Week 3: Fundamental quantum mechanics, particle in a box, spherical coordinates

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- Q6.13 Explain the following statement: if $\hbar = 0$, it would be possible to measure the position and momentum of a particle exactly and simultaneously.
- Q6.15 How would the results of the Stern-Gerlach experiment be different if they had used a Mg beam instead of an Ag beam? What about a beam of Hydrogen atoms?

Polar coordinates and spherical coordinates 1

- In general, we can represent a point in D dimensions by it's length r, and D-1 angles $\theta, \phi, \dots$ uniquely.
- So we can write any function $f(x, y, z, \dots)$ as $f(r, \theta, \phi, \dots)$
- In two dimensions, we have
  - $x = r\cos(\theta)$, $y = r\sin(\theta)$ where $r \in [0, \infty]$, $\theta \in [0, 2\pi]$.
  - So we can write any function as $f(x, y) = f(r, \theta)$.
  - When integrating, one has to be careful to take the determinant of the Jacobian into account:

$$\mathbf{J_F}(r, \theta) = \begin{bmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} \end{bmatrix} = \begin{bmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{bmatrix}$$

and $dxdy = \det(J_F(r, \theta))drd\theta = rdrd\theta$

Polar coordinates and spherical coordinates 2

In three dimensions, we have

$$
\begin{aligned}
x &= r\sin\theta\cos\phi, & r &= \sqrt{x^2+y^2+z^2} \\
y &= r\sin\theta\sin\phi, & \phi &= \arctan\left(\frac{y}{x}\right) \\
z &= r\cos\theta, & \theta &= \arccos\left(\frac{z}{r}\right)
\end{aligned}
$$

where $r \in [0,\infty], \theta \in [0,\pi]$ and $\phi \in [0, 2\pi]$. And the Jacobian reads

$$
\mathbf{J_F}(r,\theta,\phi) = \begin{bmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} & \frac{\partial x}{\partial \phi} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} & \frac{\partial y}{\partial \phi} \\ \frac{\partial z}{\partial r} & \frac{\partial z}{\partial \theta} & \frac{\partial z}{\partial \phi} \end{bmatrix} = \begin{bmatrix} \sin\theta\cos\phi & r\cos\theta\cos\phi & -r\sin\theta\sin\phi \\ \sin\theta\sin\phi & r\cos\theta\sin\phi & r\sin\theta\cos\phi \\ \cos\theta & -r\sin\theta & 0 \end{bmatrix}
$$

Then the volume element becomes

$$
dxdydz = r^2\sin(\theta)drd\theta d\phi
$$

Example exercises calculated by me

- Calculate the volume of a sphere of radius r.
- Write $\frac{\partial}{\partial x}$ in spherical coordinates.
- P6.7 Evaluate the commutator $\left[\left(d^2/dy^2\right), y\right]$ by applying the operators to an arbitrary function $f(y)$.
- Show that the state

$$\Psi(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega}{2\hbar}x^2\right)$$

has minimum uncertainty $\sigma_x \sigma_p = \frac{\hbar}{2}$.

Exercises on quantum mechanics

- P6.8 Evaluate the commutator $\left[d/dx, 1/x^2\right]$ by applying the operators to an arbitrary function $f(x)$.
- P6.9 Evaluate the commutator $[\hat{x}, \hat{p}_x]$ by applying the operators to an arbitrary function $f(x)$. What value does the commutator $[\hat{p}_x, \hat{x}]$ have?
- P6.13 For linear operators A, B, C, show that $[A, BC] = [A, B]C + B[A, C]$.
- Consider the particle in a box of length a. For the energy eigenstates $\Psi_n(x)$, calculate the expectation values $\langle x \rangle$,$\langle x^2 \rangle$, $\langle p \rangle$ and $\langle p^2 \rangle$. (Hint: $\langle x \rangle$, $\langle p^2 \rangle$ and $\langle p \rangle$ can be solved without doing any integrals.) Calculate the standard deviations $\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ and $\sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$ and the product $\sigma_x \sigma_p$. Indeed, Heisenbergs uncertainty principle states that $\sigma_x \sigma_p \geq \frac{\hbar}{2}$. Did you get that?

Exercises on mathematics

- Solve the integral

$$I = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\frac{1}{a}\sqrt{x^2+y^2+z^2}} dxdydz$$

- Quite challenging: Write $\frac{\partial}{\partial z}$ in spherical coordinates.
- Challenging: Write $\frac{\partial^2}{\partial z^2}$ in spherical coordinates.
- **Very** challenging: Show that the Laplacian, which in Cartesian coordinates reads

$$\Delta f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

reads in spherical coordinates

$$\Delta f = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial f}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial f}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2 f}{\partial \phi^2}$$