

Quantum Mechanics

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Identical particles

- Until now, our focus has largely been on the study of quantum mechanics of *individual* particles.
- However, most physical systems involve interaction of many (ca. 10^{23} !) particles, e.g. electrons in a solid, atoms in a gas, etc.
- In classical mechanics, particles are always distinguishable – at least formally, “trajectories” through phase space can be traced.
- In quantum mechanics, particles can be **identical** and **indistinguishable**, e.g. electrons in an atom or a metal.
- The intrinsic uncertainty in position and momentum therefore demands separate consideration of distinguishable and indistinguishable quantum particles.
- Here we define the quantum mechanics of many-particle systems, and address (just) a few implications of particle indistinguishability.

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Quantum statistics: preliminaries

- Consider two identical particles confined to one-dimensional box.
By “identical”, we mean particles that can not be discriminated by some internal quantum number, e.g. electrons of same spin.
- The two-particle wavefunction $\psi(x_1, x_2)$ only makes sense if

$$|\psi(x_1, x_2)|^2 = |\psi(x_2, x_1)|^2 \Rightarrow \psi(x_1, x_2) = e^{i\alpha} \psi(x_2, x_1)$$

- If we introduce **exchange operator** $\hat{P}_{\text{ex}}\psi(x_1, x_2) = \psi(x_2, x_1)$, since $\hat{P}_{\text{ex}}^2 = \mathbb{I}$, $e^{2i\alpha} = 1$ showing that $\alpha = 0$ or π , i.e.

$$\begin{array}{ll} \psi(x_1, x_2) = \psi(x_2, x_1) & \text{bosons} \\ \psi(x_1, x_2) = -\psi(x_2, x_1) & \text{fermions} \end{array}$$

Quantum statistics: preliminaries

- But which sign should we choose?

$$\psi(x_1, x_2) = \psi(x_2, x_1) \quad \text{bosons}$$

$$\psi(x_1, x_2) = -\psi(x_2, x_1) \quad \text{fermions}$$

- All elementary particles are classified as fermions or bosons:

- Particles with **half-integer spin are fermions** and their wavefunction must be antisymmetric under particle exchange.
e.g. electron, positron, neutron, proton, quarks, muons, etc.
- Particles with **integer spin (including zero) are bosons** and their wavefunction must be symmetric under particle exchange.
e.g. pion, kaon, photon, gluon, etc.

Three Generations of Matter (Fermions)

	I	II	III	
mass→	5 MeV	1.24 GeV	172.5 GeV	0
charge→	$\frac{2}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	0
spin→	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
name→	u	c	t	γ
	up	charm	top	photon
	6 MeV	95 MeV	4.2 GeV	0
	$-\frac{1}{3}$	$-\frac{1}{3}$	$-\frac{1}{3}$	0
	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1
	d	s	b	g
	down	strange	bottom	gluon
	<2 eV	<0.19 MeV	<18.2 MeV	90.2 GeV
	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0
	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1
	ν_e	ν_μ	ν_τ	Z
	electron neutrino	muon neutrino	tau neutrino	weak force
	0.511 MeV	106 MeV	1.78 GeV	80.4 GeV
	-1	-1	-1	± 1
	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1
	e	μ	τ	W
	electron	muon	tau	weak force

Quarks

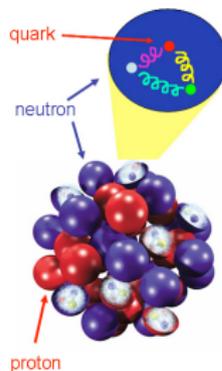
Leptons

Bosons (Forces)

Quantum statistics: remarks

- Within non-relativistic quantum mechanics, correlation between spin and statistics can be seen as an empirical law.
- However, the **spin-statistics relation** emerges naturally from the unification of quantum mechanics and special relativity.
- The rule that fermions have half-integer spin and bosons have integer spin is internally consistent:

e.g. Two identical nuclei, composed of n nucleons (fermions), would have integer or half-integer spin and would transform as a “composite” fermion or boson according to whether n is even or odd.



Quantum statistics: fermions

- To construct wavefunctions for three or more fermions, let us suppose that they do not interact, and are confined by a spin-independent potential,

$$\hat{H} = \sum_i \hat{H}_s[\hat{\mathbf{p}}_i, \mathbf{r}_i], \quad \hat{H}_s[\hat{\mathbf{p}}, \mathbf{r}] = \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r})$$

- Eigenfunctions of Schrödinger equation involve products of states of single-particle Hamiltonian, \hat{H}_s .
- However, simple products $\psi_a(1)\psi_b(2)\psi_c(3)\cdots$ do not have required antisymmetry under exchange of any two particles.
Here a, b, c, \dots label eigenstates of \hat{H}_s , and $1, 2, 3, \dots$ denote *both* space and spin coordinates, i.e. 1 stands for (\mathbf{r}_1, s_1) , etc.

Quantum statistics: fermions

- We could achieve antisymmetrization for particles 1 and 2 by subtracting the same product with 1 and 2 interchanged,

$$\psi_a(1)\psi_b(2)\psi_c(3) \mapsto [\psi_a(1)\psi_b(2) - \psi_a(2)\psi_b(1)]\psi_c(3)$$

- However, wavefunction must be antisymmetrized under *all* possible exchanges. So, for 3 particles, we must add together all 3! permutations of 1, 2, 3 in the state a, b, c with factor -1 for each particle exchange.
- Such a sum is known as a **Slater determinant**:

$$\psi_{abc}(1, 2, 3) = \frac{1}{\sqrt{3!}} \begin{vmatrix} \psi_a(1) & \psi_b(1) & \psi_c(1) \\ \psi_a(2) & \psi_b(2) & \psi_c(2) \\ \psi_a(3) & \psi_b(3) & \psi_c(3) \end{vmatrix}$$

and can be generalized to N , $\psi_{i_1, i_2, \dots, i_N}(1, 2, \dots, N) = \det(\psi_{i_j}(n))$

Quantum statistics: fermions

$$\psi_{abc}(1, 2, 3) = \frac{1}{\sqrt{3!}} \begin{vmatrix} \psi_a(1) & \psi_b(1) & \psi_c(1) \\ \psi_a(2) & \psi_b(2) & \psi_c(2) \\ \psi_a(3) & \psi_b(3) & \psi_c(3) \end{vmatrix}$$

- Antisymmetry of wavefunction under particle exchange follows from antisymmetry of Slater determinant, $\psi_{abc}(1, 2, 3) = -\psi_{abc}(1, 3, 2)$.
- Moreover, determinant is non-vanishing only if all three states a , b , c are different – manifestation of **Pauli's exclusion principle**: two identical fermions can not occupy the same state.
- Wavefunction is exact for non-interacting fermions, and provides a useful platform to study weakly interacting systems from a perturbative scheme.

Quantum statistics: bosons

- In bosonic systems, wavefunction must be symmetric under particle exchange.
- Such a wavefunction can be obtained by expanding all of terms contributing to Slater determinant and setting all signs positive.
i.e. bosonic wave function describes uniform (equal phase) superposition of all possible permutations of product states.

Space and spin wavefunctions

- When Hamiltonian is spin-independent, wavefunction can be factorized into spin and spatial components.
- For two electrons (fermions), there are four basis states in spin space: the (antisymmetric) spin $S = 0$ singlet state,

$$|\chi_S\rangle = \frac{1}{\sqrt{2}} (|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle)$$

and the three (symmetric) spin $S = 1$ triplet states,

$$|\chi_T^1\rangle = |\uparrow_1\uparrow_2\rangle, \quad |\chi_T^0\rangle = \frac{1}{\sqrt{2}} (|\uparrow_1\downarrow_2\rangle + |\downarrow_1\uparrow_2\rangle), \quad |\chi_T^{-1}\rangle = |\downarrow_1\downarrow_2\rangle$$

Space and spin wavefunctions

- For a general state, total wavefunction for two electrons:

$$\Psi(\mathbf{r}_1, s_1; \mathbf{r}_2, s_2) = \psi(\mathbf{r}_1, \mathbf{r}_2)\chi(s_1, s_2)$$

where $\chi(s_1, s_2) = \langle s_1, s_2 | \chi \rangle$.

- For two electrons, total wavefunction, Ψ , must be antisymmetric under exchange.
i.e. spin singlet state must have symmetric spatial wavefunction;
spin triplet states have antisymmetric spatial wavefunction.
- For three electron wavefunctions, situation becomes challenging...
- The conditions on wavefunction antisymmetry imply spin-dependent correlations even where the Hamiltonian is spin-independent, and leads to numerous physical manifestations...

Example I: Specific heat of hydrogen H₂ gas

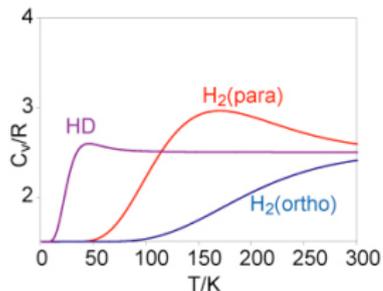
- With two spin 1/2 proton degrees of freedom, H₂ can adopt a spin singlet (parahydrogen) or spin triplet (orthoxygen) wavefunction.
- Although interaction of proton spins is negligible, spin statistics constrain available states:

Since parity of state with rotational angular momentum ℓ is given by $(-1)^\ell$, parahydrogen having symmetric spatial wavefunction has ℓ even, while for orthohydrogen ℓ must be odd.

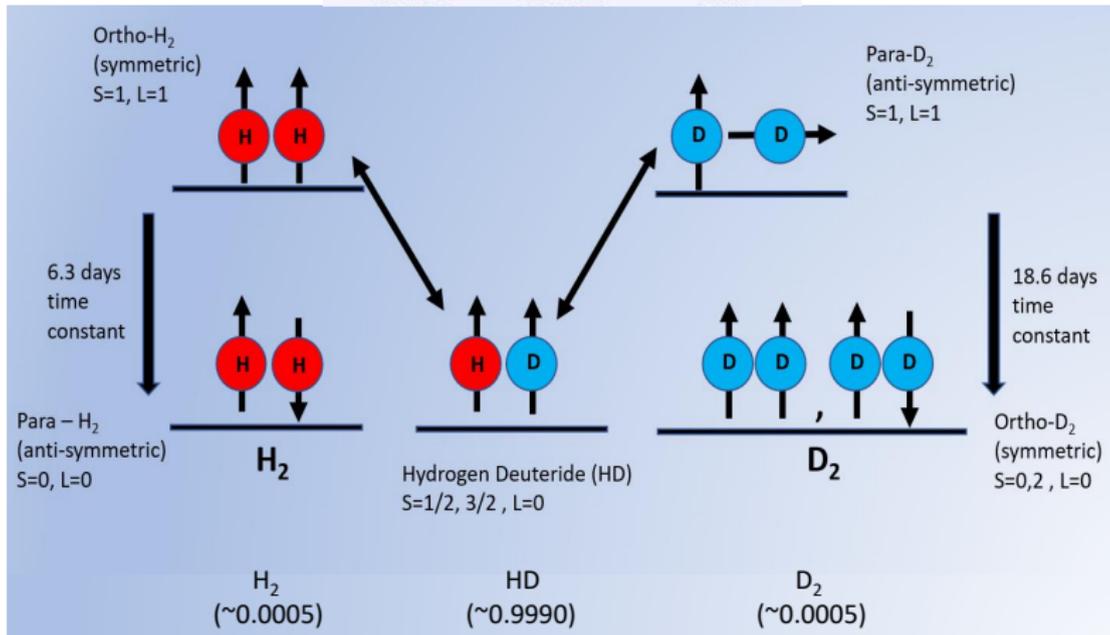
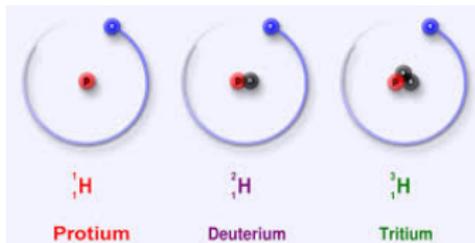
- Energy of rotational level with angular momentum ℓ is

$$E_\ell^{\text{rot}} = \frac{1}{2I} \hbar^2 \ell(\ell + 1)$$

where I denotes moment of inertia \rightsquigarrow
very different specific heats

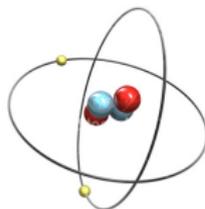


Specific heat \rightsquigarrow amount of heat required to change unit mass of substance by one degree in temperature



Example II: Excited states spectrum of Helium

$$\hat{H}^{(0)} = \sum_{n=1}^2 \left[\frac{\hat{\mathbf{p}}_n^2}{2m} + V(r_n) \right]$$



- In this approximation, ground state wavefunction involves both electrons in 1s state \rightsquigarrow antisymmetric spin singlet wavefunction, $|\Psi_{\text{g.s.}}\rangle = (|100\rangle \oplus |100\rangle)|\chi_S\rangle$.
- ground state energy is perturbed by electron-electron interaction

$$\hat{H}^{(1)} = \frac{1}{4\pi\epsilon_0} \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

- What are implications of particle statistics on spectrum of lowest excited states?

Example II: Excited states spectrum of Helium

- Ground state wavefunction belongs to class of states with symmetric spatial wavefunctions, and antisymmetric spin (singlet) wavefunctions – **parahelium**.
- In the absence of electron-electron interaction, $\hat{H}^{(1)}$, first excited states in the same class are degenerate:

$$|\psi_{\text{para}}\rangle = \frac{1}{\sqrt{2}} (|100\rangle \otimes |2\ell m\rangle + |2\ell m\rangle \otimes |100\rangle) |\chi_S\rangle$$

- Second class have antisymmetric spatial wavefunction, and symmetric (triplet) spin wavefunction – **orthohelium**. Excited states are also degenerate:

$$|\psi_{\text{ortho}}\rangle = \frac{1}{\sqrt{2}} (|100\rangle \otimes |2\ell m\rangle - |2\ell m\rangle \otimes |100\rangle) |\chi_T^{m_s}\rangle$$

Example II: Excited states spectrum of Helium

$$|\psi_{p,o}\rangle = \frac{1}{\sqrt{2}} (|100\rangle \otimes |2\ell m\rangle \pm |2\ell m\rangle \otimes |100\rangle) |\chi_{S,T}^{m_s}\rangle$$

- Despite degeneracy, since off-diagonal matrix elements between different m, ℓ values vanish, we can invoke first order perturbation theory to determine energy shift for ortho- and parahelium,

$$\begin{aligned} \Delta E_{n\ell}^{p,o} &= \langle \psi_{p,o} | \hat{H}^{(1)} | \psi_{p,o} \rangle \\ &= \frac{1}{2} \frac{e^2}{4\pi\epsilon_0} \int d^3r_1 d^3r_2 \frac{|\psi_{100}(\mathbf{r}_1)\psi_{n\ell 0}(\mathbf{r}_2) \pm \psi_{n\ell 0}(\mathbf{r}_1)\psi_{100}(\mathbf{r}_2)|^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \end{aligned}$$

(+) parahelium and (-) orthohelium.

- N.B. since matrix element is independent of m , $m = 0$ value considered here applies to all values of m .

Recap: Identical particles

- In quantum mechanics, all elementary particles are classified as fermions and bosons.
 - ① Particles with half-integer spin are described by fermionic wavefunctions, and are antisymmetric under particle exchange.
 - ② Particles with integer spin (including zero) are described by bosonic wavefunctions, and are symmetric under exchange.
- Exchange symmetry leads to development of **(ferro)magnetic spin correlations** in Fermi systems even when Hamiltonian is spin independent.
- Also leads to **Pauli exclusion principle for fermions** – manifest in phenomenon of **degeneracy pressure**.
- For an ideal gas of fermions, the ground state is defined by a filled Fermi sea of particles with an energy density

$$\frac{E_{\text{tot}}}{L^3} = \frac{\hbar^2}{20\pi^2 m} (6\pi^2 n)^{5/3}$$

Example II: Degeneracy pressure

- Cold stars are prevented from collapse by the pressure exerted by “squeezed” fermions.



Crab pulsar

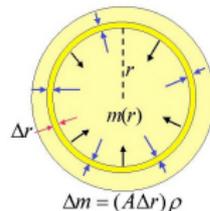
- **White dwarfs** are supported by electron-degenerate matter, and **neutron stars** are held up by neutrons in a much smaller box.

Example II: Degeneracy pressure

- From thermodynamics, $dE = \mathbf{F} \cdot d\mathbf{s} = -PdV$, i.e. pressure

$$P = -\partial_V E_{\text{tot}}$$

- To determine point of star collapse, we must compare this to the pressure exerted by gravity:



- With density ρ , gravitational energy,

$$E_G = - \int \frac{GMdm}{r} = - \int_0^R \frac{G(\frac{4}{3}\pi r^3 \rho)4\pi r^2 dr \rho}{r} = - \frac{3GM^2}{5R}$$

- Since mass of star dominated by nucleons, $M \simeq NM_N$,
 $E_G \simeq -\frac{3}{5}G(NM_N)^2(\frac{4\pi}{3V})^{\frac{1}{3}}$, and gravitational pressure,

$$P_G = -\partial_V E_G = -\frac{1}{5}G(NM_N)^2 \left(\frac{4\pi}{3}\right)^{1/3} V^{-4/3}$$

Example II: Degeneracy pressure

$$P_G = -\partial_V E_G = -\frac{1}{5} G(NM_N)^2 \left(\frac{4\pi}{3}\right)^{1/3} V^{-4/3}$$

- At point of instability, P_G balanced by degeneracy pressure. Since fermi gas has energy density $\frac{E_{\text{tot}}}{L^3} = \frac{\hbar^2}{20\pi^2 m} (6\pi^2 n)^{5/3}$, with $n = \frac{N_e}{V}$,

$$E_{\text{WD}} = \frac{\hbar^2}{20\pi^2 m_e} (6\pi^2 N_e)^{5/3} V^{-2/3}$$

- From this expression, obtain degeneracy pressure

$$P_{\text{WD}} = -\partial_V E_{\text{WD}} = \frac{\hbar^2}{30\pi^2 m_e} (6\pi^2 N_e)^{5/3} V^{-5/3}$$

- Leads to critical radius of white dwarf:

$$R_{\text{white dwarf}} \approx \frac{\hbar^2 N_e^{5/3}}{G m_e M_N^2 N^2} \simeq 7,000 \text{ km}$$

Example II: Degeneracy pressure

- White dwarf is remnant of a normal star which has exhausted its fuel fusing light elements into heavier ones (mostly ${}^6\text{C}$ and ${}^8\text{O}$).
- If white dwarf acquires more mass, E_F rises until electrons and protons abruptly combine to form neutrons and neutrinos – supernova – leaving behind neutron star supported by degeneracy.



- From $R_{\text{white dwarf}} \approx \frac{\hbar^2 N_e^{5/3}}{G m_e M_N^2 N^2}$ we can estimate the critical radius for a neutron star (since $N_N \sim N_e \sim N$),

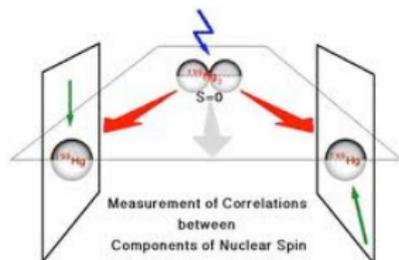
$$\frac{R_{\text{neutron}}}{R_{\text{white dwarf}}} \simeq \frac{m_e}{M_N} \simeq 10^{-3}, \quad \text{i.e.} \quad R_{\text{neutron}} \simeq 10\text{km}$$

- If the pressure at the center of a neutron star becomes too great, it collapses forming a **black hole**.

QM & causality:

■ Entanglement

- A spin-zero particle decays into two spin- $\frac{1}{2}$ particles
- If left-side particle (LSP) is measured along a chosen direction as $+\frac{1}{2}$, then right-side particle (RSP) is measured as $-\frac{1}{2}$ along this same chosen direction (because angular momentum conserved)
- In this state of affairs the spins are “entangled”; that is, they’re correlated
- Since the state of the LSP is, in general, a superposition of $+\frac{1}{2}$ & $-\frac{1}{2}$, it’s spin is **unknown** until measured
- Then the state of the RSP is fixed (along the chosen direction) **seemingly instantaneously**?!
 - And this is weird.
 - Or, at least, appears to conflict with special relativity (Einstein)
 - But it doesn’t conflict: there’s no way to transfer information using these entangled states



Einstein, Podolsky, & Rosen were upset by this state of affairs. They were right to be upset. But QM has proven itself.