Indistinguishable Particles in Quantum Mechanics

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Outline:

1. Spin and Indistiguishable Particles
2. Systems of Indistinguishable Particles
3. Reduced Density Matrices
4. Non-interacting N Body Systems

Spin and Indistiguishable Particles

Spin

- The Spin can be defined as the intrinsic angular momentum of the particle, which is independent of its orbital motion. It is an additional degree of freedom to the spatial ones, associated to the particle.

- The spin of a particle is characterized by its spin number or quantic value, denoted by $S \in \mathbb{N} \setminus \{0\}$ or $S = (2k-1)/2, k \in \mathbb{N}$, which arises from Representation Theory.

  S determines the dimension $2S+1$ of the vector space of the degrees of freedom of the spin $\mathbb{C}^{2S+1}$, i.e. the number of possible configurations of the spin. For example, the electron has $S = 1/2$, meaning that we have two possible configurations of the spin.

Spin and Indistiguishable Particles

Overall, when decribing a quantum particle, we have the following result:

Hilbert Space of a particle with Spin S

The Hilbert space of a particle ($N = 1$) with Spin S is given by the tensor product:

$$\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^{2S+1}$$

a collection of $2S + 1$ wave functions in $\mathcal{H} = L^2(\mathbb{R}^3)$.

Spin and Indistiguishable Particles

Having defined the spin we can now say what we mean by indistinguishable particles:

Indistiguishable Particles

Indistinguishable particles in Quantum Mechanics are those that have the same mass, electric charge and spin.

Systems of Indistinguishable Particles

Systems of N Indistinguishable particles

- If at some point in time we look at a system of identical particles, the wave function representing its state is given by means of products of individual wave packets which partially overlap in general.

  This inevitable overlapping gives rise to indistinguishability.

- Mathematically, the particles in the system are identical if and only if the following requirement holds:

$$[H, P] = 0$$

  where H is the Hamiltonian of the system and $P \in P_N$ any permutation in the permutation group of N elements.

Systems of Indistinguishable Particles

Given $P \in P_N$ and its action as $(P\psi)(x_1, ..., x_N) = \psi(x_{\pi_{(1)}}, ..., x_{\pi_{(N)}})$ with π permutation of N objects, we introduce a symmetry property of $\psi \in L^2(\mathbb{R}^{dN})$ under permutations:

Completely symmetric wave functions

For any $i < j$ in 1,...,N:
$(P_{i,j}\psi)(x_1, ..., x_i, ..., x_j, ..., x_N) = \psi(x_1, ..., x_j, ..., x_i, ..., x_N) = \psi(x_1, ..., x_N)$

Completely antisymmetric wave functions

For any $i < j$ in 1,...,N: $(P_{i,j}\psi)(x_1, ..., x_i, ..., x_j, ..., x_N) = -\psi(x_1, ..., x_N)$

Systems of Indistinguishable Particles

Example for a system of 3 particles, if we call the particles 1,2 and 3:

in case of completely symmetric wave functions, the wave function of the system remains the same if we exchange particle 1 and 2:
$\psi(1, 2, 3) = \psi(1, 3, 2)$.

in case of completely antisymmetric wave functions, the wave function of the system changes in sign if we exchange particle 1 and 2:
$\psi(1, 2, 3) = -\psi(1, 3, 2) = \psi(2, 3, 1)$.

Systems of Indistinguishable Particles

Therefore, the Hilbert space $\mathcal{H}_= L^2(\mathbb{R}^{dN})$ we had initially defined is now comprehensive of two subspaces:

- $\mathcal{H}_s = L^2_s(\mathbb{R}^{dN})$ of the completely symmetric states;
- $\mathcal{H}_a = L^2_a(\mathbb{R}^{dN})$ of the completely antisymmetric states;

Now we can introduce the 6th postulate of Quantum Mechanics:

Sixth Postulate of Quantum Mechanics

A pure state of a system of indistinguishable particles must be completely symmetric or antisymmetric under the permutation of any two of them.

Systems of Indistinguishable Particles

Boson

A Quantum Particle is a boson if its Spin is $S \in \mathbb{N}$.

Fermion

A Quantum Particle is a fermion if its Spin is $S = (2k-1)/2, k \in \mathbb{N}$.

Spin-Statistics Theorem

- The pure state of a system of bosonic indistinguishable particles is completely symmetric.
- The pure state of a system of fermionic indistinguishable particles is completely antisymmetric.

Systems of Indistinguishable Particles

How do we build a fermionic or bosonic state for a system of indistinguishable particles?

We need to make sure that the symmetry contraints on $\psi(x_1, ..., x_N)$ are satisfied.

Symmetry operators

- $S_N : L^2(\mathbb{R}^{3N}) \to L^2_s(\mathbb{R}^{3N})$ as

$$(S_N\psi)(x_1, ..., x_N) = 1/N! \sum_{\pi in P_N} \psi(x_{\pi_{(1)}}, ..., x_{\pi_{(N)}})$$

- $A_N : L^2(\mathbb{R}^{3N}) \to L^2_a(\mathbb{R}^{3N})$ as

$$(A_N\psi)(x_1, ..., x_N) = 1/N! \sum_{\pi in P_N} (-1)^{|\pi|}\psi(x_{\pi_{(1)}}, ..., x_{\pi_{(N)}})$$

with $|\pi|$ is the parity of the permutation.

Systems of Indistinguishable Particles

Example: Let's take two orthonormal states, ψ_1, ψ_2, and see which pure states we can build:

- Bosons : $1/\sqrt{2}(\psi_1(x_1)\psi_2(x_2) + \psi_1(x_2)\psi_2(x_1))$
- Fermions : $1/\sqrt{2}(\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1))$

Problem: what if we have $\psi_1 = \psi_2$? Pauli Exclusion Principle.

Systems of Indistinguishable Particles

Bosons obey the Bose-Einstein statistics while fermions obey the Fermi-dirac statistics.

Bose-Einstein statistics allow multiple identical bosons to occupy the same quantum state simultaneously. This leads to phenomena such as Bose-Einstein condensation, where a large number of bosons occupy the lowest energy state.

Fermi-Dirac statistics, on the other hand, enforce the Pauli exclusion principle, which states that no two identical fermions can occupy the same quantum state.

Reduced Density Matrices

Density Matrix

A quantum system in a given state , can be characterized through its Density Matrix $\Gamma \in \mathcal{L}^1(L^2(\mathbb{R}^{3N}))$, which can be decomposed as

$$\Gamma = \sum_{j=1}^{\infty} \lambda_j \left|\psi_j\right\rangle \left\langle\psi_j\right|$$

with λ_j eigenvalues.

Properties:

$$Tr(\Gamma) = 1 \ , 0 \leq \Gamma \leq 1$$

Reduced Density Matrices

Γ as an integral operator

Γ can be seen as an integral operator with kernel:

$$\Gamma(X, Y) = \sum_{j=1}^{\infty} \lambda_j \psi_j^*(X)\psi_j(Y)$$

where $X = (x_1, ..., x_N)$ and $Y = (y_1, ..., y_N)$.

If Γ is a mixed or pure state of a system of N indistinguishable particles then the ψ_j must satisfy the symmetry properties of the Spin and Statistics Theorem. i.e. the kernel must be separately symmetric/antisymmetric under the permutation of any two particles in X,Y.

Reduced Density Matrices

Consequences: if we study a subsystem of $k \leq N$ particles we can define a simplified operator that contains all the information about the subsystems of k particles.

Reduced Density Matrix

Given $\Gamma \in \mathcal{L}^1(L^2(\mathbb{R}^{3N}))$, the reduced density matrix is $\gamma^{(k)} \in \mathcal{L}^1(L^2(\mathbb{R}^{3k}))$ with $k \leq N$

$\gamma^{(k)}(x_1, ..., x_N, y_1, ..., y_N) =$

$$N!/(N-k)! \int_{\mathbb{R}^{3(N-k)}} dy_{k+1}...dy_N \Gamma(x_1, ..., x_k, y_{k+1}, .., y_N; Y)$$

which will be simply indicated as indicate as $\gamma^{(k)} = Tr_{N-k}\Gamma$

Reduced Density Matrices

Given the Hamiltonian of N interacting particles

$$H = \sum_{j=1}^{N} (-1/2\Delta_j + V(x_j)) + \sum_{1 \le j \le i \le N} I(x_i, x_j)$$

the expectation over a generic state ψ can be expressed in terms of the reduced density matrices $\gamma^{(1)}, \gamma^{(2)}$:

$$(*)\ \epsilon[\psi] = \langle\psi| H |\psi\rangle = Tr_{L^2(\mathbb{R}^3)}(h\gamma^{(1)}) + 1/2\, Tr_{L^2(\mathbb{R}^6)}(I\gamma^{(2)})$$

where $h = -1/2\Delta_j + V(x_j)$.

Find the fundamental state:which Trace operators on $L^2(\mathbb{R}^3)$ and $L^2(\mathbb{R}^6)$ are reduced density matrices associated to a bosonic/fermionic state?

N-representability Problem.

Reduced Density Matrices

Representability problem is solved for k=1:

Properties of Reduced Density Matrices

Let $\gamma^{(1)} = Tr_{N-1}\Gamma$ be the reduced density matrix for $k = 1$ associated to a state Γ, then:

- $\gamma^{(1)}$ is self-adjoint and $\gamma^{(1)} \geq 0$;
- $\gamma^{(1)} \in \mathcal{L}^1(L^2(\mathbb{R}^3))$ and $Tr(\gamma^{(1)}) = N$;
- if Γ is a fermionic state , then $\gamma^{(1)} \leq 1$.

Any trace operator over $L^2(\mathbb{R}^3)$ that satisfies such properties is the reduced density matrix of an N body state Γ.

Non-interacting N Body Systems

$(*)$ is useless in case of interacting N body systems i.e. for $k \geq 2$, but in case of N body systems where we leave interactions among the particles out of the description of the system :

$$H = \sum_{j=1}^{N} (-\Delta_j + V(x_j))$$

we can use $(*)$ to calculate the ground state: only dependence on $\gamma^{(1)}$.

Non-interacting N Body Systems

Given $-\infty < e_0 < e_1 \leq ... \leq e_{M-1} < 0$, M bound states for $-\Delta_j + V(x_j)$ with $\psi_0, ..., \psi_{M-1}$ orthonormal eigenfunctions, the energy of the ground bosonic/fermionic state is given by:

$$E_0^{b/f} = inf\,\sigma(H) = inf_{\psi \in L^2_{s/a}(R^{3N}), ||\psi||=1} \langle\psi| H |\psi\rangle$$

In particular:

Ground State for N non-interacting Bosons

$E_0^b = e_0 N$ with $\psi_0 = \prod_{i=0}^{N-1} \psi_0(x_i)$.

Ground State for N non-interacting Fermions

- if $M \geq N$, $E_0^f = \sum_{i=0}^{N-1} e_i$ with $\psi_0 = \psi_0 \wedge ... \wedge \psi_{N-1}$;
- if $M < N$, $E_0^f = \sum_{i=0}^{M-1} e_i$ no ψ_0 exists.

Proof.

1.Find an estimate from below:

Given $\psi \in L^2_a(\mathbb{R}^{3N})$,$\Gamma_\psi$ trace operator, and $\gamma^{(1)}$, there exists a c.o.n.s. $\{\phi_j\}$ and $0 \leq \lambda_j \leq 1$ such that $\sum_j \lambda_j = N$ and $\gamma^{(1)} = \sum_j \lambda_j \left|\phi_j\right\rangle \left\langle\phi_j\right|$.

Rewrite $\epsilon[\psi] = \sum_j \lambda_j \left\langle\phi_j\right| h \left|\phi_j\right\rangle$.

If ψ_j are o.n.,$\phi_j = \sum_{l=0}^{M-1} c_{jl}\psi_l + \chi_j$, $\chi_j \in span\{\psi_0, ..., \psi_{M-1}\}^\perp$.

calculating $\|\phi_j\|^2 = 1$ implies $\sum_{l=0}^{M-1}|c_{jl}|^2 \leq 1$.
while $\chi_j \in span\{\psi_0, ..., \psi_{M-1}\}^\perp$ implies $\left\langle\chi_j\right| h \left|\chi_j\right\rangle \geq 0$.

Also orthonormality implies $\left\langle\psi_j\right| h \left|\psi_k\right\rangle = \epsilon_J\delta_{jk}$ and $\left\langle\chi_j\right| h \left|\psi_k\right\rangle = 0$.

Putting everything together we can rewrite:
$\epsilon[\psi] \geq \sum_{j \in N} \lambda_j \sum_{l=0}^{M-1} |c_{jl}|^2 e_l = \sum_{l=0}^{M-1} \mu_l e_l$.

where $\mu_l = \sum_j \lambda_j |c_{jl}|^2 \leq \sum_j |c_{jl}|^2 = \sum_j |\langle \phi_j| \, |\psi_l\rangle|^2 = \sum_j \|\psi_l\|^2 = 1$

and $\sum_{l=0}^{M-1} \mu_l = \sum_j \lambda_j |c_{jl}|^2 \leq \sum_j \lambda_j = N$.

Solve the minimization problem for $\mu_l = 1$ and $M < N$ or $M \geq N$:

$\epsilon[\psi] \geq \inf\{\sum_{l=0}^{M-1} \mu_l e_l \text{ s.t. } 0 \leq \mu_l \leq 1 \, , \, \sum_{l=0}^{M-1} \mu_l = N\}$.

2.Find an estimate from above:

Build a succession of states of the form:

$$\psi_0 \wedge ... \wedge \psi_{M-1} \wedge \xi_1 \wedge ... \wedge \xi_{N-M}$$

where $\xi_1 \wedge ... \wedge \xi_{N-M}$ are:

1. orthonormal and $\in E_h[0, +\infty)$ $L^2(R^3)$;
2. almost eigenstates and with energy going to zero.

Example: Take a potential with compact support with ray R_0.(Hypothesis)

Build ξ_j through a sequence of approximating functions C^∞ of the charachteristic functions of the annulus with rays in between R and R+j and s.t. $R >> 1$ and $R > R_0$.

Make R go to infinity and obtain the energies for $M < N$ or $M \geq N$.

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