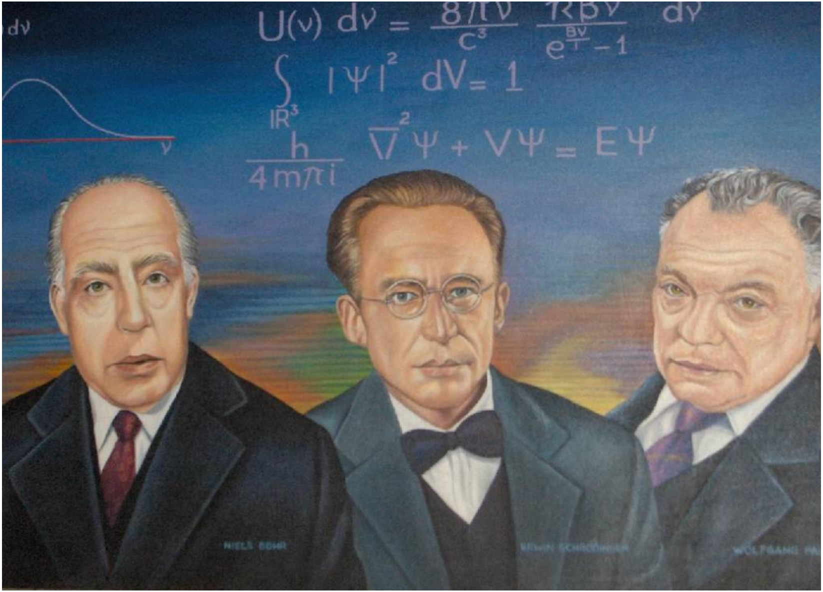
Modern Physics

Luis A. Anchordoqui

Department of Physics and Astronomy
Lehman College, City University of New York

Lesson XI
November 2, 2023

Table of Contents


$\int_{IR^3} |\Psi|^2 \, dV = 1$
$\frac{h}{4m\pi i} \nabla^2 \Psi + V\Psi = E\Psi$

- Prescription to obtain 3D Schrödinger equation for free particle:
  - substitute into classical energy momentum relation

$$E = \frac{|\vec{p}\,|^2}{2m} \tag{1}$$

  - differential operators

$$E \to i\hbar \frac{\partial}{\partial t} \quad \text{and} \quad \vec{p} \to -i\hbar\vec{\nabla} \tag{2}$$

  - resulting operator equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi = i\hbar\frac{\partial}{\partial t}\psi \tag{3}$$

  acts on complex wave function $\psi(\vec{x}, t)$
- Interpret $\rho = |\psi|^2$ as ☞ probability density
  $|\psi|^2 d^3x$ gives probability of finding particle in volume element d^3x

Continuity equation

- We are often concerned with moving particles
  e.g. collision of particles
- Must calculate density flux of particle beam $\vec{j}$
- From conservation of probability
  rate of decrease of number of particles in a given volume
  is equal to total flux of particles out of that volume

$$-\frac{\partial}{\partial t}\int_V \rho \, dV = \int_S \vec{j}\cdot\hat{n}\, dS = \int_V \vec{\nabla}\cdot\vec{j}\, dV \tag{4}$$

(last equality is Gauss' theorem)

- Probability and flux densities are related by continuity equation

$$\frac{\partial \rho}{\partial t} + \vec{\nabla}\cdot\vec{j} = 0 \tag{5}$$

Flux

To determine flux...

- First form $\partial\rho/\partial t$ by substracting wave equation multiplied by $-i\psi^*$ from the complex conjugate equation multiplied by $-i\psi$

$$\frac{\partial\rho}{\partial t} - \frac{\hbar}{2m}(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*) = 0 \qquad (6)$$

- Comparing this with continuity equation ☞ probability flux density

$$\vec{j} = -\frac{i\hbar}{2m}(\psi^*\nabla\psi - \psi\nabla\psi^*) \qquad (7)$$

- Example ☞ free particle of energy E and momentum $\vec{p}$

$$\psi = Ne^{i\vec{p}\cdot\vec{x}-iEt} \qquad (8)$$

has ☞ $\rho = |N|^2$ and $\vec{j} = |N^2|\,\vec{p}/m$

Time-independent Schrödinger equation for central potential

- Potential depends only on distance from origin

$$V(\vec{r}) = V(|\vec{r}\,|) = V(r) \tag{9}$$

  hamiltonian is spherically symmetric

- Instead of using cartesian coordinates $\vec{x} = \{x, y, z\}$
  use spherical coordinates $\vec{x} = \{r, \vartheta, \varphi\}$ defined by

$$\left\{ \begin{array}{l} x = r \sin\vartheta \cos\varphi \\ y = r\sin\vartheta \sin\varphi \\ z = r\cos\vartheta \end{array} \right\} \Leftrightarrow \left\{ \begin{array}{l} r = \sqrt{x^2 + y^2 + z^2} \\ \vartheta = \arctan\left(z/\sqrt{x^2+y^2}\right) \\ \varphi = \arctan(y/x) \end{array} \right\} \tag{10}$$

- Express the Laplacian ∇^2 in spherical coordinates

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta \frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2} \tag{11}$$

To look for solutions...

- Use separation of variable methods ☞ $\psi(r,\vartheta,\varphi) = R(r)Y(\vartheta,\varphi)$

$$-\frac{\hbar^2}{2m}\left[\frac{Y}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{R}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial Y}{\partial\vartheta}\right) + \frac{R}{r^2\sin^2\vartheta}\frac{\partial^2 Y}{\partial\varphi^2}\right] + V(r)RY = ERY$$

- Divide by RY/r^2 and rearrange terms

$$-\frac{\hbar^2}{2m}\left[\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)\right] + r^2(V-E) = \frac{\hbar^2}{2mY}\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial Y}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2 Y}{\partial\varphi^2}\right]$$

- Each side must be independently equal to a constant ☞ $\varkappa = -\frac{\hbar^2}{2m}l(l+1)$
- Obtain two equations

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}(V-E) = l(l+1) \quad (12)$$

$$\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial Y}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2 Y}{\partial\varphi^2} = -l(l+1)Y \quad (13)$$

- What is the meaning of operator in angular equation?

Angular momentum operator

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}} = -i\hbar\, \hat{\vec{r}} \times \hat{\vec{\nabla}} \tag{14}$$

in cartesian coordinates

$$\begin{aligned}
\hat{L}_x &= \hat{y}\hat{p}_z - \hat{p}_y\hat{z} = -i\hbar\left(y\frac{\partial}{\partial z} - \frac{\partial}{\partial y}z\right) \\
\hat{L}_y &= \hat{z}\hat{p}_x - \hat{p}_z\hat{x} = -i\hbar\left(z\frac{\partial}{\partial x} - \frac{\partial}{\partial z}x\right) \\
\hat{L}_z &= \hat{x}\hat{p}_y - \hat{p}_x\hat{y} = -i\hbar\left(x\frac{\partial}{\partial y} - \frac{\partial}{\partial x}y\right)
\end{aligned} \tag{15}$$

commutation relations

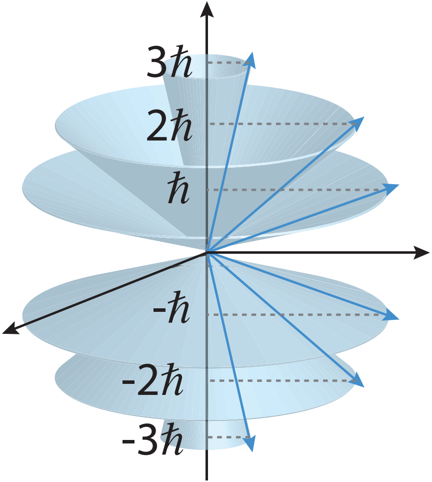
$$[\hat{L}_i, \hat{L}_j] = i\hbar\, \varepsilon_{ijk}\, \hat{L}_k \quad \text{and} \quad [\hat{L}^2, \hat{L}_x] = [\hat{L}^2, \hat{L}_y] = [\hat{L}^2, \hat{L}_z] = 0 \tag{16}$$

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

We can always know:

length of angular momentum plus one of its components

E.g. ☞ choosing the z-component



- Angular momentum vector in spherical coordinates

$$\hat{L}_x = i\hbar\left(\sin\varphi\frac{\partial}{\partial\theta} + \cot\varphi\cos\varphi\frac{\partial}{\partial\varphi}\right)$$
$$\hat{L}_y = -i\hbar\left(\cos\varphi\frac{\partial}{\partial\vartheta} - \cot\vartheta\sin\varphi\frac{\partial}{\partial\varphi}\right)$$
$$\hat{L}_z = -\hbar\frac{\partial}{\partial\varphi} \qquad (17)$$

- Form of $\hat{L}^2$ should be familiar

$$\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right] \qquad (18)$$

- Eigenvalue equations for $\hat{L}^2$ and $\hat{L}_z$ operators:

$$\hat{L}^2 Y(\vartheta,\varphi) = \hbar^2 l(l+1)Y(\vartheta,\varphi) \quad \text{and} \quad \hat{L}_z Y(\vartheta,\varphi) = \hbar m Y(\vartheta,\varphi)$$

Solution of angular equation

$$\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial Y_l^m(\vartheta,\varphi)}{\partial\vartheta}\right)+\frac{1}{\sin^2\vartheta}\frac{\partial^2 Y_l^m(\vartheta,\varphi)}{\partial\varphi^2}=-l(l+1)Y_l^m(\vartheta,\varphi)$$

- Use separation of variables ☞ $Y(\vartheta,\varphi)=\Theta(\vartheta)\Phi(\varphi)$
- By multiplying both sides of the equation by $\sin^2\vartheta/Y(\vartheta,\varphi)$

$$\frac{1}{\Theta(\vartheta)}\left[\sin\vartheta\frac{d}{d\vartheta}\left(\sin\vartheta\frac{d\Theta}{d\vartheta}\right)\right]+l(l+1)\sin^2\vartheta=-\frac{1}{\Phi(\varphi)}\frac{d^2\Phi}{d\varphi^2} \quad (19)$$

- 2 equations in different variables ☞ introduce constant m^2:

$$\frac{d^2\Phi}{d\varphi^2}=-m^2\Phi(\varphi) \quad (20)$$

$$\sin\vartheta\frac{d}{d\vartheta}\left(\sin\vartheta\frac{d\Theta}{d\vartheta}\right)=[m^2-l(l+1)\sin^2\vartheta]\Theta(\vartheta) \quad (21)$$

Solution of angular equation

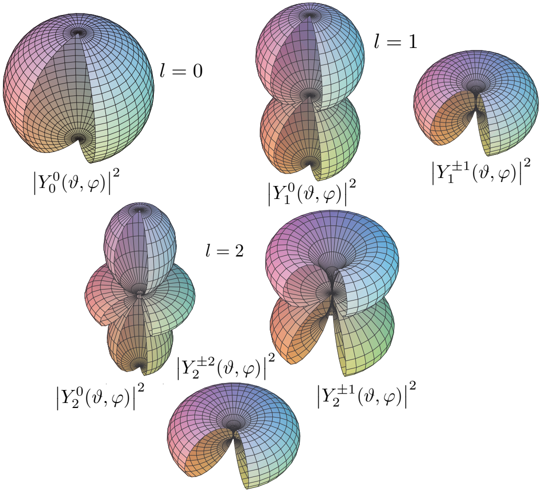
- First equation is easily solved to give ☞ $\Phi(\varphi) = e^{im\varphi}$
- Imposing periodicity $\Phi(\varphi + 2\pi) = \Phi(\varphi)$ ☞ $m = 0, \pm 1, \pm 2, \cdots$
- Solutions to the second equation ☞ $\Theta(\vartheta) = AP_l^m(\cos\vartheta)$
- P_l^m ☞ associated Legendre polynomials
- Normalized angular eigenfunctions

$$Y_l^m(\vartheta, \varphi) = \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-m)!}{(l+m)!}} \, P_l^m(\cos\vartheta) e^{im\varphi} \tag{22}$$

- Spherical harmonics are orthogonal:

$$\int_0^\pi \int_0^{2\pi} Y_l^{m*}(\vartheta, \varphi) \, Y_{l'}^{m'} \sin\vartheta d\vartheta d\varphi = \delta_{ll'} \delta_{mm'} \,, \tag{23}$$

l \ m	0	1	2	3
0	$P_0^0 = 1$			
1	$P_1^0 = \cos\vartheta$	$P_1^1 \sin\vartheta$		
2	$P_2^0 = (3\cos^2\vartheta - 1)/2$	$P_2^1 = 3\cos\vartheta\sin\vartheta$	$P_2^2 = 3\sin^2\vartheta$	
3	$P_3^0(5\cos^3\vartheta - 3\cos\vartheta)/2$	$P_3^1 = 3(5\cos^2\vartheta - 1)/2\,\sin\vartheta$	$P_3^2 = 15\cos\vartheta\sin^2\vartheta$	$P_3^3 = 15\sin^3\vartheta$



Solution of radial equation

$$\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) - \frac{2mr^2}{\hbar^2}(V-E) = l(l+1)R(r) \quad (24)$$

- to simplify solution ☞ $u(r) = rR(r)$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V + \frac{\hbar}{2m}\frac{l(l+1)}{r^2}\right]u(r) = Eu(r) \quad (25)$$

- define an effective potential

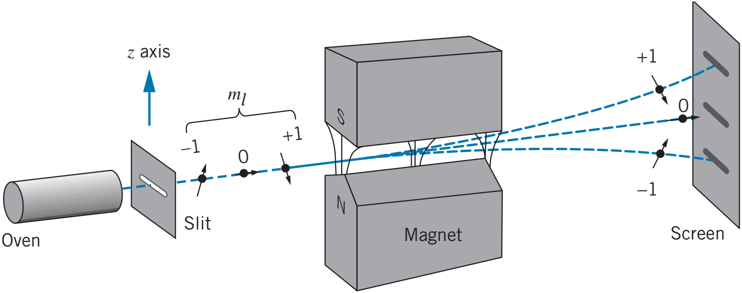
$$V'(r) = V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} \quad (26)$$

(25) is very similar to the one-dimensional Schrödinger equation

- Wave function ☞ need 3 quantum numbers (n, l, m)

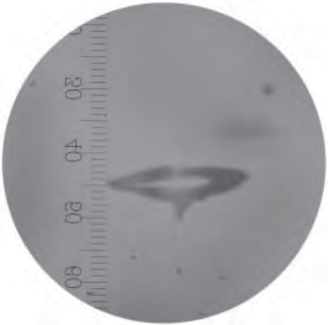
$$\psi_{n,l,m}(r,\vartheta,\varphi) = R_{n,l}(r)Y_l^m(\vartheta,\varphi) \quad (27)$$

Stern-Gerlach apparatus



- Beam of atoms passes through a region where there is nonuniform $\vec{B}$-field
- Atoms with their magnetic dipole moments in opposite directions experience forces in opposite directions

Results of Stern-Gerlach experiment



- Image of slit with field turned off (left)
- With the field on ☞ two images of slit appear
- Small divisions in the scale represent 0.05 mm

Uhlenbeck-Goudsmit-Pauli hypothesis

- Magnetic moment ☞ connected via intrinsic angular momentum

$$\vec{\mu}_S = -\frac{e}{2m_e} g_e \vec{S} \tag{28}$$

- For intrinsic spin ☞ only matrix representation is possible
  - Spin up $|\uparrow\rangle$ and down $|\downarrow\rangle$ are defined by

$$\text{spin up} \quad \Leftrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{spin down} \quad \Leftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} . \tag{29}$$

  - $\hat{S}_z$ spin operator is defined by

$$\hat{S}_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{30}$$

- $\hat{S}_z$ acts on up and down states by ordinary matrix multiplication

$$\hat{S}_z|\uparrow\rangle = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}|\uparrow\rangle \quad (31)$$

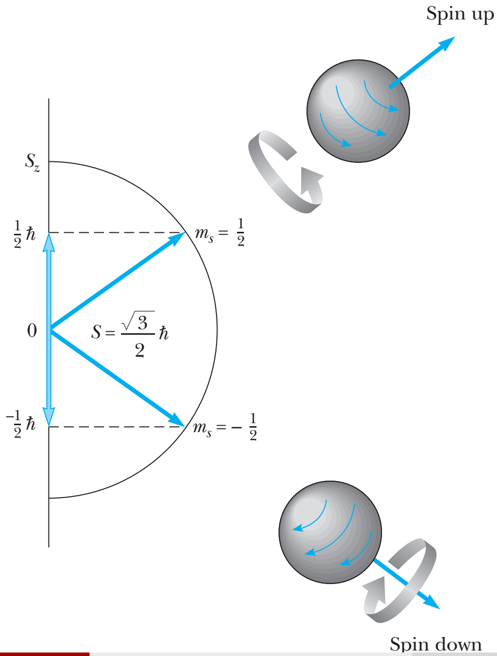
$$\hat{S}_z|\downarrow\rangle = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\hbar}{2}|\uparrow\rangle \quad (32)$$

- As for orbital angular momentum $[\hat{S}_i, \hat{S}_j] = i\hbar\,\epsilon_{ijk}\hat{S}_k$

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (33)$$

- Only 4 hermitian 2-by-2 matrices ☞ indentity + Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (34)$$


Spin up
S_z
$\frac{1}{2}\hbar$
$m_s = \frac{1}{2}$
0
$S = \frac{\sqrt{3}}{2}\hbar$
$-\frac{1}{2}\hbar$
$m_s = -\frac{1}{2}$
Spin down

Relativistic wave equation

- Schrodinger equation violates Lorentz invariance and is not suitable for particle moving relativistically
- Making the operator substitution starting from relativistic energy momentum relation

$$-\frac{\partial^2\psi}{\partial t^2} + \nabla^2\psi = m^2\psi \qquad (\hbar = c = 1) \tag{35}$$

- Introducing the covariant form ☞ $p^\mu \to i\partial^\mu$

$$\partial^\mu = \left(\partial_t, -\vec{\nabla}\right) \quad \text{and} \quad \partial_\mu = \left(\partial_t, \vec{\nabla}\right) \tag{36}$$

we can form invariant (D'Alembertian) operator $\Box^2 \equiv \partial_\mu\partial^\mu$

$$\partial_\mu\partial^\mu\psi + m^2\psi \equiv (\Box^2 + m^2)\psi = 0 \tag{37}$$

- Recall $\psi(\vec{x}, t)$ is scalar complex-valued wave function

Negative probability density?

- Multiplying KG by $-i\psi^*$ minus complex conjugate equation by $-i\psi$

$$\partial_t \underbrace{[i(\psi^* \partial_t \psi - \psi \partial_t \psi^*)]}_{\rho} + \vec{\nabla}. \underbrace{[-i(\psi^* \vec{\nabla} \psi - \psi \nabla \psi^*)]}_{\vec{j}} = 0 \qquad (38)$$

- Consider motion free particle of energy E and momentum $\vec{p}$

$$\psi = N\, e^{i(\vec{p}.\vec{x} - Et)} \qquad (39)$$

from (38) ☞ $\rho = 2\,E\,|N|^2$ and $\vec{j} = 2\,\vec{p}\,|N|^2$

- Probability density ρ is timelike component of 4-vector

$$\rho \propto E = \pm(\vec{p}^{\,2} + m^2)^{1/2} \qquad (40)$$

- In addition to acceptable $E > 0$ solutions
  we have negative energy solutions
  which have associated negative probability density!

Antimatter

- Pauli and Weisskopf ☞ inserted charge e in continuity equation

$$j^\mu = -i\, e\, (\psi^* \, \partial^\mu \psi - \psi \, \partial^\mu \psi^*) \tag{41}$$

  interpreting j^μ as electromagnetic charge-current density

- j^0 represents a charge density ☞ not a probability density and so the fact that it can be negative is no longer objectable

- Stückelberg and Feynman ☞ negative energy solution describes a particle which propagates backwards in time or positive energy *antiparticle* propagating forward in time


IF I ROTATE MY HAMMER FAST ENOUGH, IT WILL EMIT ANTI-MATTER PARTICLES! THERE-- IT IS WORKING!

Thor's "spinless" positron

- Consider spin-0 particle with $(E, \vec{p}, e)$
  generally referred to as the "spinless electron"
- Electromagnetic 4-vector current is

$$j^{\mu}(e^{-}) = -2e|N|^{2}(E,\ \vec{p}) \tag{42}$$

- Taking antiparticle e^{+} of same $(E, \vec{p})$

$$j^{\mu}(e^{+}) = +2e|N|^{2}(E, \vec{p}) = -2e|N|^{2}(-E, -p) \tag{43}$$

  exactly same current of the original particle with $-E, -\vec{p}$
- As far as system is concerned ☞ emission of antiparticle with energy E is same as absorption of particle of energy $-E$
- Negative-energy particle solutions going backward in time
  describe
  positive-energy antiparticle solutions going forward in time