Quantum Many-Body Theory

Presentation 1

Tim Lund

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Preliminaries

States

- The state of a quantum object is described by a **state vector** $|\psi\rangle$
- The set of state vectors is the **state space** $\mathcal{H}$, which is a vector space isomorphic to $\mathbb{C}^2$

Observables

- **Physical observables** (position, velocity, etc.) of quantum objects are represented by nonsingular Hermitian operators on $\mathcal{H}$
- The eigenvectors of an observable are referred to as its **eigenstates**

Since the eigenstates of an observable span $\mathcal{H}$, any state vector can be expressed as a linear combination thereof

$$|\psi\rangle = \sum_i \underset{\substack{\uparrow \\ c_i \in \mathbb{C}}}{c_i} \overset{\substack{\textit{Eigenstate} \\ \downarrow}}{|\varphi_i\rangle}$$

Measurement

- A measurement of an observable must interact with the quantum state, causing it to jump to an eigenstate of the observable

$$\underset{\substack{\uparrow \\ \textit{Physical observable}}}{\mathbf{A}} \overset{\substack{\textit{State to which the object jumps} \\ \downarrow}}{|\varphi_i\rangle} = \underset{\substack{\uparrow \\ \textit{Measured value}}}{a_i} |\varphi_i\rangle$$

- The state to which an object jumps upon measurement is random, occurring with probability $|c_i|^2$

Preliminaries

Uncertainty

- Two observables can only be measured simultaneously if they can be diagonalized using the same eigenstates

  The necessary and sufficient condition for this is that the commutator must equal zero

$$[\mathbf{A}, \mathbf{B}] := \mathbf{AB} - \mathbf{BA}$$

Additional Notes

- The inner product between two state vectors $|\varphi\rangle,\ |\psi\rangle \in \mathcal{H}$ is denoted by $\langle\varphi|\psi\rangle$
- The physical meanings of the state vectors $|\psi\rangle$ and $c|\psi\rangle$ are the same for all $c \neq 0$; we may therefore assume that $\langle\psi|\psi\rangle = 1$

The Shrödinger Equation

The Shrödinger equation describes the evolution of a quantum state $|\psi(t)\rangle$ over time

$$\mathrm{i}\partial_t|\psi(t)\rangle = \mathbf{H}(t)|\psi(t)\rangle$$

Where the Hamiltonian operator **H** *gives the total energy of the system*

The Shrödinger Equation

We consider the solution to the Shrödinger equation when the Hamiltonian is time-independent

The Hamiltonian is diagonalized via

$$\mathbf{H}|\varphi_i\rangle = E_i|\varphi_i\rangle$$

Case 1

If the initial state $|\psi(t_0)\rangle$ is an eigenstate of $\mathbf{H}$, then the solution to the Shrödinger equation is

$$|\psi(t)\rangle = e^{-\mathrm{i}E_i(t-t_0)}|\psi(t_0)\rangle$$

The Shrödinger Equation

Case 2

If the initial state is *not* an eigenstate of $\mathbf{H}$, recall that we may express it as a linear combination of the eigenstates

$$|\psi(t_0)\rangle = \sum_i c_i |\varphi_i\rangle$$

This yields the solution

$$|\psi(t)\rangle = \sum_i c_i e^{-\mathrm{i}E_i(t-t_0)} |\varphi_i\rangle.$$

Particle in One Dimension

- Hilbert space

$$\mathcal{H} = \left\{ f \,\middle|\, \int_{\mathbb{R}} |f(x)|^2 \mathrm{d}x < \infty \right\}$$

- Inner product

$$\langle \varphi | \psi \rangle = \int_{\mathbb{R}} \varphi^*(x) \psi(x) \mathrm{d}x$$

- Normalization condition

$$\langle \psi | \psi \rangle = \int_{\mathbb{R}} |\psi(x)|^2 \mathrm{d}x = 1$$

Representing Real Space

Particle in One Dimension

- Position operator $\mathbf{x}$
- Momentum operator $\mathbf{p}$

$$\mathbf{p} = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}$$

- We note that the position and momentum operators do not commute

$$[\mathbf{x}, \mathbf{p}] = \mathrm{i}$$

This is the canonical commutation relation, which gives us the Heisenberg uncertainty principle

Particle in Three Dimensions

- Position operator $\mathbf{r} = (\mathbf{x}, \mathbf{y}, \mathbf{z})^\mathsf{T}$
- Momentum operator $\mathbf{p} = (\mathbf{p}_x, \mathbf{p}_y, \mathbf{p}_z)^\mathsf{T}$
- We introduce the angular momentum operator $\mathbf{L}$

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} = \mathbf{r} \times (-\mathrm{i}\nabla_\mathbf{r})$$

- We often work with the square magnitude of the angular momentum $\mathbf{L}^2 = \mathbf{L}_x^2 + \mathbf{L}_y^2 + \mathbf{L}_z^2$

  In spherical coordinates

$$\mathbf{L}^2 = -\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right) - \frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\varphi^2}$$

  We observe that this is independent of radial direction

Eigenfunctions of $\mathbf{L}^2$

We consider the eigenproblem

$$\mathbf{L}^2 Y(\theta, \varphi) = EY(\theta, \varphi)$$

We make the ansatz

$$Y(\theta, \varphi) = \Theta(\theta), \Phi(\varphi)$$

Substituting gives us

$$\left(-\frac{1}{\sin(\theta)} \frac{\partial}{\partial \theta} \left(\sin(\theta) \frac{\partial}{\partial \theta} \right) - \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial \varphi^2} \right) \Theta(\theta) \Phi(\varphi) = E\Theta(\theta)\Phi(\varphi)$$

Eigenfunctions of $\mathbf{L}^2$

Separating out the φ variable

$$-\frac{\partial^2 \Phi}{\partial \varphi^2} = m^2 \Phi$$

Where m^2 is an eigenvalue

This yields solutions of the form

$$\Phi(\varphi) = A e^{\mathrm{i} m \varphi} + B e^{-\mathrm{i} m \varphi}$$

We find that m must be an integer

Eigenfunctions of $\mathbf{L}^2$

Separating out the θ variable

$$-\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial\Theta}{\partial\theta}\right)+\frac{m^2}{\sin^2(\theta)}\Theta=k\Theta$$

Where k is an eigenvalue; we find that $k=l(l+1)$ for $l\in\mathbb{N}$

Applying the change of variables $\zeta=\cos(\theta)$, $\xi(\cos(\theta))=\Theta(\theta)$ yields

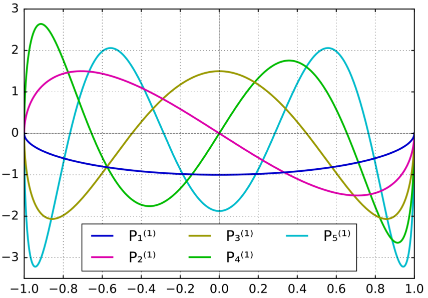
$$\frac{\mathrm{d}}{\mathrm{d}\zeta}\left[(1-\zeta^2)\frac{\mathrm{d}\xi}{\mathrm{d}\zeta}\right]+\left[k-\frac{m^2}{1-\zeta^2}\right]\xi=0$$

With $k=l(l+1)$, this is equivalent to the general Legendre equation

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x}P_l^m(x)\right]+\left[l(l+1)-\frac{m^2}{1-x^2}\right]P_l^m(x)=0$$

Eigenfunctions of $\mathbf{L}^2$

The solutions $P_l^m(x)$ to the general Legendre equation are called the associated Legendre polynomials



https://en.wikipedia.org/wiki/Associated_Legendre_polynomials#/media/File:Mplwp_legendreP15a1.svg

Therefore, our solutions to the eigenproblem in θ are of the form

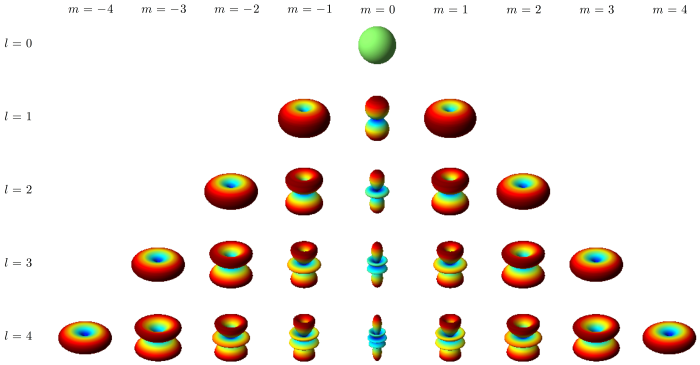
$$\Theta(\theta) = P_l^m(\cos(\theta))$$

Eigenfunctions of $\mathbf{L}^2$

All eigenfunctions $Y(\theta, \varphi)$ for $\mathbf{L}^2$ are therefore given by

$$Y_{lm}(\theta, \varphi) = C_{lm} P_l^m(\cos(\theta)) e^{im\varphi}$$

Where C_{lm} is a normalization factor



http://opticaltweezers.org/chapter-5-electromagnetic-theory/figure-5-2-spherical-harmonics/

The Hamiltonian in Real Space

Particle in One Dimension

$$\mathbf{H} = \underbrace{\frac{\mathbf{p}^2}{2}}_{\text{Kinetic energy}} + \overbrace{V(\mathbf{x})}^{\text{Potential field}}$$

Particle in Three Dimensions

$$\mathbf{H} = -\frac{1}{2}\Delta_{\mathbf{r}} + V(\mathbf{r})$$

Where $\Delta_{\mathbf{r}} = \partial_x^2 + \partial_y^2 + \partial_z^2$ *is the Laplacian*

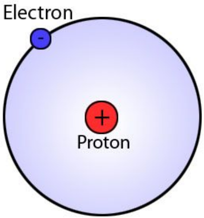
Representing the Hydrogen Atom

Time-Independent Shrödinger Equation

The stationary state of the time-independent Shrödinger equation can be found by solving the eigenproblem

$$\left(-\frac{1}{2}\Delta_{\mathbf{r}} + V(\mathbf{r})\right)\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

The hydrogen atom is the only element on the periodic table for which the Shrödinger equation has a closed-form solution



https://www.pinterest.com/pin/144678206755850918/

Representing the Hydrogen Atom

We consider the nucleus to be fixed at the origin, so that

$$V(\mathbf{r}) = -\frac{1}{r}$$

Where $r = |\mathbf{r}|$

Since representation in spherical coordinates is helpful, we express the Laplacian accordingly

$$\begin{aligned}\Delta_{\mathbf{r}} &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2(\theta)}\frac{\partial^2}{\partial\varphi^2} \\ &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{r^2}\mathbf{L}^2\end{aligned}$$

Representing the Hydrogen Atom

We make the ansatz

$$\psi(r,\theta,\varphi) = R(r)Y_{lm}(\theta,\varphi)$$

This allows us to separate out the radial component of the eigenproblem

$$-\frac{1}{2r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{l(l+1)}{2r^2}R(r) - \frac{1}{r}R(r) = ER(r)$$

Where $\tilde{V}(r) = \frac{l(l+1)}{2r^2} - \frac{1}{r}$

Applying the change of variables $u(r) = rR(r)$

$$-\frac{1}{2}\frac{\partial^2}{\partial r^2}u(r) + \tilde{V}(r)u(r) = Eu(r)$$

Representing the Hydrogen Atom

As $r \to \infty$, $\tilde{V}(r) \to 0$, so the equation looks like

$$-\frac{1}{2}\frac{\partial^2}{\partial r^2}u(r) = Eu(r)$$

If $E > 0$, we have $u(r) \sim c_1 e^{i\sqrt{2E_r}} + c_2 e^{i\sqrt{2E_r}}$, which is not square integrable

Therefore for $E < 0$, we can solve for the eigenvalues as

$$E_{kl} = -\frac{1}{2(k+l)^2}$$