Quantum Mechanics I

Kinematics vs. Dynamics

Transformations
Symmetries
Application

Tristan Hübsch

Department of Physics and Astronomy, Howard University, Washington DC

http://physics1.howard.edu/~thubsch/

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

QMI

Kinematics vs. Dynamics

Transformations

- Disclaimer: focus on pure states $\hat{\boldsymbol{\rho}} = |\psi\rangle\langle\psi|$
  - extend results to mixed states using that for all mixed states

$$\hat{\boldsymbol{\rho}} = \sum_n \rho_n\,|\rho_n\rangle\langle\rho_n| \qquad \hat{\boldsymbol{\rho}}\,|\rho_n\rangle = \rho_n\,|\rho_n\rangle \quad 0 \leqslant \rho_n \leqslant 1,\ \sum_n \rho_n = 1$$

$$= \sum_n \varrho_n\,|n\rangle\langle n| \qquad \forall\,|n\rangle \in \mathscr{D}_{\hat{\boldsymbol{\rho}}},\ \langle n'|n\rangle = \delta_{n',n},\ \sum_n |n\rangle\langle n| = \mathbb{1}$$

$$0 \leqslant \varrho_n \leqslant 1,\ \sum_n \varrho_n = 1$$

- Among other things,

$$|\chi\rangle = \mathsf{A}\,|\psi\rangle \qquad \Rightarrow \quad |\chi\rangle\langle\chi| = \mathsf{A}\,|\psi\rangle\langle\psi|\,\mathsf{A}^\dagger$$

in fact, all operators, in general

$$\hat{\boldsymbol{\rho}}\,' = \mathsf{A}\,\hat{\boldsymbol{\rho}}\,\mathsf{A}^\dagger$$ for all states, pure and mixed

- Also,

$$\langle \mathsf{R}\rangle_{\hat{\boldsymbol{\rho}}} = \mathrm{Tr}[\hat{\boldsymbol{\rho}}\,\mathsf{R}] = \mathrm{Tr}[\sum_n \varrho_n\,|n\rangle\langle n|\,\mathsf{R}] = \sum_n \varrho_n\,\mathrm{Tr}[|n\rangle\langle n|\,\mathsf{R}]$$

$$= \sum_n \varrho_n\,\mathrm{Tr}[\langle n|\,\mathsf{R}\,|n\rangle] = \sum_n \varrho_n \langle n|\mathsf{R}|n\rangle \quad = \langle\psi|\mathsf{R}|\psi\rangle \text{ if } \varrho_n = \delta_{n,\psi}$$

QMI

Kinematics vs. Dynamics

Transformations

- Laws of nature—& observables—are coordinate-independent
  - up to proper coordinate transformations (such as rotation, $F_x \to \mathbf{R}\cdot F_x$)
- Thus, $A\,|\phi_n\rangle = a_n\,|\phi_n\rangle \quad \Rightarrow \quad A'\,|\phi'_n\rangle = a_n\,|\phi'_n\rangle$

$$|\psi\rangle = \sum_n c_n\,|\phi_n\rangle \quad \Rightarrow \quad |\psi'\rangle = \sum_n c'_n\,|\phi'_n\rangle$$

$$|c_n|^2 = |c'_n|^2 \qquad \textit{i.e.,} \qquad \big|\langle\phi_n|\psi\rangle\big|^2 = \big|\langle\phi'_n|\psi'\rangle\big|^2$$

- BTW: Classical probabilistic physics (stat. mech.) may be phrased in terms of probabilities.

conservation of probability

- Quantum mechanics is phrased in terms of (complex!) probability *amplitudes*
- Probability = | probability amplitude | ^{2}
  - the (overall) phase of the probability amplitude is not observable
  - relative phases induce interference—QM hallmark

Kinematics vs. Dynamics

Symmetries

- Theorem [Wigner]:
- Any mapping of a vector space (of pure states) onto itself
  - preserving amplitudes of probability may be implemented by a U
  - which is either unitary (& linear) or antiunitary (and antilinear).
- Unitary (& linear): $UU^{\dagger} = U^{\dagger}U = \mathbf{1}$

$$\langle\phi'|\psi'\rangle = \big(\langle\phi|\,U^{\dagger}\big)\big(U|\psi\rangle\big) = \langle\phi|\,\underbrace{U^{\dagger}U}_{=\mathbb{1}}|\psi\rangle \quad = \langle\phi|\psi\rangle$$

Unitary:
$UAU^{\dagger} = UAU^{-1}$
(similarity tr.)

- Antiunitary (& antilinear): $A\,c\,|\psi\rangle = c^{*}A\,|\psi\rangle$

$$\langle\phi'|\psi'\rangle = \big\langle\phi A^{\dagger}\big|A\psi\big\rangle = \langle\phi|\psi\rangle^{*}$$

- $\mathbf{1}$ is unitary.
- Continuous transformations “tunable” to $\mathbf{1}$ must be unitary
- Discrete transformations can be either of the two.

QMI

Kinematics vs. Dynamics

Symmetries

- For all unitary transformations
- operators transform as $A \to A' = UAU^{\dagger} = UAU^{-1}$
- Physical transformations *concatenate*
- For a $U(s)$ such that $U(0)=\mathbf{1}$ and $U(s_1)U(s_2)=U(s_1+s_2)$,
- In general, [Unitary operator] = $e^{\,i\,[\text{Hermitian operator}]}$
  Hermitian operator: *generator*
- Non-relativistic space-time symmetries
  - (1) Time translation: $t \to t' = t + t_0$
  - (3) Space translation: $\boldsymbol{r} \to \boldsymbol{r}' = \boldsymbol{r} + \boldsymbol{r}_0$
  - (3) Space rotation: $\boldsymbol{r} \to \boldsymbol{r}' = R(\boldsymbol{r}) = \boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{r}) + (\boldsymbol{n}\times\boldsymbol{r})\sin\theta + [\boldsymbol{r}-\boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{r})]\cos\theta$
  - (3) Constant-velocity boosts: $\boldsymbol{v} \to \boldsymbol{v}' = \boldsymbol{v} + \boldsymbol{v}_0$
  - These 10 transformations comprise the Galilean group
  - Notice: $\text{boost}(\boldsymbol{r}) = \boldsymbol{r} + \boldsymbol{v}_0 t$, but $\text{boost}(t) = t$

Kinematics vs. Dynamics

Symmetries

- Generators:
  - time-translation: H
  - space-translation: P_α
  - space-rotation: J_α
  - velocity boost: G_α not very familiar…
- In general: $e^{i\varepsilon A} e^{i\varepsilon B} e^{-i\varepsilon A} e^{-i\varepsilon B} = 1 + \varepsilon^2[A,B] + \ldots$
- Using only geometry and the Jacobi identities* (essentially, meaning and consistency)

(a)	$[P_\alpha, P_\beta] = 0$	(f)	$[G_\alpha, P_\beta] = i\delta_{\alpha\beta}\hbar M \mathbb{1}$
(b)	$[G_\alpha, G_\beta] = 0$	(g)	$[P_\alpha, H] = 0$
(c)	$[J_\alpha, J_\beta] = i\varepsilon_{\alpha\beta\gamma}\hbar J_\gamma$	(h)	$[J_\alpha, H] = 0$
(d)	$[J_\alpha, P_\beta] = i\varepsilon_{\alpha\beta\gamma}\hbar P_\gamma$	(i)	$[G_\alpha, H] = i\hbar P_\alpha \mathbb{1}$
(e)	$[J_\alpha, G_\beta] = i\varepsilon_{\alpha\beta\gamma}\hbar G_\gamma$		

* $[A,[B,C]] + [B,[C,A]] + [C,[A,B]] = 0$

Q M I

Kinematics vs. Dynamics

Identifications, i.e. Application

- Galilean symmetries

Space-Time Transformation	**Unitary Operator**	**Generator**
Rotation about the α-axis		(angular momentum)
$\boldsymbol{r} \to R_\alpha(\theta)\cdot\boldsymbol{r}$	$\exp\{-i\theta J_\alpha/\hbar\}$	J_α
Translation along the α-axis		(linear momentum)
$x_\alpha \to x_\alpha + a$	$\exp\{-iaP_\alpha/\hbar\}$	P_α
Velocity boost along the α-axis		(Galilean boost)
$x_\alpha \to x_\alpha + v_0 t$	$\exp\{iv_0 G_\alpha/\hbar\}$	G_α
Time-translation		(Hamiltonian)
$t \to t + t_0$	$\exp\{it_0 H/\hbar\}$	H

Kinematics vs. Dynamics

Identifications, i.e. Application

- We need a way to assess position. Define Q_α as the Hermitian (Cartesian coordinate) position operator
- Then, $Q_\alpha\,|\boldsymbol{r}\rangle = x_\alpha\,|\boldsymbol{r}\rangle \qquad [Q_\alpha, Q_\beta] = 0 \qquad -\infty \leqslant x_\alpha \leqslant +\infty$
- From the geometric meaning of P_α, and J_α, it follows that

$$Q'_\alpha = e^{-i\boldsymbol{a}\cdot\boldsymbol{P}/\hbar}\,Q_\alpha\,e^{+i\boldsymbol{a}\cdot\boldsymbol{P}/\hbar} \stackrel{!}{=} Q_\alpha - a_\alpha\,\mathbb{1}$$

space translations translate Q_α

$$[Q_\alpha, P_\beta] = i\hbar\delta_{\alpha\beta}\,\mathbb{1}$$

CCR

$$Q'_\alpha = e^{-i\boldsymbol{\theta}\cdot\boldsymbol{J}/\hbar}\,Q_\alpha\,e^{+i\boldsymbol{\theta}\cdot\boldsymbol{J}/\hbar} \stackrel{!}{=} Q_\alpha + \varepsilon_\alpha{}^{\beta\gamma}\,\theta_\beta Q_\gamma\,\mathbb{1} \qquad [J_\alpha, Q_\beta] = i\hbar\varepsilon_{\alpha\beta}{}^{\gamma}Q_\gamma\,\mathbb{1}$$

space rotations… rotate Q_α

$$Q'_\alpha = e^{-i\boldsymbol{v}\cdot\boldsymbol{G}(t)/\hbar}\,Q_\alpha\,e^{+i\boldsymbol{v}\cdot\boldsymbol{G}(t)/\hbar} \stackrel{!}{=} Q_\alpha - v_\alpha t\,\mathbb{1} \qquad G_\alpha(t) = M\,Q_\alpha - tP_\alpha$$

velocity boosts… t-dependently translate Q_α …for a free particle

Try exercise 3.7. Then check Ballentine's solution on p. 621–622

Kinematics vs. Dynamics

Identifications, i.e. Application

- Finally, define V_α such that $\langle V_\alpha \rangle := \frac{\mathrm{d}}{\mathrm{d}t}\langle Q_\alpha \rangle = \frac{\mathrm{d}}{\mathrm{d}t}\langle \Psi | Q_\alpha | \Psi \rangle$
- Calculate:

measuring position is time-independent

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \Psi | Q_\alpha | \Psi \rangle = \left(\frac{\mathrm{d}}{\mathrm{d}t}\langle \Psi |\right) Q_\alpha |\Psi\rangle + \langle \Psi | \left(\frac{\mathrm{d}}{\mathrm{d}t} Q_\alpha\right) |\Psi\rangle + \langle \Psi | Q_\alpha \left(\frac{\mathrm{d}}{\mathrm{d}t}|\Psi\rangle\right)$$

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

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

$$\langle \Psi | V_\alpha | \Psi \rangle = \left(-\tfrac{1}{i\hbar}\langle \Psi(t)| H^{\dagger}\right) Q_\alpha |\Psi(t)\rangle + \langle \Psi(t)| Q_\alpha \left(\tfrac{1}{i\hbar} H |\Psi(t)\rangle\right)$$

$$= \tfrac{i}{\hbar}\langle \Psi(t)|\,[H, Q_\alpha]\,|\Psi(t)\rangle$$

$$V_\alpha := \tfrac{i}{\hbar}[H, Q_\alpha]$$

general definition

- Verify:

$$V'_\alpha = e^{iv\cdot G/\hbar}\, V_\alpha\, e^{-iv\cdot G/\hbar} = V_\alpha - v_\alpha \mathbb{1}$$

Kinematics vs. Dynamics

Identifications, i.e. Application

- Verify that $L_\alpha := i\hbar\,\varepsilon_\alpha{}^{\beta\gamma}\,Q_\beta P_\gamma$ satisfies $[L_\alpha, L_\beta] = i\hbar\,\varepsilon_{\alpha\beta}{}^{\gamma}\,L_\gamma$
- So define $J_\alpha := L_\alpha + S_\alpha$, where $[L_\alpha, S_\beta] = 0$ and $[S_\alpha, S_\beta] = i\hbar\,\varepsilon_{\alpha\beta}{}^{\gamma}\,S_\gamma$
- Now, define the (space) coordinate representation:

$$\Psi(\boldsymbol{r},t) := \langle \boldsymbol{r}|\Psi(t)\rangle \qquad R\Psi(\boldsymbol{r},t) := \langle \boldsymbol{r}|R|\Psi(t)\rangle$$

state-*function* (over space)

- Then

$$e^{-i\theta\cdot J}\Psi(\boldsymbol{r},t) = \left\langle \boldsymbol{r}\middle|e^{-i\theta\cdot J}\middle|\Psi(t)\right\rangle = \left\langle \boldsymbol{r}\middle|e^{-i\theta\cdot(L+S)}\middle|\Psi(t)\right\rangle$$

- Thus: L_α is "positional," while S_α is "directional."
  - Historically: L_α is "orbital," while S_α is "spin."
- On the other hand, $i\hbar\,P_\alpha = [G_\alpha, H] = [MQ_\alpha - t\,P_\alpha, H]$
- fits $H = \frac{1}{2M}\left|\vec{P} + \vec{A}(Q)\right|^2 + W(Q)$

most general non-relativistic Hamiltonian

Potential ⇒ no t-dependent transl.

Quantum Mechanics I

Now, go forth and calculate!!

Hübsch

Department of … University, Washington DC

http://physics1.howar…