PHY 571: Quantum Physics

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The Transition to Quantum Mechanics

Module 1, Lecture 6, 7 and 8

Postulates of Quantum Mechanics

- Describe waves/particles via the Wave function, $\psi(\mathbf{r},t)$
- Wave function evolves in time (Schrödinger) or the Operator evolves in time (Heisenberg): equivalent, but they appear to be very different (*several math tools*, *interacting with one physics; many to one relationship*, *discuss...*)
- Interpretation of the wave function (Born): Probability, P, of observing particle is proportional to $|\psi|^2$; normalized to $P = 1$
- Schrödinger equation (SE) is a (deterministic) operator equation; the order of the operations is important: it "operates" on the wave function. Basic is the time-dependent SE, but most useful (in materials/ nanoscience) is the time-independent SE.
- Download Transition to Quantum Mechanics document

The Schrödinger Equation(s)

- time-dependent write out: $i\hbar\partial/\partial t(\psi) = H(\psi)$
- time-independent: $H(\psi) = E(\psi)$
- What is H? This is the Hamiltonian, classical expression for the Energy = K(kinetic) + V(potential),
- In 1-dimension (1D), $K= -(\hbar^2/2m)\partial^2/\partial x^2$ and $V= V(x)$
- In 3D, $K = -(\hbar^2/2m)\nabla^2$ and $V = V(\mathbf{r})$; $\mathbf{r} = [x, y, z]$, rectangular or $[r, \theta, \phi]$, radial-angular coordinates
- ***Whoa!*** keep it simple to start with, 1D examples... Each of these topics rate whole chapters or books, etc

The transition to Quantum Mechanics

☺ We want to make the transition from particles $\mathbf{r}(t)$ and waves $\omega(\mathbf{k})$ to the wave function $\psi(\mathbf{r},t)$ which is either/or (or is it) both/and...

a) This function $\psi(\mathbf{r},t)$ can be associated with (a spread of) energies $E = \hbar\omega$ and momenta $\mathbf{p} = \hbar\mathbf{k}$

b) $\psi(x,t)$ satisfies: $i\hbar\partial/\partial t(\psi) = -(\hbar^2/2m)\partial^2\psi/\partial x^2 + V(x)\psi$: this is the time-dependent SE in 1D

c) Probability $P(\mathbf{r},t) = |\psi|^2 = \psi^*\psi$ (of finding particle at position $\mathbf{r}$ and time t)

☹ Final element is the role of Measurement which "collapses $\psi(\mathbf{r},t)$ onto an Eigenstate"... *not trivial, take your time to understand all this*

Do the various authors agree on pedagogy?

- Feynman lecture video: guess $\rightarrow$ prescription (model); prescription $\rightarrow$ consequences, comparison with expt.
- Griffiths book *states* b) and c) on p1-2; Gasiorowicz *argues towards* b) and c), but only for a free particle (chapter 2).
- So either way it is a guess, a jump, a *Quantum Leap*! (*Life looks different after you have taken the bait*): a fishy story, but now you see Classical Mechanics as the *incoherent* limit of Quantum Mechanics.
- In QM we add amplitudes and then take $\psi^*\psi$ to get (probabilistic) intensities; in CM we add intensities; understand the importance of phases (coherence)

Example: Real and Complex potentials

- Probability current and particle number conservation *leads to a general expression for the current* $\mathbf{j}(\mathbf{r})$ that works for free particles and when $V(\mathbf{r})$ is real
- If $V(\mathbf{r})$ is complex, particles can be absorbed (or created). Example: transmission of electrons through a thin film: *the simplest model of the Transmission Electron Microscope (TEM).*
- For a beam in free space $\psi(\mathbf{r},t) = \psi_0 \exp[i(\mathbf{k}.\mathbf{r}-\omega t)]$ and $\mathbf{j} = (\hbar\mathbf{k}/m)\psi_0^*\psi_0$. This for real $V(\mathbf{r})$, note vectors in 3D
- If there is an imaginary part of the potential $V_i(\mathbf{r})$, there is absorption, $\mathbf{k} \rightarrow \mathbf{k} + i\mathbf{q}$, and then (in 1D) the current $j(x)$ reduces with distance: $j = (\hbar k/m)\psi_0^*\psi_0 \exp(-2qx)$

Example: The Importance of Phases

- The 2-slit interference experiment: If ψ_1 and ψ_2 are coherent, we add amplitudes and then form intensities.
- Exercise: take $\psi_1 = A\exp(ik_1 y)$ and $\psi_2 = B\exp(ik_2 y)$, where A and B can be complex (i.e. can have phases ϕ_1 and ϕ_2 respectively).
- Work out the intensity $I = \psi^*\psi$, where $\psi = \psi_1 + \psi_2$, keeping proper track of all the complex numbers
- Express the answer in terms of trigonometric functions (cos, sin, etc) if it simplifies, and if it doesn't, find the conditions under which it does (e.g. $|A|=|B|$, $A=B$, or $A = B = 1$). *Note I is real...*
- *Keep your (right) answers at your bedside for future reference..*

Expectation values, Averages and Operators

- Probability P = $\psi^*\psi$: But how is this related to classical probability? In classical physics the order of operations doesn't matter, but in quantum physics it does...
- <f>(t) the Average = $\int f(x)P(x,t)dx$ in classical physics. In quantum physics the same quantity is the
- Expectation Value = $\int \psi^* f(x) \psi dx$; *note order*
- f(x) ***operates*** on ψ. Operators may ***not commute***
- Examples: the free particle SE, operators for **p**, x or **r** V(**r**) and E; Relationship to measurement and the Uncertainty Principle; Poisson brackets and Representations (x and **p**). ...***Whoa again!***

Operators for **p**, x or **r,** V(**r**) and E

- In the SE, the kinetic energy $K = -(\hbar^2/2m)\partial^2/\partial x^2\psi$; this is equivalent to $p^2/2m$ (low energy, non-relativistic)
- In operator language p^2 means the operator p acting twice (sequentially from the right); so we choose the operator $p = (\hbar/i)\partial/\partial x$ (or should it be $-1/i = i$?). In 3D, the momentum operator $\mathbf{p} = (\hbar/i)\nabla$. ($\nabla$ = "nabla", gradient, called grad, a vector operator)
- The operators x, **r** are simple multiplications, and also for V(x or **r**), *provided that there is no t-dependence*
- The Energy operator is the Hamiltonian H = K + V

Example: back to the Current operator, j(**r**)

- Probability current and particle number conservation *leads to* $\partial P/\partial t + \nabla.\mathbf{j}(\mathbf{r}) = 0$, that works for free particles and when $V(\mathbf{r})$ is real
- 1D result: $\mathbf{j}(\mathbf{x}) = (\hbar/2im)(\psi^* \partial/\partial x(\psi) - \psi\partial/\partial x(\psi^*))$.
  Exercise: *Write down the 3D result by analogy, and*
- Try this out on a beam in free space, where $\psi(\mathbf{r},t) = \psi_0\exp[i(\mathbf{k}.\mathbf{r}-\omega t)]$ and show that $\mathbf{j} = (\hbar\mathbf{k}/m)\psi_0^*\psi_0$. This for real $V(\mathbf{r})$, vectors in 3D; start with 1D: $\mathbf{r}\rightarrow x$, $\mathbf{k}\rightarrow k$
- If there is an imaginary part of the potential $V_i(\mathbf{r})$, there is absorption, $\mathbf{k} \rightarrow \mathbf{k} + i\mathbf{q}$, and then (in 1D) the current $j(x)$ reduces with distance: $j = (\hbar k/m)\psi_0^*\psi_0\exp(-2qx)$

Relationship of operators to H's UP

- If operators commute, can be measured simultaneously Example p and H. Check that [pH-Hp]ψ = 0
- If operators do not commute, *cannot be measured simultaneously*, the quantities obey H's UP. Example x and p_x. Check that $[xp_x - p_x x]\psi = (\hbar/i)\,\psi$
- [ ] is called a commutator, and is written [p,H] or $[x,p_x]$. The commutator $[x,p_x] = \hbar/i$ states Heisenberg's Uncertainty Principle precisely: an *Operator equation*.
- In classical physics [ ] is called a Poisson bracket. As $\hbar \to 0$ we get classical results. One way to start quantum mechanics. *Operator theorems*, true for any ψ

Representations: position and momentum

- Just as with vectors, operator theorems are independent of the coordinate system. However, to work out real problems, coordinates are usually needed.
- The equivalent in Quantum is the Representation. Some problems fit naturally into x- or **r**-representation $\psi(\mathbf{r},t)$, whereas others are easier to visualize in momentum (p_x or **p**)-representation, $\phi(\mathbf{p},t)$.
- For a beam in free space $\psi(\mathbf{r},t) = \psi_0 \exp[i(\mathbf{k}.\mathbf{r}-\omega t)]$ and $\mathbf{j} = (\hbar\mathbf{k}/m)\psi_0^*\psi_0$. This wave function is best considered in momentum representation $\phi(\mathbf{k}$ or $\mathbf{p}) = \delta(\mathbf{p}-\hbar\mathbf{k})$. Generally true for particle beams with $E > 0$; normalization current/ unit area.
- For bound states with $E < 0$, $\psi(\mathbf{r})$ is a localized function, and is preferred, But $\psi(\mathbf{r})$ and $\phi(\mathbf{k}$ or $\mathbf{p})$ are related as FT pairs...