FY2045 Quantum Mechanics I

Fall 2023

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Week 7

Spin $\frac{1}{2}$

Abstract formulation

For $s = \frac{1}{2}$ we have two possible eigenvectors of $\mathbf{S}^2$ and S_z:

$$\left|\frac{1}{2}, +\frac{1}{2}\right\rangle \equiv |+\rangle \equiv |\uparrow\rangle\,,$$
$$\left|\frac{1}{2}, -\frac{1}{2}\right\rangle \equiv |-\rangle \equiv |\downarrow\rangle\,,$$

forming a complete set in a two-dimensional Hilbert space.

Can expand arbitrary vector $|\chi\rangle$ in the 2D Hilbert space:

$$\begin{aligned} |\chi\rangle &= \langle\uparrow|\chi\rangle\,|\uparrow\rangle + \langle\downarrow|\chi\rangle\,|\downarrow\rangle \\ &\equiv a_+\,|\uparrow\rangle + a_-\,|\downarrow\rangle\,. \end{aligned}$$

$a_\pm$: probability amplitude of measuring spin up (down) and leaving the spin in state $|\uparrow\rangle$ ($|\downarrow\rangle$).

Matrix formulation

Represent state $|\chi\rangle$ by two-element column matrix

$$\chi = \begin{pmatrix} a_+ \\ a_- \end{pmatrix},$$

called a **spinor**. The adjoint state $\langle\chi|$ is represented by the adjoint matrix

$$\chi^\dagger = (\chi^T)^* = \begin{pmatrix} a_+^* & a_-^* \end{pmatrix}.$$

Require normalization,

$$\chi^\dagger \chi = 1.$$

Eigenspinors of S_z

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \text{ spin up,}$$

$$\chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \text{ spin down.}$$

Orthonormal:

$$\chi_\sigma^\dagger \chi_{\sigma'} = \delta_{\sigma\sigma'}$$

Matrix formulation

Operators represented by 2×2 matrices

$$\mathbf{S}^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{3}{4}\hbar^2 \mathbb{1},$$

and

$$S_x = \frac{\hbar}{2}\sigma_x, \quad S_y = \frac{\hbar}{2}\sigma_y, \quad S_z = \frac{\hbar}{2}\sigma_z.$$

Connection between matrix and abstract operator:

$$F = \begin{pmatrix} ++ & +- \\ -+ & -- \end{pmatrix} = \begin{pmatrix} \langle + | \hat{F} | + \rangle & \langle + | \hat{F} | - \rangle \\ \langle - | \hat{F} | + \rangle & \langle - | \hat{F} | - \rangle \end{pmatrix}.$$

Pauli matrices

Dimensionless matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

satisfying

$$[\sigma_i, \sigma_j] = \sigma_i\sigma_j - \sigma_j\sigma_i = 2i\epsilon_{ijk}\sigma_k,$$

$$\{\sigma_i, \sigma_j\} = \sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}\mathbb{1}.$$

The spin direction

Expectation value of observable F in state χ given by

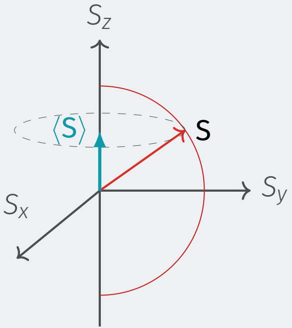
$$\langle F \rangle_\chi = \chi^\dagger F \chi.$$

The direction of

$$\langle \mathbf{S} \rangle = \langle S_x \rangle \hat{x} + \langle S_y \rangle \hat{y} + \langle S_z \rangle \hat{z}.$$

is often called the **spin direction**.

NB: The direction of **S** is **not** an observable since the components S_i do not commute.



Eigenstates along other directions

If we measure the x or y component of the spin we can also get the values $\pm\hbar/2$. The normalized eigenstates for all three spatial directions are

$\underline{S_x:}$ $\underline{S_y:}$ $\underline{S_z:}$

$$\chi_+^{(x)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \chi_+^{(y)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} \qquad \chi_+^{(z)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad +\frac{\hbar}{2}$$

$$\chi_-^{(x)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \qquad \chi_-^{(y)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} \qquad \chi_-^{(z)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad -\frac{\hbar}{2}$$

Measuring the spin along direction i leaves the spin in one of the eigenstates of S_i — **measurements change the state of the spin.**

Electron in a magnetic field

Magnetic moment $\boldsymbol{\mu} = \gamma_e \mathbf{S}$, ($\gamma_e < 0$), and Hamiltonian $H = -\boldsymbol{\mu} \cdot \mathbf{B}$. From Schrödinger equation $i\hbar \frac{\partial \chi}{\partial t} = H\chi$ we get

$$\chi(t) = a_+ \chi_+ e^{-iE_+ t/\hbar} + a_- \chi_- e^{-iE_- t/\hbar},$$

with $E_\pm = \mp \gamma_e B_0 \hbar / 2$ when $\mathbf{B} = B_0 \hat{z}$.

The spin expectation value precesses with the Larmor frequency $\omega = \gamma_e B_0$:

$$\langle \mathbf{S} \rangle = \hbar a_+ a_- \left[\cos \omega t \, \hat{x} - \sin \omega t \, \hat{y} + \frac{a_+^2 - a_-^2}{a_+ a_-} \hat{z} \right],$$

where a_+, a_- are assumed real.

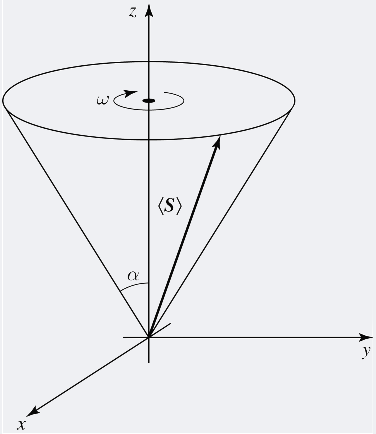


Figure from Griffiths and Schroeter, ©Cambridge University Press 2018

Identical particles

Two-particle Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 + V(\mathbf{r}_1, \mathbf{r}_2),$$

Non-interacting particles

If $V(\mathbf{r}_1, \mathbf{r}_2) = V(\mathbf{r}_1) + V(\mathbf{r}_2)$, we can write $\hat{H} = \hat{H}_1 + \hat{H}_2$ and use separation of variables:

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2),$$

with single-particle states $\psi_{a/b}$ satisfying $\hat{H}_1\psi_a = E_a\psi_a$ and $\hat{H}_2\psi_b = E_b\psi_b$.

Indistinguishable particles

Identical particles not distinguishable in quantum mechanics — must have

$$|\Psi(\mathbf{r}_1, \mathbf{r}_2, t)|^2 = |\Psi(\mathbf{r}_2, \mathbf{r}_1, t)|^2.$$

In 3D we have two possibilities:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = \begin{cases} +\Psi(\mathbf{r}_2, \mathbf{r}_1, t) & \text{for bosons,} \\ -\Psi(\mathbf{r}_2, \mathbf{r}_1, t) & \text{for fermions.} \end{cases}$$

In 2D it is possible to have particle with in-between statistics — *anyons*. See, e.g., The story behind the mysterious anyon particles.

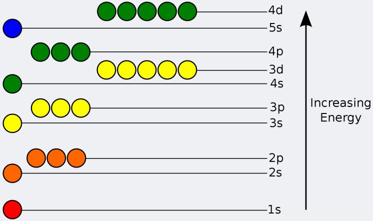
Two non-interacting particles

$$\psi(\mathrm{r}_1, \mathrm{r}_2) = \begin{cases} \frac{1}{\sqrt{2}}[\psi_a(\mathrm{r}_1)\psi_b(\mathrm{r}_2) + \psi_b(\mathrm{r}_1)\psi_a(\mathrm{r}_2)], & \text{bosons} \\ \frac{1}{\sqrt{2}}[\psi_a(\mathrm{r}_1)\psi_b(\mathrm{r}_2) - \psi_b(\mathrm{r}_1)\psi_a(\mathrm{r}_2)], & \text{fermions} \end{cases}$$

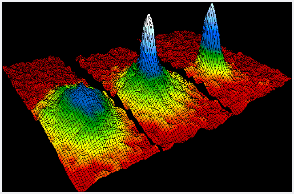
Pauli exclusion principle

Fermions cannot be in the same single-particle state.

Electrons in an atom



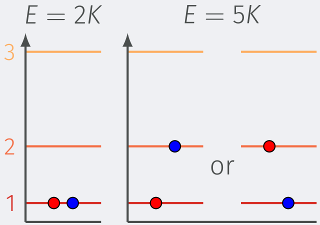
Bose-Einstein condensation



Figures by Richard Parsons and National Institute of Standards and Technology (NIST)

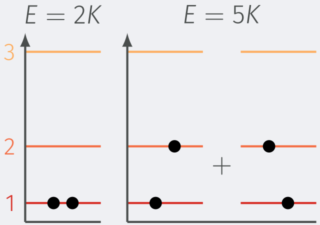
Example — Two non-interacting particles in an infinite square well

Distinguishable particles



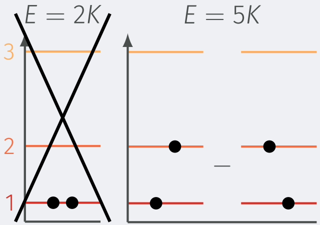
Doubly degenerate first excited state.

Bosons



Indistinguishable — non-degenerate first excited state.

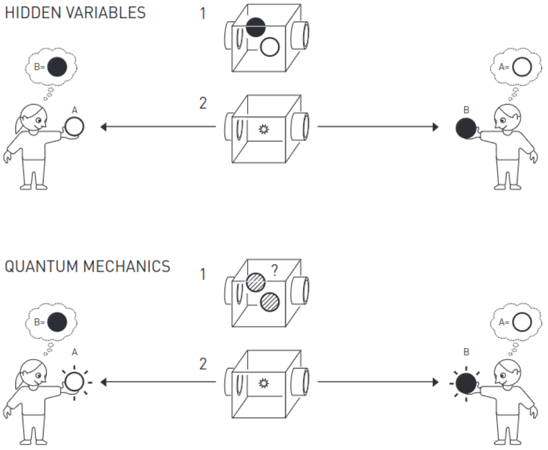
Fermions



Pauli principle: Two fermions cannot occupy the same state!

Entanglement

Nobel prize in physics 2022: “for experiments with entangled photons, establishing the violation of Bell inequalities and pioneering quantum information science”[1]



[1] For more info see e.g. the summary from the Nobel foundation.