Quantum Mechanics I

Quantum Dynamics

Quantization & Compositeness
Equations of Motion
Conservation Laws

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Pink Floyd: "Another Brick in the Wall (Pt. II)"

Quantum Dynamics

Quantization and Compositeness

- Frequent approach: "quantizing a classical model"
  - Ambiguous: classically $AB = BA$, quantum-ly $AB \neq BA$
  - Normal ordering: a pre-agreed ordering
    - Cannot remove all issues [LEB, p. 88, last 4 lines]
- On general grounds, quantum → classical
  - That is, classical = [$\hbar \to 0$]-special case of quantum
    - Subtle: details: Ch.14 & 15
  - Classical *should not* be able to "cover" all of quantum
  - Approach: build quantum physics from ground up
    - such that it recovers classical physics in the correct "limit"
    - N. Bohr's "correspondence principle"
    - Not sufficient: just as $f(x)$ is not determined from $f(0)$ alone
    - There exist "purely" quantum phenomena
    - Real space (of positions) *vs*. Hilbert space (of states)

Quantum Dynamics

Quantization and Compositeness

Must start *somewhere*
…might as well from classical

- Canonical quantization
  - Assign $A \to \mathsf{A} = \omega(A)$ according to any fixed ordering scheme
  - Compute the *anomaly*, $\Delta_{AB} := [\omega(A), \omega(B)] - \omega(\{A,B\}_{\mathrm{PB}})$
    - If A, B generate a gauge symmetry (e.g., EM), Δ_{AB} must vanish
    - If A, B generate a non-gauge symmetry, Δ_{AB} must be conserved
      - Useful in phase-transition: "anomaly matching conditions"
    - This assumes a classical formulation is known, for comparison
  - In general, classical observables $f(p,q)$ over phase space
    - But, $[\mathsf{Q}_\alpha, \mathsf{P}_\beta] = i\hbar\,\delta_{\alpha\beta}\mathbb{1} \Rightarrow \mathsf{Q}_\alpha$ and P_β cannot both be "just" variables
    - Some half of them must act as derivatives w.r.t. the other half
    - Choice of "polarization" ⇒ Geometric Quantization program
- Other quantization frameworks
  - …must work in all known / understood applications
  - …and work (better) where canonical quantization fails

Quantum Dynamics

Quantization and Compositeness

- Everything is composite
  - System = composite, comprised of sub-systems
  - Sub-systems are *separable* if one is describable w/o reference to the other
  - If the state-vector factorizes,

$$|\Psi\rangle = |\psi\rangle\,|\chi\rangle\,|\xi\rangle\ldots$$

  - …just like when separating coordinates.
  - Otherwise, they are *non-separable*

$$|\Psi\rangle = \sum_n c_n\,|\psi_n\rangle\,|\chi_n\rangle\,|\xi_n\rangle\ldots = c_1\,|\psi_1\rangle\,|\chi_1\rangle\,|\xi_1\rangle\ldots + c_2\,|\psi_2\rangle\,|\chi_2\rangle\,|\xi_2\rangle\ldots$$

    - …with no common factors; non-factorizable.
    - This, in fact, is the generic (non-special) case.
    - When the summand-factors refer to "individual" particles, this is oft-called "entanglement" [E. Schrödinger], which is a …misnomer.

Sub-systems *may* refer to particles, or to *qualites*

Quantum Dynamics

Quantization and Compositeness

- When a system is comprised of sub-systems that otherwise can be identified with "individual" particles
- We refer to the sub-systems as 1-particle systems
- …and to the composite as an *k*-particle system
- The *k*-particle states may be formed by tensor products

$$|\Psi(1,2)\rangle := \sum_n c_n |\psi_n^{(1)}\rangle \otimes |\psi_n^{(2)}\rangle \qquad \mathsf{A} := \mathsf{A}^{(1)} \otimes \mathsf{A}^{(2)}$$

  - such that

$$\mathsf{A}\,|\Psi(1,2)\rangle := \sum_n c_n \left(\mathsf{A}^{(1)}|\psi_n^{(1)}\rangle\right) \otimes \left(\mathsf{A}^{(2)}|\psi_n^{(2)}\rangle\right)$$

  - When the coefficients reduce to $c_n = \delta_{n,n'}$ for some fixed n', the *k*-particle state is factorizable, *i.e.*, separable.

- We often write $|\psi_1, \psi_2, \ldots\rangle := |\psi_1\rangle \otimes |\psi_2\rangle \otimes \ldots$

Quantum Dynamics

Equations of Motion

- Time-dependence

$$\frac{\mathrm{d}}{\mathrm{d}t}|\Psi\rangle := \lim_{\epsilon\to 0}\frac{|\Psi(t+\epsilon)\rangle - |\Psi(t)\rangle}{\epsilon} = \lim_{\epsilon\to 0}\frac{e^{-i\epsilon H/\hbar}|\Psi(t)\rangle - |\Psi(t)\rangle}{\epsilon}$$

$$= \lim_{\epsilon\to 0}\frac{[\mathbb{1} - i\epsilon H/\hbar + \ldots]\,|\Psi(t)\rangle - |\Psi(t)\rangle}{\epsilon} = \tfrac{1}{i\hbar}H\,|\Psi(t)\rangle$$

- Therefore, the Schrödinger equation

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\Psi(t)\rangle = H\,|\Psi(t)\rangle$$

- is a consequence of space-time geometry, mathematical consistency and the axioms of quantum mechanics.
- For any state operator

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho} = [H,\hat{\rho}]$$

Quantum Dynamics

Equations of Motion

- Physics deals with observables
- ...and their expectation values (comp. w/experiments)

$$\langle R\rangle(t) := \mathrm{Tr}[\hat{\rho}\, R] \;= \mathrm{Tr}\left[\,|\Psi(t)\rangle\,\langle\Psi(t)|\, R\right]$$

$$= \left(\langle\Psi(t_0)|U^\dagger(t,t_0)\right) R \left(U(t,t_0)|\Psi(t_0)\rangle\right) \quad U(t,t_0) := e^{i(t-t_0)H/\hbar}$$

$$= \langle\Psi(t_0)|\, \underbrace{U^\dagger(t,t_0) R\, U(t,t_0)}_{:= R_H(t)}\, |\Psi(t_0)\rangle$$

- Define the Heisenberg picture:

$$R_H(t) := U^\dagger(t,t_0) R\, U(t,t_0) \qquad |\Psi\rangle_H := |\Psi(t_0)\rangle$$

- Refer to the initial picture as the Schrödinger picture.

Quantum Dynamics

Equations of Motion

$$U(t,t_0) := e^{i(t-t_0)H/\hbar}$$

- In the Heisenberg picture:

$$R_H(t) := U^\dagger(t,t_0)\, R\, U(t,t_0) \qquad |\Psi\rangle_H := |\Psi(t_0)\rangle$$

- Then,

$$\frac{\mathrm{d}}{\mathrm{d}t} R_H(t) = \left(\frac{\partial U^\dagger}{\partial t}\right) R\, U + U^\dagger \left(\frac{\partial R}{\partial t}\right) U + U^\dagger R \left(\frac{\partial U}{\partial t}\right)$$

- where

$$\frac{\partial U}{\partial t} = \frac{\partial}{\partial t} e^{i(t-t_0)H/\hbar} = \frac{i}{\hbar} H\, e^{i(t-t_0)H/\hbar} = \frac{i}{\hbar} H\, U(t,t_0) \qquad \frac{\partial U^\dagger}{\partial t} = -\frac{i}{\hbar} U^\dagger(t,t_0)\, H^\dagger$$

- so

$$\frac{\mathrm{d}}{\mathrm{d}t} R_H(t) = \left(\frac{1}{i\hbar} U^\dagger H\right) R\, U + U^\dagger R \left(\frac{i}{\hbar} H\, U\right) + U^\dagger \left(\frac{\partial R}{\partial t}\right) U$$

$$\frac{\mathrm{d}}{\mathrm{d}t} R_H(t) = \frac{1}{i\hbar} U^\dagger [H,R] U + i\hbar U^\dagger \left(\frac{\partial R}{\partial t}\right) U$$

Heisenberg equation of motion

Quantum Dynamics

Equations of Motion

- Easy to show: $\langle R\rangle(t) = \langle\Psi(t)|R|\Psi(t)\rangle = \langle\Psi(t_0)|R_H|\Psi(t_0)\rangle$
- Then,

$$\frac{\mathrm{d}\langle R_S\rangle}{\mathrm{d}t} = \left\langle \frac{\mathrm{d}R_S}{\mathrm{d}t} \right\rangle = \mathrm{Tr}\left[\widehat{\rho}_S(t)\,\frac{\partial R_S}{\partial t} - \frac{1}{i\hbar}\widehat{\rho}_S(t)\,[H, R_S]\right] \qquad \text{Schrödinger picture}$$

$$= \mathrm{Tr}\left[\widehat{\rho}_H(t_0)\left(\frac{\partial R}{\partial t}\right)_H - \frac{1}{i\hbar}\widehat{\rho}_H(t_0)\,[H, R_H]\right] \qquad \text{Heisenberg picture}$$

- where, in general

$$A_H := U^\dagger(t, t_0) A_S U(t, t_0)$$

- Caution:

$$\left(\frac{\partial R}{\partial t}\right)_H = U^\dagger(t, t_0)\left(\frac{\partial R_S}{\partial t}\right)U(t, t_0) \neq \left(\frac{\partial R_H}{\partial t}\right)$$

- Toggle freely between the two pictures
  - equation by equation; not in the middle of an equation!

Quantum Dynamics

Conservation laws

- For *any* observable and *any* transformation

$$R \to R' = U(s) R U^\dagger(s) = U(s) R U^{-1}(s)$$

$$R' = R \quad \Rightarrow \quad U(s) R U^{-1}(s) = R \quad \Rightarrow \quad U(s) R = R U(s)$$

$$[U(s), R] = 0$$
$$\Updownarrow$$

- Since

$$U(s) = e^{isK} \quad \Rightarrow \quad [K, R] = 0$$

- In particular, when $R = H$
  - (the Hamiltonian is invariant w.r.t. a transformation)

$$[H, U(s)] = 0 \quad \Leftrightarrow \quad [H, K] = 0$$

$$\frac{\mathrm{d}\langle K\rangle}{\mathrm{d}t} = \left\langle \frac{\mathrm{d}K}{\mathrm{d}t} \right\rangle = \mathrm{Tr}\left[\widehat{\rho}(t)\,\frac{\partial K}{\partial t} - \frac{1}{i\hbar}\widehat{\rho}(t)\,[H, K]\right]$$

$$\frac{\mathrm{d}\langle f(K)\rangle}{\mathrm{d}t} = \left\langle \frac{\mathrm{d}f(K)}{\mathrm{d}t} \right\rangle = \mathrm{Tr}\left[\widehat{\rho}(t)\,\frac{\partial K}{\partial t} f'(K) - \frac{1}{i\hbar}\widehat{\rho}(t)\,[H, f(K)]\right]$$

$$\frac{\partial K}{\partial t} = 0 = [H, K]$$
$$\Rightarrow \quad \frac{\mathrm{d}\langle K\rangle}{\mathrm{d}t} = 0$$

Quantum Dynamics

Conservation laws

- So, *if* the generator of a transformation
  - (a) does not explicitly depend on time
  - (b) commutes with the total Hamiltonian
  - ***then*** it represents a conserved quantity

Constant of motion

Symmetry*	Implemented by	Generator, K	Conserved Quantity
Time-translation	$e^{+i\tau H/\hbar}$	H	Total energy
Space-translation	$e^{-ia\cdot P/\hbar}$	P_α	Linear momentum
Space-rotation	$e^{-i\theta\cdot J/\hbar}$	J_α	Angular momentum

* A transformation generated by K is a symmetry if $\frac{\partial K}{\partial t} = 0 = [H, K]$

- 1. $[H,H] \equiv 0$; E-conservation then needs only $\frac{\partial H}{\partial t} = 0$
- 2. Exceptionally, cancellation in Tr[…] $\frac{d\langle f(K)\rangle}{dt} = \mathrm{Tr}\left[\hat{\rho}(t)\,\frac{\partial K}{\partial t}\,f'(K) - \frac{1}{i\hbar}\hat{\rho}(t)\,[H, f(K)]\right]$

I'LL BE BACK

Quantum Dynamics

Conservation laws

- Stationary states (when $\partial_t H = 0$)

$$H\,|\Psi(t)\rangle = E_n\,|\Psi(t)\rangle \quad \Rightarrow \quad i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\,|\Psi(t)\rangle = E_n\,|\Psi(t)\rangle$$

$$\Rightarrow \quad |\Psi(t)\rangle = e^{-iE_n t/\hbar}\,|E_n\rangle$$

stationary state

$$H\,|E_n\rangle = E_n\,|E_n\rangle$$

H-eigenstate

- Then

$$\langle R\rangle(t) = \langle E_n|e^{+itE_n/\hbar}\,R\,e^{-itE_n/\hbar}|E_n\rangle = \langle E_n|R|E_n\rangle$$

$$\frac{\mathrm{d}\langle R\rangle_{\text{stat.}}}{\mathrm{d}t} = \frac{\mathrm{d}\langle E_n|R|E_n\rangle}{\mathrm{d}t} = 0$$

Stationary state expectation values of all observables are constant in time

$$R\,e^{-itE_n/\hbar}\,|E_n\rangle = e^{-itE_n/\hbar}R\,|E_n\rangle \qquad \text{even if } R = f(\tfrac{\mathrm{d}}{\mathrm{d}t})$$

$$f(\tfrac{\mathrm{d}}{\mathrm{d}t})\Big(e^{-iE_n t/\hbar}\,|E_n\rangle\Big) = f(\tfrac{E_n}{i\hbar})\Big(e^{-iE_n t/\hbar}\,|E_n\rangle\Big) = \Big(e^{-iE_n t/\hbar}f(\tfrac{1}{i\hbar}H)\,|E_n\rangle\Big)$$

- Finally,

$$\frac{\partial f(H)}{\partial t} = \frac{\partial H}{\partial t}f'(H) = 0 \quad \text{since } \frac{\partial H}{\partial t} = 0$$

Quantum Dynamics

Miscellanea

- Signs: $e^{-i\mathbf{a}\cdot\mathbf{P}}\Psi(\mathbf{r},t) := \langle\mathbf{r}|e^{-i\mathbf{a}\cdot\mathbf{P}}|\Psi(t)\rangle$

$$e^{-i\theta\cdot(\mathbf{L}+\mathbf{S})}\Psi(\mathbf{r},t) := \langle\mathbf{r}|e^{-i\theta\cdot(\mathbf{L}+\mathbf{S})}|\Psi(t)\rangle$$

- but

$$e^{+i\tau H}\Psi(\mathbf{r},t) := \langle\mathbf{r}|e^{+i\tau H}|\Psi(t)\rangle$$

- Recall the possible "exceptional" cancellation:

$$0 = \mathrm{Tr}\left[\widehat{\rho}(t)\left(\frac{\partial K}{\partial t}f'(K) - \frac{1}{i\hbar}[H, f(K)]\right)\right]$$

projection(s) — needs to cancel only within the projection(s) — state-dependent

- As this ***may*** be true, the "quantum conservation theorem"

$$\frac{\mathrm{d}\langle K\rangle}{\mathrm{d}t} = 0 \quad \Leftarrow \!\!\!\!\!\not\Rightarrow \quad \frac{\partial K}{\partial t} = 0 = [H, K]$$

state-dependent

Not "if and only if"

(as is E. Noether's, in classical physics)

Quantum Mechanics I

Now, go forth and calculate!!

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