdots \alpha_N\rangle \}$$

Ortogonaliad

$$\langle \alpha_1 \alpha_2 \cdots \alpha_N | \alpha_{1'} \alpha_{2'} \cdots \alpha_{N'} \rangle = \delta_{\alpha_1, \alpha_{1'}} \cdots \delta_{\alpha_N, \alpha_{N'}}$$

Función de onda de muchas partículas

$$\mathscr{H}_N = \mathscr{H}^{(1)} \otimes \mathscr{H}^{(2)} \otimes \cdots \otimes \mathscr{H}^{(N)}$$



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

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

Vive en $\mathscr{H}_N$

Función de onda de muchos cuerpos no antimetrizada

Está normalizada?

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

Estado de muchas partículas sin interacción

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

Antisimetrización y normalización

Espacio abstracto de N-partículas antisimetrizadas

Espacio de Hilbert

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

$$|\alpha_1 \alpha_2 \cdots \alpha_N\rangle_{\mathscr{A}} = \text{combinacion lineal}: |\alpha_1\rangle\,|\alpha_2\rangle \cdots |\alpha_{\text{N}}\rangle$$

Determinante de Slatter

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

Función de onda de muchos cuerpos antisimétrica

Base

$$\{\, |\alpha_1 \alpha_2 \cdots \alpha_N\rangle_{\mathscr{A}} \}$$

Espacio abstracto de N-partículas antisimetrizadas

Espacio de Hilbert

$$\mathscr{H}_N^{\mathscr{A}} = \text{sub}:\mathscr{H}^{(1)} \otimes \mathscr{H}^{(2)} \otimes \cdots \otimes \mathscr{H}^{(\mathrm{N})}$$

Base

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

Completitud

$$I = \sum_{\alpha_i} |\alpha_1\alpha_2\cdots\alpha_N\rangle_{\mathscr{A}}\langle\alpha_1\alpha_2\cdots\alpha_N|$$

Ortogonalidad

$$_{\mathscr{A}}\langle\alpha_1\alpha_2\cdots\alpha_N|\alpha_{1'}\alpha_{2'}\cdots\alpha_{N'}\rangle_{\mathscr{A}} = \delta_{\alpha_1,\alpha_{1'}}\cdots\delta_{\alpha_N,\alpha_{N'}}$$

Determinante de Slater

Representación coordenada

Función de onda

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

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

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

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

Determinante de Slatter

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

Hacer como ejemplo el caso de dos partículas

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

Antisimetrización y normalización con acople:
Dos Partículas

Función de onda de dos partículas acopladas

Función de onda no antisimetrizada

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

Función de onda de partícula simple

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

$$a = \{nlj\}$$

Propiedad

$$\Psi^{JM}_{j_1 j_2}(\boldsymbol{r}_2, \boldsymbol{r}_1) = (-)^{j_1 + j_2 - J} \Psi^{JM}_{j_2 j_1}(\boldsymbol{r}_1, \boldsymbol{r}_2)$$

Ortogonalidad

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

Función de onda de dos partículas acopladas y antisimetrizadas

Función de onda antisimetrizada

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

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

Considerar comparar con segunda cuantización

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

Ortogonalidad

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

$$\int d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 N_{j_1 j_2} N_{j_1' j_2'}\left[\Psi^{JM}_{j_1 j_2}(\boldsymbol{r}_1, \boldsymbol{r}_2) - (-)^{j_1+j_2-J}\Psi^{JM}_{j_2 j_1}(\boldsymbol{r}_1, \boldsymbol{r}_2)\right]^\dagger$$

$$\left[\Psi^{JM}_{j_1' j_2'}(\boldsymbol{r}_1, \boldsymbol{r}_2) - (-)^{j_1'+j_2'-J}\Psi^{JM}_{j_2' j_1'}(\boldsymbol{r}_1, \boldsymbol{r}_2)\right] =_3 \delta_{j_1\, j_1'}\delta_{j_2\, j_2'}$$

$$N_{j_1 j_2} N_{j_1' j_2'}\left[2\delta_{j_1 j_1'}\delta_{j_2 j_2'} - 2(-)^{j_2+j_1-J}\delta_{j_1 j_2'}\delta_{j_2 j_1'}\right] =_3 \delta_{j_1\, j_1'}\delta_{j_2\, j_2'}$$

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

Propiedad

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

Luego repetiremos las cuentas en 2da cuantización

Función de onda de dos partículas acopladas y antisimetrizadas: propiedades

Función de onda antisimetrizada

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

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

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

Propiedades

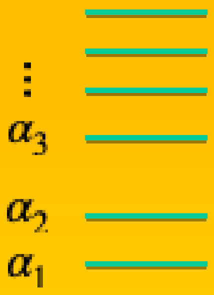
$$\tilde{\Psi}^{JM}_{ab}(\boldsymbol{x}_2, \boldsymbol{x}_1) = (-)^{j_a + j_b - J}\, \tilde{\Psi}^{JM}_{ba}(\boldsymbol{x}_1, \boldsymbol{x}_2)$$

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

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

Operadores de creación - Preliminar

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



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

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

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

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

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

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

Función de onda de dos partículas acopladas y antisimetrizadas
EN SEGUNDA CUANTIZACION

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

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

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

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

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

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

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

Hacer desarrollo...

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

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

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

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

Luego, repetimos con Wick

Sistemas con número de partículas NO CONSTANTE

Definiciones

Operadores de creación/destrucción

Vacío

$|0\rangle$

Operador de creación

$c_\alpha^\dagger$

Operador de destrucción

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

$c_\alpha |0\rangle = 0$

Estados de uno, dos, … partículas

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

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

$$\vdots$$

$$|\alpha_1\alpha_2\cdots\alpha_N\rangle = c_{\alpha_1}^\dagger c_{\alpha_2}^\dagger \cdots c_{\alpha_N}^\dagger |0\rangle \rightarrow$$

Espacio de N partículas

$$\mathscr{H}_N = \mathscr{H}^{(1)} \otimes \mathscr{H}^{(2)} \otimes \cdots \otimes \mathscr{H}^{(N)}$$

Espacio de Fock

Espacio de Fock

Motivación…

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

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

$$\mathscr{F} = \mathscr{H}_1 \oplus \mathscr{H}_2 \oplus \cdots \mathscr{H}_N \oplus \cdots$$

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

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

Representación número de partícula

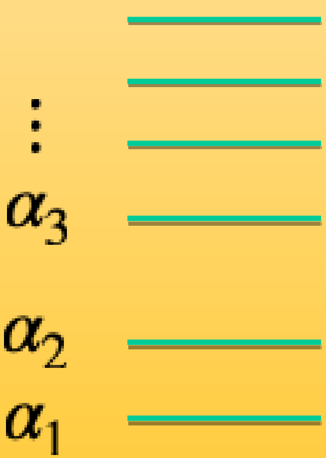
Estado número de partículas

Vacío de Fock

$$\mathscr{F} = \mathscr{H}_1 \oplus \mathscr{H}_2 \oplus \cdots \mathscr{H}_N \oplus \cdots$$

$$|0\rangle = |000\cdots\rangle$$

En cada estado i hay 0 partículas



Espectro de una partícula

(no degenerado)

Estado número de ocupación

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

La particula está en un estado alfa_i

En cada estado i hay n_i partículas

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

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

Ejemplificar

partícula 1 partícula 2 partícula N

Estado número de partículas

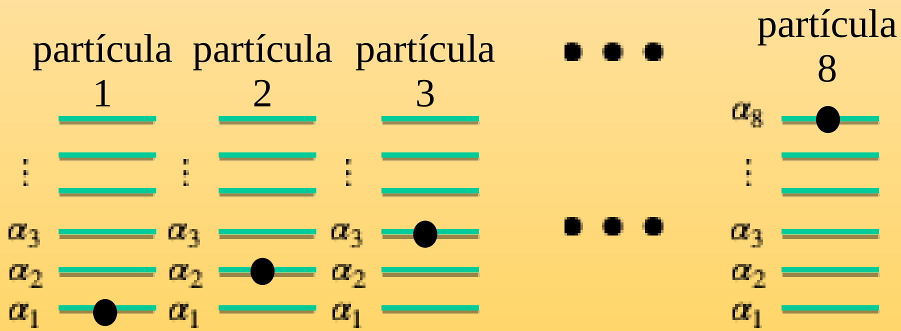
Vacío de Fock

$$\mathscr{F} = \mathscr{H}_1 \oplus \mathscr{H}_2 \oplus \cdots \mathscr{H}_N \oplus \cdots$$

$$|0\rangle = |000\cdots\rangle$$

Estado número de ocupación

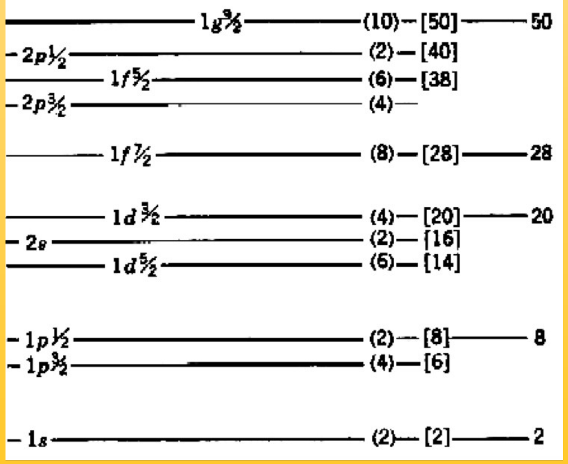
$$|\alpha_1\alpha_2\cdots\alpha_N\rangle = |n_1n_2n_3\cdots\rangle$$



$\alpha_1 = \{1s_{1/2}, m = 1/2\}$ $\alpha_3 = \{1p_{3/2}, m = 3/2\}$ $\alpha_8 = \{1p_{1/2}, m = -1/2\}$

$\alpha_2 = \{1s_{1/2}, m = -1/2\}$

Espectro de una partícula



$$|g.s.\rangle = |\alpha_1\alpha_2\cdots\alpha_N\rangle = |1\,1\cdots1\,0\,0\cdots\rangle \qquad \sum_{i=1}^{\infty} n_i = 8$$

$$|Ex_1\rangle = |\alpha_1\alpha_2\cdots\alpha_N\rangle = |0\,1\cdots1\,1\,0\,\cdots\rangle$$

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

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

$$i\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_A, t) = H\Psi(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_A, t)$$

$$\Psi(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_A, t) = \sum_{\alpha'_1, \cdots, \alpha'_A} C(\alpha'_1, \cdots, \alpha'_A, t)\phi_{\alpha'_1}(\boldsymbol{r}_1)\cdots\phi_{\alpha'_A}(\boldsymbol{r}_A)$$

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

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

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

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

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

Ecuación de Schroedinger

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

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

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

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

$$| \Psi \rangle = \sum_{\alpha_1', \cdots, \alpha_A'} C(\alpha_1', \cdots, \alpha_A', t) | \alpha_1' \cdots \alpha_A' \rangle$$

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

Ecuación de Schroedinger

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

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

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

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

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

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

Ecuación de Schroedinger

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

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

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

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

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

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

Redefinición de coeficientes

$$\tilde{C}(n_1, n_2, \cdots, n_\infty, t) \equiv C(\alpha_1, \alpha_2, \cdots, \alpha_1, \alpha_A, t)$$

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

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

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

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

$$\sum_{i=1}^{\infty} n_{\mathbf{i}} = A$$

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

Redefinición de coeficientes

$$\tilde{C}(n_1, n_2, \cdots, n_\infty, t) \equiv C(\alpha_1, \alpha_2, \cdots, \alpha_1, \alpha_A, t)$$

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

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

$$\sum_{i=1}^{\infty} n_1 = A$$

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

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

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

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

Redefinición de coeficientes

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

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

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

$$\sum_{i=1}^{\infty} n_1 = A$$

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

Lo vamos a usar más adelante…

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

$$\sum_{i=1}^{\infty} n_1 = A$$

Volviendo a la Ecuación de Schroedinger

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

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

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

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

$$= \sum_{i=1}^{A} \sum_{\beta'} \tilde{C}(n_1, \cdots, n_{\alpha_i} - 1, \cdots, n_{\beta'} + 1, \cdots, n_\infty, t) \langle \alpha_i | t(\boldsymbol{r}) | \beta' \rangle + \frac{1}{2} \cdots$$

Esto expone el hecho que el estado α_i aparece una vez menos, mientras el estado β' una vez más

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

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

Volviendo a la Ecuación de Schroedinger

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

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

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

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

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

Volviendo a la Ecuación de Schroedinger

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

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

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

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

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

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

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

Volviendo a la Ecuación de Schroedinger

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

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

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

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

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

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

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

Operador de una partícula

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

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

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

Aplicarlo al Hamiltoniano de campo medio

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

Ejemplo:

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

Operadores en segunda cuantización

Ejemplo operador de una partícula

Proyección Momento angular

J_z

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

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

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

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

Operadores en segunda cuantización

Operador de dos partículas

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

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

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

Operadores en segunda cuantización

Interacción de dos partículas

$$V = \sum_{i<j} v(\boldsymbol{r}_i, \boldsymbol{r}_j) = \frac{1}{2} \sum_{i \neq j} v(\boldsymbol{r}_i, \boldsymbol{r}_j) \qquad V = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma$$

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

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

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

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

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

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

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

Orden normal:

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

Ejemplo:

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

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

Contracción

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

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

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

Ejemplos:

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

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

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

Teorema de Wick

Contracción: $\wick{\c A \c B} = AB - \mathcal{N}[AB] = \langle \Psi_0 | AB | \Psi_0 \rangle$

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

Teorema de Wick:

$$
\begin{aligned}
ABCDEF... \quad = \quad & \mathcal{N}[ABCDEF...] \\
& + \mathcal{N}[\wick{\c A \c B CDEF...}] + \mathcal{N}[\wick{\c A B \c C DEF...}] + \ldots \\
& + \mathcal{N}[\wick{\c1 A \c1 B \c2 C \c2 D EF...}] + \mathcal{N}[\wick{\c1 A \c1 B \c2 C D \c2 E F...}] + \ldots \\
& \vdots \\
& + \text{todos los pares contraídos}
\end{aligned}
$$

Aplicación: valor medio vacío

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

Aplicación de Wick en las ecuaciones de Hartree-Fock

Campo Medio: Hartree-Fock

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

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

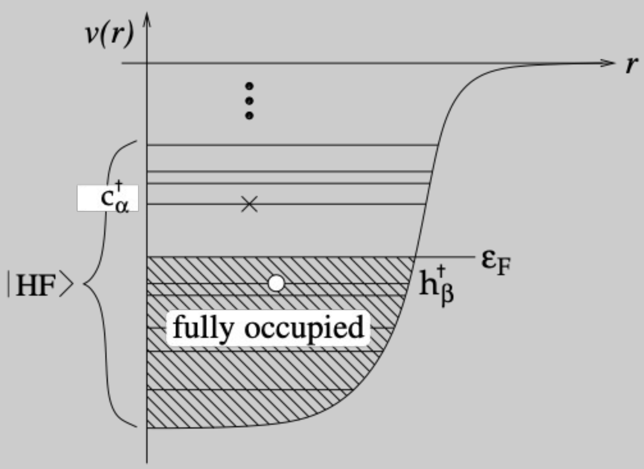
Interacción: $V = \frac{1}{4}\sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta}\, c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma$ $\qquad \bar{v}_{\alpha\beta\gamma\delta} = v_{\alpha\beta\gamma\delta} - v_{\alpha\beta\delta\gamma}$

Única contracción no nula

$$\langle HF|c^\dagger_a c_b|HF\rangle = \delta_{ab}$$

$$\varepsilon_h < \varepsilon_F$$

$$\begin{aligned}
4V = & \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta}\mathcal{N}[c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma] \\
& - \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta}\langle HF|c^\dagger_\alpha c_\delta|HF\rangle\mathcal{N}[c^\dagger_\beta c_\gamma] \\
& + \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta}\langle HF|c^\dagger_\alpha c_\gamma|HF\rangle\mathcal{N}[c^\dagger_\beta c_\delta] \\
& + \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta}\langle HF|c^\dagger_\beta c_\delta|HF\rangle\mathcal{N}[c^\dagger_\alpha c_\gamma] \\
& - \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta}\langle HF|c^\dagger_\beta c_\gamma|HF\rangle\mathcal{N}[c^\dagger_\alpha c_\delta] \\
& - \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta}\langle HF|c^\dagger_\alpha c_\delta|HF\rangle\langle HF|c^\dagger_\beta c_\gamma]|HF\rangle \\
& + \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta}\langle HF|c^\dagger_\alpha c_\gamma|HF\rangle\langle HF|c^\dagger_\beta c_\delta]|HF\rangle
\end{aligned}$$



Crédito: Suhonen

Campo Medio: Hartree-Fock

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

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

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

Interacción: $V = \frac{1}{4}\sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta}\, c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma$ $\quad \bar{v}_{\alpha\beta\gamma\delta} = v_{\alpha\beta\gamma\delta} - v_{\alpha\beta\delta\gamma}$

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

$$\langle HF|c^\dagger_a c_b|HF\rangle = \delta_{ab}$$

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

Campo Medio: Hartree-Fock

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

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

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

Interacción: $V = \frac{1}{4}\sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta}\, c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma$ $\quad \bar{v}_{\alpha\beta\gamma\delta} = v_{\alpha\beta\gamma\delta} - v_{\alpha\beta\delta\gamma}$

Propiedades

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

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

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

Campo Medio: Hartree-Fock

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

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

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

Interacción: $V = \frac{1}{4}\sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta}\, c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma$ $\quad \bar{v}_{\alpha\beta\gamma\delta} = v_{\alpha\beta\gamma\delta} - v_{\alpha\beta\delta\gamma}$

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

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

Operador de una partícula →

$$+\sum_{\alpha\beta}\left(\sum_{\substack{\gamma \\ \varepsilon_\gamma \leq \varepsilon_F}} \bar{v}_{\gamma\alpha\gamma\beta}\right) c^\dagger_\alpha c_\beta$$

Escalar →

$$-\frac{1}{2}\sum_{\substack{\alpha\beta \\ \varepsilon_\alpha \leq \varepsilon_F \\ \varepsilon_\beta \leq \varepsilon_F}} \bar{v}_{\alpha\beta\alpha\beta}$$

Campo Medio: Hartree-Fock

Hamiltoniano de muchos cuerpos:

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

$$
\begin{aligned}
T &= \sum_{i=1}^{A} t(\boldsymbol{r}_i) \\
V &= \sum_{i<j} v(\boldsymbol{r}_i, \boldsymbol{r}_j) = \frac{1}{2}\sum_{i\neq j} v(\boldsymbol{r}_i, \boldsymbol{r}_j)
\end{aligned}
$$

Ecuación de autovalores de HF:

$$
t_{\alpha\beta} + \sum_{\substack{\gamma \\ \varepsilon_\gamma \leq \varepsilon_F}} \bar{v}_{\gamma\alpha\gamma\beta} = \varepsilon_{\alpha\beta}\, \delta_{\alpha\beta}
$$

Hamiltoniano campo medio:

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

$$
H_{HF} = \sum_{\alpha} \varepsilon_\alpha c^\dagger_\alpha c_\alpha \qquad V_{Res} = \frac{1}{4}\sum_{\alpha\beta\gamma\delta} \bar{V}_{\alpha\beta\gamma\delta}\mathcal{N}[c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma] - \frac{1}{2}\sum_{\substack{\alpha\beta \\ \varepsilon_\alpha \leq \varepsilon_F \\ \varepsilon_\beta \leq \varepsilon_F}} \bar{V}_{\alpha\beta\alpha\beta}
$$

Ecuación de Hartree-Fock en coordenadas

Ecuación de autovalores de HF:

$$t_{\alpha\beta} + \sum_{\substack{\gamma \\ \varepsilon_\gamma \leq \varepsilon_F}} \bar{v}_{\gamma\alpha\gamma\beta} = \varepsilon_{\alpha\beta}\,\delta_{\alpha\beta}$$

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

Representación coordenada:

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

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

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

Hamiltoniano en segunda cuantización acoplado

(recordemos)Función de onda de dos partículas acopladas

Función de onda antisimetrizada

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

Función de onda de partícula simple

$$\psi_{am_a}(\boldsymbol{r})=\frac{u_a(r)}{r}\mathscr{Y}_{ljm}$$

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

Representación coordenada

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

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

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

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

Operador destrucción de dos partículas acopladas

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

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

Hamiltoniano en 2da cuantización acoplado(informativo)

Hamiltoniano coordenadas

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

Hamiltoniano 2da cuantización

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

Hamiltoniano acoplado

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

Hamiltoniano en 2da cuantización acoplado

Hamiltoniano coordenadas

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

Hamiltoniano acoplado

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

Elementos de matriz

$$E_J(ab, cd) = < \Phi^{JM}_{ab} | V | \Phi^{JM}_{cd} >$$

Propiedades

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

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

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

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:

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

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

Normalización:

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

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

Ecuación de autovalores:

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

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

Interacción delta de Dirac

Función de onda correlacionada:

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

Ecuación de autovalores:

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

Interacción delta:

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

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

Expansión en ondas parciales:

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

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

Elementos de matriz:

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

Recordar R0 $\qquad V(r) = 1$

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

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

Comparación con experimento

Función de onda correlacionada:

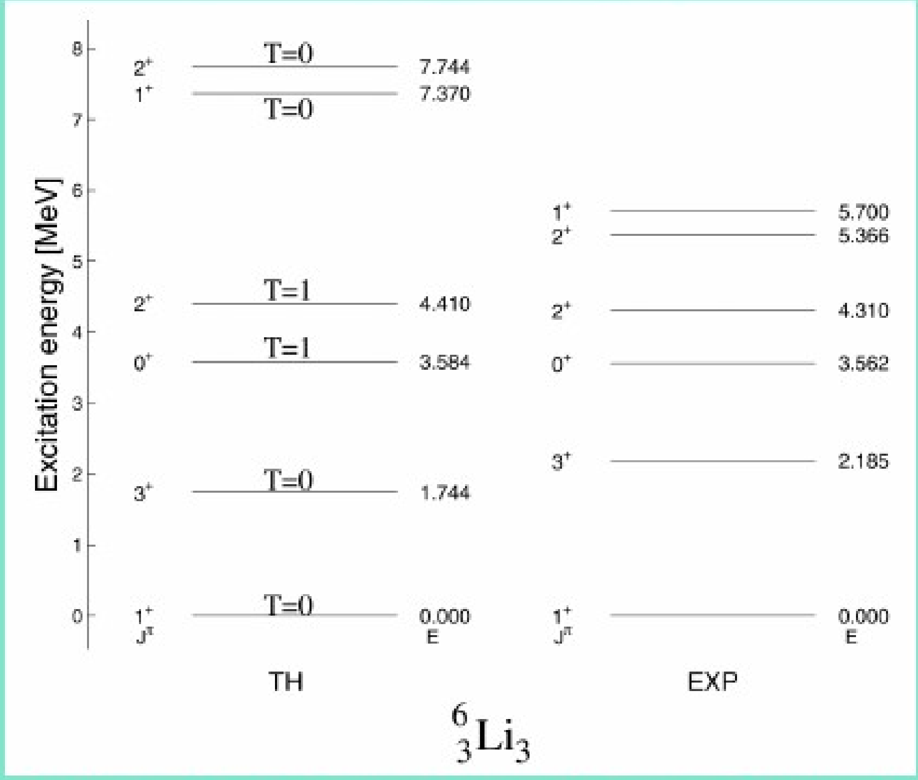
$$\Psi_{EJM}(\boldsymbol{r}_1, \boldsymbol{r}_2) \quad = \quad \sum_{d \leq c} X_{cd,EJ} \Phi_{cd}^{JM}(\boldsymbol{r}_1, \boldsymbol{r}_2)$$

Ecuación de autovalores:

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

Elementos de matriz:

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



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

Ejemplo: Hamiltoniano de apareamiento

Volviendo a la Interacción Separable

Hamiltoniano

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

Elementos de matriz

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

Ground state $J = 0$

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

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

Solución Exacta de Many-Body: Hamiltoniano de apareamiento

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

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

$$H = \sum_{am_a} \varepsilon_a c^\dagger_{am_a} c_{am_a} - G P^\dagger P$$

Time reverse

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

Operador de pairing

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

Forma escalar del Hamiltoniano y tensor

Sobre tensores

Definición

$$[J_z, T_{kq}] = qT_{kq}$$
$$[J_\pm, T_{kq}] = \sqrt{(k \pm q - 1)(k \mp q)}\,T_{kq\pm1}$$

Tensor

$A^\dagger_{JM}$

$$A^\dagger_{JM}(ab) = \frac{1}{\sqrt{1+\delta_{ab}}} \sum_{m_a m_b} \langle j_a m_a j_b m_b | JM \rangle c^\dagger_{am_a} c^\dagger_{bm_b}$$

$$|\Phi^{JM}_{ab}\rangle = A^\dagger_{JM}(ab)|0\rangle$$

No tensor

$$A_{JM}(cd) = \left[A^\dagger_{JM}(cd)\right]^\dagger$$

Tensor

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

Producto escalar

<u>Acople de tensores</u>

$$A^{\dagger}_{JM}$$

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

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

Hamiltoniano en forma escalar

Hamiltoniano coordenadas

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

Hamiltoniano acoplado

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

Hamiltoniano manifiestamente escalar

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

Fin