

La clase pasada vimos:

- Sistemas cuánticos de varias partículas
- Definición del problema de partículas idénticas
- Postulado de simetrización con dos partículas
- Operadores de permutación de  $N$  partículas

En esta clase veremos:

- Kets completamente simétricos y antisimétricos
- Postulado de simetrización
- Construcción de estados
- Simetrización de observables
- Ejemplo: dos electrones

## Definición: Partículas idénticas

Son partículas que tienen las mismas propiedades intrínsecas:

Masa, carga, espín, etc. Ejemplos: electrones, protones, neutrones.

Electrón y positrón difieren (sólo) en la carga eléctrica, no son idénticos.

Descripción matemática del estado físico con un espín **up** y otro **down**

$$\alpha | +, - \rangle + \beta | -, + \rangle$$

$$|\alpha|^2 + |\beta|^2 = 1$$

¿Cuál estado tomamos? —————> Degeneración de intercambio

## Operador Permutación: dos partículas idénticas

$$\left. \begin{aligned} P_{21}|\psi_S\rangle &= |\psi_S\rangle \\ P_{21}|\psi_A\rangle &= -|\psi_A\rangle \end{aligned} \right\} \text{Autovectores simétricos y antisimétricos} \\ \text{con respecto al intercambio de partículas}$$

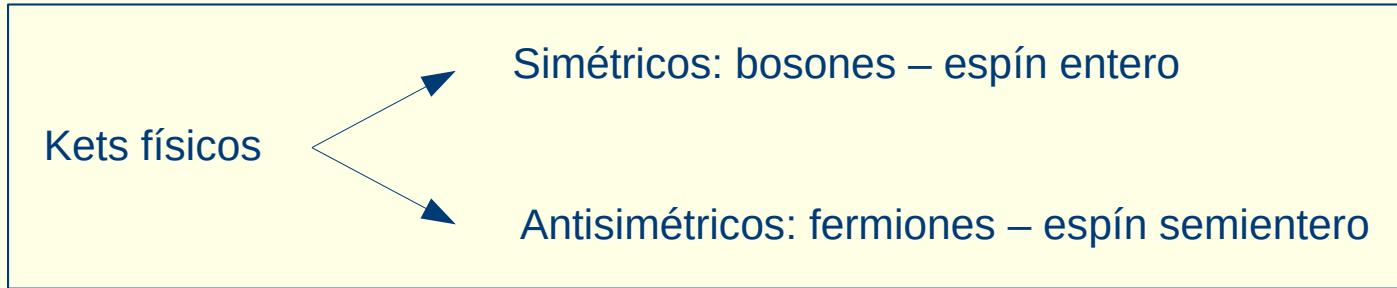
Operador simétrico:  $[\mathcal{O}(1, 2), P_{21}] = 0$

**Simetrizador y antisimetrizador**

$$S \equiv \frac{1}{2}(1 + P_{21})$$

$$A \equiv \frac{1}{2}(1 - P_{21})$$

## Postulado de simetrización



## Más partículas: N=3

$$P_{123}, P_{312}, P_{231}, P_{132}, P_{213}, P_{321}$$

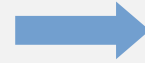
transposiciones  
6 operadores de permutación

$$P_{npq} | 1 : u_i; 2 : u_j; 3 : u_k \rangle = | n : u_i; p : u_j; q : u_k \rangle$$

## **Kets completamente simétricos y antisimétricos**

Consideremos **sistemas con N general**

Los operadores de permutación  
no conmutan todos entre sí



No hay una base de  
autoestados comunes

Sea  $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_N)$  una permutación arbitraria de  $(1, 2, \dots, N)$

Sea  $P_\alpha$  el operador de permutación asociado:

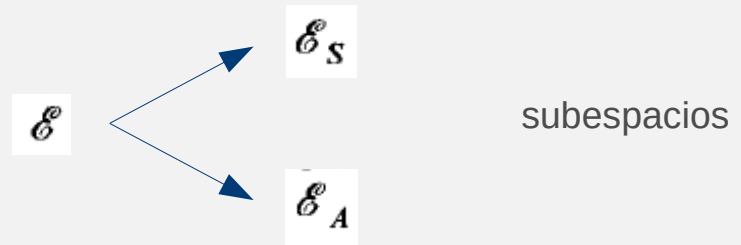
$$P_\alpha |1 : u_{i_1}, 2 : u_{i_2}, \dots, N : u_{i_N}\rangle = |\alpha_1 : u_{i_1}, \alpha_2 : u_{i_2}, \dots, \alpha_N : u_{i_N}\rangle$$

# Kets completamente simétricos y antisimétricos

Definimos kets completamente simétricos  $|\psi_S\rangle$  :  $\longrightarrow$   $P_\alpha |\psi_S\rangle = |\psi_S\rangle$

Kets completamente antisimétricos  $|\psi_A\rangle$  :

$\longrightarrow$   $P_\alpha |\psi_A\rangle = \varepsilon_\alpha |\psi_A\rangle$  con  $\left\{ \begin{array}{l} \varepsilon_\alpha = +1 \\ \varepsilon_\alpha = -1 \end{array} \right.$  permutaciones pares  
permutaciones impares



## Simetrizador y antisimetrizador

$$\begin{aligned} S &= \frac{1}{N!} \sum_{\alpha} P_{\alpha} \\ A &= \frac{1}{N!} \sum_{\alpha} \varepsilon_{\alpha} P_{\alpha} \end{aligned} \quad \xrightarrow{\text{proyectores en}} \quad \begin{aligned} \mathcal{E}_S \\ \mathcal{E}_A \end{aligned}$$

## Propiedades

(1) S y A son hermíticos

$$\begin{aligned} S^{\dagger} &= S \\ A^{\dagger} &= A \end{aligned}$$

$P_{\alpha}^{\dagger}$  es otro operador de permutación (más precisamente  $P_{\alpha}^{\dagger} = P_{\alpha}^{-1}$ )

Al sumar sobre todos ellos se obtiene la misma suma con el orden de los sumandos cambiado.



$$S = \frac{1}{N!} \sum_{\alpha} P_{\alpha}$$

$$A = \frac{1}{N!} \sum_{\alpha} \varepsilon_{\alpha} P_{\alpha}$$

## Propiedades

(2) Sea  $P_{\alpha_0}$  un operador de permutación. Entonces:

$$P_{\alpha_0} S = S P_{\alpha_0} = S$$

$$P_{\alpha_0} A = A P_{\alpha_0} = \varepsilon_{\alpha_0} A$$

Demostración: como

$$P_{\alpha_0} P_{\alpha} = P_{\beta}$$

también es un operador de permutación, con

$$\varepsilon_{\beta} = \varepsilon_{\alpha_0} \varepsilon_{\alpha}$$

Entonces:

$$P_{\alpha_0} S = \frac{1}{N!} \sum_{\alpha} P_{\alpha_0} P_{\alpha} = \frac{1}{N!} \sum_{\beta} P_{\beta} = S$$

$$P_{\alpha_0} A = \frac{1}{N!} \sum_{\alpha} \varepsilon_{\alpha} P_{\alpha_0} P_{\alpha} = \frac{1}{N!} \varepsilon_{\alpha_0} \sum_{\beta} \varepsilon_{\beta} P_{\beta} = \varepsilon_{\alpha_0} A$$

$$S = \frac{1}{N!} \sum_{\alpha} P_{\alpha}$$
$$A = \frac{1}{N!} \sum_{\alpha} \varepsilon_{\alpha} P_{\alpha}$$

## Propiedades

(3) S y A son idempotentes

$$S^2 = S$$
$$A^2 = A$$

$$S^2 = \frac{1}{N!} \sum_{\alpha} P_{\alpha} S = \frac{1}{N!} \sum_{\alpha} S = S$$
$$A^2 = \frac{1}{N!} \sum_{\alpha} \varepsilon_{\alpha} P_{\alpha} A = \frac{1}{N!} \sum_{\alpha} \varepsilon_{\alpha}^2 A = A$$

(4) Son algo así como disjuntos u ortogonales

$$AS = SA = 0$$

$$AS = \frac{1}{N!} \sum_{\alpha} \varepsilon_{\alpha} P_{\alpha} S = \frac{1}{N!} S \sum_{\alpha} \varepsilon_{\alpha} = 0$$

$$S = \frac{1}{N!} \sum_{\alpha} P_{\alpha}$$

$$A = \frac{1}{N!} \sum_{\alpha} \varepsilon_{\alpha} P_{\alpha}$$

## Propiedades

(5) S y A son proyectores, proyectan sobre  $\mathcal{E}_S$  and  $\mathcal{E}_A$

$$P_{x_0} S |\psi\rangle = S |\psi\rangle$$

$$P_{x_0} A |\psi\rangle = \varepsilon_{x_0} A |\psi\rangle$$

(6) Para  $N > 2$ , S y A no son proyectores sobre subespacios suplementarios

En otras palabras:  $\mathcal{E} \neq \mathcal{E}_S \oplus \mathcal{E}_A$

Por ejemplo, para  $N = 3$  vemos que:

$$S + A = \frac{1}{3} (P_{123} + P_{231} + P_{312}) \neq 1$$

# Postulado de simetrización

## Postulado de simetrización

When a system includes several identical particles, only certain kets of its state space can describe its physical states. Physical kets are, depending on the nature of the identical particles, either completely symmetric or completely antisymmetric with respect to permutation of these particles. Those particles for which the physical kets are symmetric are called *bosons*, and those for which they are antisymmetric, *fermions*.

From the point of view of this postulate, particles existing in nature are divided into two categories. All currently known particles obey the following *empirical rule*<sup>★</sup>: particles of half-integral spin (electrons, positrons, protons, neutrons, muons, etc.) are fermions, and particles of integral spin (photons, mesons, etc.) are bosons.

<sup>★</sup> The “spin-statistics theorem”, proven in quantum field theory, makes it possible to consider this rule to be a consequence of very general hypotheses. However, these hypotheses may not all be correct, and discovery of a boson of half-integral spin or a fermion of integral spin remains possible. It is not inconceivable that, for certain particles, the physical kets might have more complex symmetry properties than those envisaged here.

Pablo:

Please be more specific about the hypotheses of the theorem, that is, which are the assumptions on which it is based

ChatGPT

The spin-statistics theorem is a deep result in quantum field theory, and it can be derived from certain assumptions about the nature of quantum fields and their symmetries. Here are the key assumptions or hypotheses on which the theorem is based:

Relativistic Invariance:

The theory in which the spin-statistics theorem is applied is assumed to be relativistically invariant, meaning that the laws of physics are the same for all observers moving at constant velocities. This is a fundamental principle in modern particle physics.

Local Commutativity or Anticommutativity:

The essential assumption is that the quantum fields representing elementary particles either commute or anticommute at spacelike separations. This property is known as local commutativity or anticommutativity. Mathematically, for spacelike separations  $x-y$ , the fields either satisfy the commutation relation  $\Phi(x)\Phi(y)=\pm\Phi(y)\Phi(x)$ , where the sign depends on the spin-statistics.

Microcausality:

Microcausality is a principle that states that measurements made at spacelike-separated events should be independent of each other. This implies that the order in which measurements are made at different spacelike-separated events should not affect the outcomes. The assumption of microcausality is closely related to the local commutativity or anticommutativity of fields.

Existence of a Vacuum State:

The theory is assumed to have a vacuum state, which is the state of lowest energy. The vacuum state is invariant under Lorentz transformations and is used as a reference state for particle states.

Poincaré Invariance:

The theory is assumed to be Poincaré invariant, meaning it is invariant under the full Poincaré group, which includes translations, rotations, and Lorentz boosts.

Given these assumptions, the spin-statistics theorem can be derived, establishing the connection between the spin of particles and the statistics they obey. The mathematical details of the proof involve sophisticated techniques from quantum field theory, and the theorem is a crucial element in understanding the consistency of quantum field theories describing elementary particles.

## **Postulado de simetrización**

Simetría de partículas elementales y compuestas

El postulado de simetrización elimina la degeneración de intercambio



# Construcción de estados

## Construcción de estados de partículas idénticas

$$H_0 = \sum_{i=1}^N \hat{h}_i = \sum_{i=1}^N \left( \frac{-\hbar^2 \nabla_i^2}{2m} + u(x_i) \right) \quad x = (\mathbf{r}, s)$$

Primero resolvemos el problema de una partícula:

$$\hat{h}\phi_\nu(x) = \varepsilon_\nu \phi_\nu(x) \quad \Longrightarrow \quad \{\phi_\nu\} \text{ base de "orbitales" } \phi_\nu$$

Ejemplo:  $u(x) = -\frac{Ze^2}{r} \quad \Longrightarrow \quad \nu = (n, \ell, m, m_s)$

**Receta:**

(1) Formar un estado producto:  $\phi_{\nu_1}(x_1) \dots \phi_{\nu_N}(x_N)$

(2) Aplicar S o A

(3) Normalizar

## Bosones

normalización

$$\phi^{(S)} = C \sum_{\alpha} P_{\alpha}[\phi_{\nu_1}(x_1) \dots \phi_{\nu_N}(x_N)]$$

### Normalización C

Si todos los  $\nu_i$  son iguales:  $\sum_{\alpha} P_{\alpha}[\phi_{\nu}(x_1) \dots \phi_{\nu}(x_N)] = N! \phi_{\nu}(x_1) \dots \phi_{\nu}(x_N)$

$\implies$  se divide por  $N! \implies C = \frac{1}{N!}$

Si todos los  $\nu_i$  son distintos, hay  $N!$  sumandos y se normaliza con  $\frac{1}{\sqrt{N!}}$

En general:  $\frac{1}{\sqrt{N!} \sqrt{\prod_k n_k!}}$

$k$ : índice de orbitales distintos

$n_k$ : número de partículas en  $k$

## Fermiones

$$\phi^{(A)} = \frac{1}{\sqrt{N!}} \sum_{\alpha} \text{sgn}(P_{\alpha}) P_{\alpha} [\phi_{\nu_1}(x_1) \dots \phi_{\nu_N}(x_N)]$$

$$\phi^{(A)} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{\nu_1}(x_1) & \dots & \phi_{\nu_1}(x_N) \\ \vdots & & \vdots \\ \phi_{\nu_N}(x_1) & \dots & \phi_{\nu_N}(x_N) \end{vmatrix}$$

Determinante de Slater

Notar que si:  $\nu_i = \nu_j \implies \phi^{(A)} = 0$

Principio de exclusión de Pauli

Los estados simetrizados son autoestados de  $H_0$

$$\begin{aligned}
 H_0 \phi^{(S/A)}(x_1, \dots, x_N) &= \sum_{i=1}^N \left[ \frac{-\hbar^2 \nabla_i^2}{2m} + u(x_i) \right] \phi^{(S/A)}(x_1, \dots, x_N) \\
 &= \underbrace{\left( \sum_{i=1}^N \varepsilon_{\nu_i} \right)}_{\text{Autovalor } E \text{ total}} \phi^{(S/A)}(x_1, \dots, x_N)
 \end{aligned}$$

Ejercicio: demostrarlo explícitamente para  $N = 2$  ( $\nu_1 \neq \nu_2$ ) donde  $H_0 = \hat{h}_1 + \hat{h}_2$

# Simetrización de observables

Los observables asociados a cantidades físicas tienen que involucrar a las  $N$  partículas simétricamente

$$\mathbf{R}_G = \frac{1}{3} (\mathbf{R}_1 + \mathbf{R}_2 + \mathbf{R}_3)$$

$$\mathbf{P} = \mathbf{P}_1 + \mathbf{P}_2 + \mathbf{P}_3$$

$$\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2 + \mathbf{L}_3$$

$$W = \frac{q^2}{4\pi\epsilon_0} \left( \frac{1}{|\mathbf{R}_1 - \mathbf{R}_2|} + \frac{1}{|\mathbf{R}_2 - \mathbf{R}_3|} + \frac{1}{|\mathbf{R}_3 - \mathbf{R}_1|} \right)$$

$$\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3$$

$$[G, P_\alpha] = 0 \quad \text{for all } P_\alpha$$



## **Ejemplo: dos electrones**

Habíamos hecho la suma de dos espines  $\frac{1}{2}$  :

$$|0, 0\rangle = \frac{1}{\sqrt{2}} [ |+, -\rangle - |-, +\rangle ]$$

singlete

$$\begin{cases} |1, 1\rangle & = |+, +\rangle \\ |1, 0\rangle & = \frac{1}{\sqrt{2}} [ |+, -\rangle + |-, +\rangle ] \\ |1, -1\rangle & = |-, -\rangle \end{cases}$$

triplete

$|\psi\rangle = |\varphi\rangle \otimes |\chi\rangle$  Debe ser antisimétrico frente al intercambio de partículas

$$|\psi\rangle = (|1 : u_i, 2 : u_j\rangle \pm |1 : u_j, 2 : u_i\rangle) \otimes |S, M\rangle$$

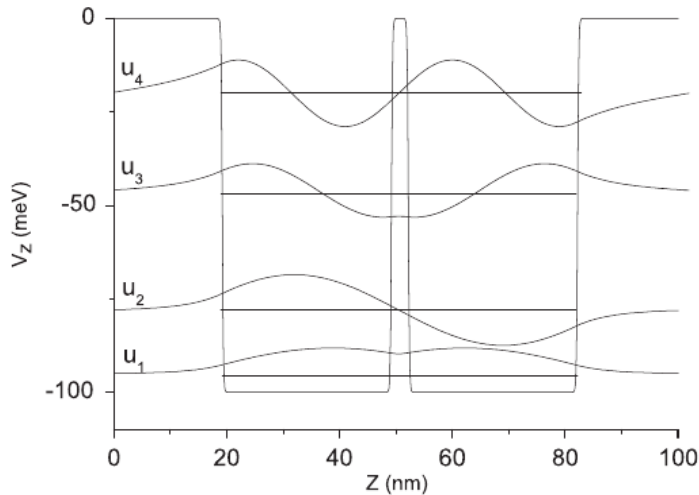


## Spin-orbit effects on two-electron states in nanowhisker double quantum dots

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**Fig. 1.** The  $\text{Al}_{0.1}\text{In}_{0.9}\text{Sb}$ - $\text{InSb}$  double-well confining potential in the longitudinal direction of the quasi-one-dimensional nanowhisker quantum dots. The single-particle eigenfunctions and energies are also shown.

As a basis set for the two-electron Hilbert space we take all the  $u_n$  ( $n = 1, 4$ ) which gives 28 two-particle basis states:

$$\varphi_i = u_i(z_1)u_i(z_2)|0, 0\rangle,$$

$$\varphi_{j+3} = (1/\sqrt{2})[u_1(z_1)u_j(z_2) + u_j(z_1)u_1(z_2)]|0, 0\rangle,$$

$$\varphi_{k+5} = (1/\sqrt{2})[u_2(z_1)u_k(z_2) + u_k(z_1)u_2(z_2)]|0, 0\rangle,$$

$$\varphi_{10} = (1/\sqrt{2})[u_3(z_1)u_4(z_2) + u_4(z_1)u_3(z_2)]|0, 0\rangle,$$

$$\varphi_{l+9} = (1/\sqrt{2})[u_1(z_1)u_l(z_2) - u_l(z_1)u_1(z_2)]|1, 1\rangle,$$

$$\varphi_{l+12} = (1/\sqrt{2})[u_1(z_1)u_l(z_2) - u_l(z_1)u_1(z_2)]|1, -1\rangle,$$

$$\varphi_{l+15} = (1/\sqrt{2})[u_1(z_1)u_l(z_2) - u_l(z_1)u_1(z_2)]|1, 0\rangle,$$

$$\varphi_{m+17} = (1/\sqrt{2})[u_2(z_1)u_m(z_2) - u_m(z_1)u_2(z_2)]|1, 1\rangle,$$

$$\varphi_{m+19} = (1/\sqrt{2})[u_2(z_1)u_m(z_2) - u_m(z_1)u_2(z_2)]|1, -1\rangle,$$

$$\varphi_{m+21} = (1/\sqrt{2})[u_2(z_1)u_m(z_2) - u_m(z_1)u_2(z_2)]|1, 0\rangle,$$

$$\varphi_{26} = (1/\sqrt{2})[u_3(z_1)u_4(z_2) - u_4(z_1)u_3(z_2)]|1, 1\rangle,$$

$$\varphi_{27} = (1/\sqrt{2})[u_3(z_1)u_4(z_2) - u_4(z_1)u_3(z_2)]|1, -1\rangle,$$

$$\varphi_{28} = (1/\sqrt{2})[u_3(z_1)u_4(z_2) - u_4(z_1)u_3(z_2)]|1, 0\rangle,$$

$$H = H_1^0 + H_2^0 + H_{1dR} + V_{int},$$

$$H_{1dR} = \sum_{i=1}^2 \frac{\gamma_R}{\hbar} \left\langle \frac{\partial V_x}{\partial x} \right\rangle p_{z,i} (\sigma_{x_i} - \sigma_{y_i}),$$

$$V_{int}(|z_2 - z_1|) = \int dx_1 dx_2 dy_1 dy_2 \times \frac{e^2 \Phi(x_1)^2 \Phi(x_2)^2 \Phi(y_1)^2 \Phi(y_2)^2}{\epsilon \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}}$$

$$\psi_i = \sum_{j=1}^{28} a_{ij} \varphi_j,$$

## Resumen de la Clase 25

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