Quantum Mechanics II

Quantum → Classical Physics

The “Classical Limit”; Ehrenfest’s Theorem; The Phase→Hamilton-Jacobi Theorem

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Quantum→Classical Physics

The "Classical Limit"

- Often dubbed the "$\hbar \to 0$" limit
- Strictly, "1.055×10^{-34} J·s $\to 0$" is as *meaningless* as "$1 \to 0$"
- A typical classical event:
  - A piece of chalk (0.01 kg) thrown against the blackboard (2 m away)
  - flies ~$\frac{1}{10}$ s so, $v \sim (2 \div \frac{1}{10} = 20)$ m/s so, $KE \sim \frac{1}{2}(0.01)(20)^2 = 2$ J
  - so, Hamilton's action $= \int \mathrm{d}t\,(KE - PE) \sim (\frac{1}{10})(2) = 0.2$ J·s

    vs. $\hbar = 1.055 \times 10^{-34}$ J·s
  - A pirouetting ballerina (60 kg), spinning at 1 Hz, *i.e.*, $\omega = 2\pi \cdot 1\ \mathrm{s}^{-1}$
  - $KE_{rot} \sim \frac{1}{2}\big(\frac{1}{2}(60)(0.20)^2\big)(2\pi)^2 = 23.69$ J, Hamilton's action ~ (1)(23.69) J·s

    (axially rotating cylinder)

    vs. $\hbar = 1.055 \times 10^{-34}$ J·s
- Instead, test whether $(\hbar/S_i) \ll 1$, for all S_i **commensurate** with $\hbar$
  - If true, classical; if false (for even one S_i), quantum.

key ratios!!!

Note: This has little to do with size, or "amounts" of position, momentum, energy, time… *per se* !!!

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Ehrenfest's Theorem

- The claim: **Expectation values of quantum operators obey classical dynamical equations**
- Expectation values are state-dependent
  - represent average trajectories, energies, momenta, …
  - need not represent any particular trajectory, energy, momentum, …
  - just like there exists no particular USA family with 2.3 children
- A (quantum) state thus ⇄ an ensemble of classical states
- Classical equation of motion:

$$\frac{\mathrm{d}R}{\mathrm{d}t} = \frac{\partial R}{\partial t} + \{\, H \,,\, R \,\}_{\mathrm{PB}} \qquad = \frac{\partial R}{\partial t} + \Big(\frac{\partial H}{\partial q^i}\frac{\partial R}{\partial p_i} - \frac{\partial R}{\partial q^i}\frac{\partial H}{\partial p_i}\Big)$$

$$\frac{\mathrm{d}\langle\widehat{R}\rangle}{\mathrm{d}t} = \frac{\partial\langle\widehat{R}\rangle}{\partial t} + \{\langle\widehat{H}\rangle, \langle\widehat{R}\rangle\}_{\mathrm{PB}} = \frac{\partial\langle\widehat{R}\rangle}{\partial t} + \Big(\frac{\partial\langle\widehat{H}\rangle}{\partial q^i}\frac{\partial\langle\widehat{R}\rangle}{\partial p_i} - \frac{\partial\langle\widehat{R}\rangle}{\partial q^i}\frac{\partial\langle\widehat{H}\rangle}{\partial p_i}\Big)$$

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Ehrenfest's Theorem

- Simple example: $\widehat{H} = \frac{\widehat{P}^2}{2M} + W(\widehat{Q}) \qquad \frac{\partial \widehat{P}}{\partial t} = 0 = \frac{\partial \widehat{Q}}{\partial t}$
- Calculate:

$$\frac{\mathrm{d}\widehat{Q}}{\mathrm{d}t} = \frac{i}{\hbar}[\widehat{H}, \widehat{Q}] = \frac{\widehat{P}}{M}$$

$$\frac{\mathrm{d}\widehat{P}}{\mathrm{d}t} = \frac{i}{\hbar}[\widehat{H}, \widehat{P}] = -W'(\widehat{Q})$$

- These are the (quantum, Heisenberg) equations of motion
- Compute the expectation values of these:

$$\frac{\mathrm{d}\langle\widehat{Q}\rangle}{\mathrm{d}t} = \frac{\langle\widehat{P}\rangle}{M} \qquad \frac{\mathrm{d}\langle\widehat{Q}\rangle}{\mathrm{d}t} = -\langle W'(\widehat{Q})\rangle \stackrel{?}{=} -W'(\langle\widehat{Q}\rangle)$$

as claimed

must be verified

- In systems w/o EM interaction, the proof reduces to proving

$$\langle W'(\widehat{Q})\rangle \stackrel{?}{=} W'(\langle\widehat{Q}\rangle)$$

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Ehrenfest's Theorem

$$\frac{\mathrm{d}R}{\mathrm{d}t} = \frac{\partial R}{\partial t} + \{\, H, R \,\}_{\text{PB}}$$

How?

- In general, $$\frac{\mathrm{d}\widehat{R}}{\mathrm{d}t} = \frac{\partial \widehat{R}}{\partial t} + \tfrac{i}{\hbar}[\,\widehat{H}, \widehat{R}\,]$$
- Expand:

$$\widehat{H} = \langle \widehat{H} \rangle + \widehat{\mathscr{H}} \qquad \widehat{R} = \langle \widehat{R} \rangle + \widehat{\mathscr{R}} \qquad \tfrac{i}{\hbar}[\widehat{H}, \widehat{R}] = F(\widehat{Q}, \widehat{P}, \widehat{R}, \dots)$$

$$F(\widehat{Q}, \widehat{P}, \widehat{R}, \dots) = F\Big((\langle \widehat{Q} \rangle + \widehat{\mathscr{Q}}), (\langle \widehat{P} \rangle + \widehat{\mathscr{P}}), (\langle \widehat{R} \rangle + \widehat{\mathscr{R}}), \dots \Big)$$

$\widehat{Q}$–$\widehat{P}$–$\widehat{R}$–… coupling! *…a complex issue!*

$$= F(\langle \widehat{Q} \rangle, \langle \widehat{P} \rangle, \langle \widehat{R} \rangle, \dots) + \Big[\frac{\partial F}{\partial \langle \widehat{R} \rangle}\Big]_0 \widehat{\mathscr{R}} + \Big[\tfrac{1}{2}\frac{\partial F}{\partial \langle \widehat{R} \rangle}\Big]_0 \widehat{\mathscr{R}}^2 + \dots$$

$$+ \text{ terms coupling with } \widehat{\mathscr{Q}}, \widehat{\mathscr{P}}, \dots$$

"quite often"

$$\stackrel{?}{=} \{\, \langle \widehat{H} \rangle, \langle \widehat{R} \rangle \,\}_{\text{PB}} + \dots$$

- It is possible (albeit tedious) to pursue this
  - "Background" expansion: vevs = classical background

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Ehrenfest's Theorem

$$\frac{dR}{dt} = \frac{\partial R}{\partial t} + \{H, R\}_{PB}$$

How?

- In general, $\frac{d\hat{R}}{dt} = \frac{\partial\hat{R}}{\partial t} + \frac{i}{\hbar}[\hat{H}, \hat{R}]$
- Expand:

$$\hat{H} = \langle\hat{H}\rangle + \hat{\mathscr{H}} \qquad \hat{R} = \langle\hat{R}\rangle + \hat{\mathscr{R}} \qquad \tfrac{i}{\hbar}[\hat{H},\hat{R}] = F(\hat{Q},\hat{P},\hat{R},\dots)$$

$$F(\hat{Q},\hat{P},\hat{R},\dots) = F\Big((\langle\hat{Q}\rangle+\hat{\mathscr{Q}}),(\langle\hat{P}\rangle+\hat{\mathscr{P}}),(\langle\hat{R}\rangle+\hat{\mathscr{R}}),\dots\Big)$$

$\hat{Q}$–$\hat{P}$–$\hat{R}$–… coupling! *…a complex issue!*

$$= F(\langle\hat{Q}\rangle,\langle\hat{P}\rangle,\langle\hat{R}\rangle,\dots) + \Big[\frac{\partial F}{\partial\langle\hat{R}\rangle}\Big]_0 \hat{\mathscr{R}} + \Big[\frac{1}{2}\frac{\partial F}{\partial\langle\hat{R}\rangle}\Big]_0 \hat{\mathscr{R}}^2 + \dots$$

$$+ \text{ terms coupling with } \hat{\mathscr{Q}}, \hat{\mathscr{P}}, \dots$$

"quite often"

$$\stackrel{?}{=} \{\langle\hat{H}\rangle, \langle\hat{R}\rangle\}_{PB} + \dots$$

- It is possible (albeit tedious) to pursue this
  - "Background" expansion: vevs = classical background
  - about which quantum observables fluctuate

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Ehrenfest's Theorem

$$\frac{\mathrm{d}R}{\mathrm{d}t} = \frac{\partial R}{\partial t} + \{\, H\,,\, R\,\}_{\mathrm{PB}}$$

- In general, $\frac{\mathrm{d}\hat{R}}{\mathrm{d}t} = \frac{\partial \hat{R}}{\partial t} + \frac{i}{\hbar}[\,\hat{H}\,,\,\hat{R}\,]$ → How?
- Expand:

$$\hat{H} = \langle \hat{H} \rangle + \widehat{\mathscr{H}} \qquad \hat{R} = \langle \hat{R} \rangle + \widehat{\mathscr{R}} \qquad \tfrac{i}{\hbar}[\hat{H},\hat{R}] = F(\hat{Q},\hat{P},\hat{R},\ldots)$$

$$F(\hat{Q},\hat{P},\hat{R},\ldots) = F\Big((\langle\hat{Q}\rangle+\widehat{\mathscr{Q}}),(\langle\hat{P}\rangle+\widehat{\mathscr{P}}),(\langle\hat{R}\rangle+\widehat{\mathscr{R}}),\ldots\Big)$$

$\hat{Q}$–$\hat{P}$–$\hat{R}$–… coupling! *…a complex issue!*

$$= F(\langle\hat{Q}\rangle,\langle\hat{P}\rangle,\langle\hat{R}\rangle,\ldots) + \Big[\frac{\partial F}{\partial\langle\hat{R}\rangle}\Big]_0 \widehat{\mathscr{R}} + \Big[\frac{1}{2}\frac{\partial F}{\partial\langle\hat{R}\rangle}\Big]_0 \widehat{\mathscr{R}}^2 + \ldots$$

$+$ terms coupling with $\widehat{\mathscr{Q}}$, $\widehat{\mathscr{P}}$, …

"quite often"

$$\stackrel{?}{=} \{\,\langle\hat{H}\rangle\,,\,\langle\hat{R}\rangle\,\}_{\mathrm{PB}} + \ldots$$

- It is possible (albeit tedious) to pursue this
  - "Background" expansion: vevs = classical background
  - about which quantum observables fluctuate
  - …aiming to reproduce the classical equations to 0^{th} order *+ a nonlinearly coupled system of quantum fluctuations…*

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Anomalies

$$\frac{\mathrm{d}R}{\mathrm{d}t} = \frac{\partial R}{\partial t} + \{\, H\,,\, R\,\}_{\text{PB}}$$

- Actually, the issue
  - the correspondence

$$\frac{\mathrm{d}\hat{R}}{\mathrm{d}t} = \frac{\partial \hat{R}}{\partial t} + \tfrac{i}{\hbar}[\,\hat{H}\,,\,\hat{R}\,]$$

commutator ↔ Poisson bracket

- …turns out to be very important!
- In classical physics, observables will satisfy some Poisson-bracket algebra: $\{A_i\,,\,A_j\}_{\text{PB}} = f_{ij}{}^{k}\,A_k$ (as do rotations)
- The corresponding quantum operators need not do so.
- Denote the (“quantization”) assignment as $A_i \mapsto \hat{A}_i := \pi(A_i)$
- Then compute: $\triangle_{ij} := \pi\Big(\{\,A_i\,,\,A_j\,\}_{\text{PB}}\Big) - \tfrac{i}{\hbar}[\,\pi(A_i)\,,\,\pi(A_j)]$
- If nonzero, then the quantization assignment $\pi(\ldots)$ does not preserve the classical relationship between observables A_i.
- This could range from irrelevant (“ignorable” A_i’s 🙈🙉🙊)
- to disastrous: gauge symmetry (EM charge conservation 😱🆘)

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Ehrenfest's Theorem

- In the "typical" cases, where $\langle F(\hat{Q})\rangle = F(\langle\hat{Q}\rangle) + \ldots$ negligible
  - …so Ehrenfest's theorem holds for position/momentum equations,
  - …Ehrenfest's theorem is not guaranteed to hold for all observables
- Also, Ehrenfest's theorem is ***insufficient*** guarantee:
  - ***Some*** systems satisfy Ehrenfest's theorem, even though they are manifestly non-classical

$$\langle W'(\hat{Q})\rangle \stackrel{\checkmark}{=} W'(\langle\hat{Q}\rangle)$$

for LHO although its energy levels are ***quantized***

- Also, Ehrenfest's theorem is ***not necessary*** a guarantee:
  - ***Some*** systems behave classically although they do not satisfy Ehrenfest's theorem
  - A particle in a box (impenetrable walls) oscillates with $k_n = n\pi/L$, energy $E_n = n^2\hbar^2\pi^2/2mL^2$, frequency $\omega_n = E_n/\hbar = n^2\hbar\pi^2/2mL^2$ and period $T_n = 2\pi/\omega_n = (4mL^2/\hbar\pi)/n^2$ — which is ***nothing*** like $T_{cl} = 2L/v$?!

    Yet, the average distribution of both cl. and q. particles are constant & flat…

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Bohr's Complementarity Principle

- Note: orbital angular momentum ~ $\ell \cdot \hbar \lll$ macroscopic value
- Bohr: in the limit $n \to \infty$, quantum should resemble classical
  - WKB:

$$\psi^{(\pm)}_{\text{WKB}}(x) = \frac{C_\pm}{\sqrt{k(x)}}\, e^{\pm i \int \mathrm{d}\xi\, k(\xi)} \qquad \overline{\left|\psi^{(\text{st.w.})}_{\text{WKB}}(x)\right|^2} = \frac{|C_\pm|^2}{k(x)}\,\frac{1}{2}$$

  - The classical probability density is proportional to the time the particle spends within Δx, i.e., $\Delta t/\Delta x = 1/v = 1/(\hbar k/M) \propto 1/k$ ☑
  - H-atom:

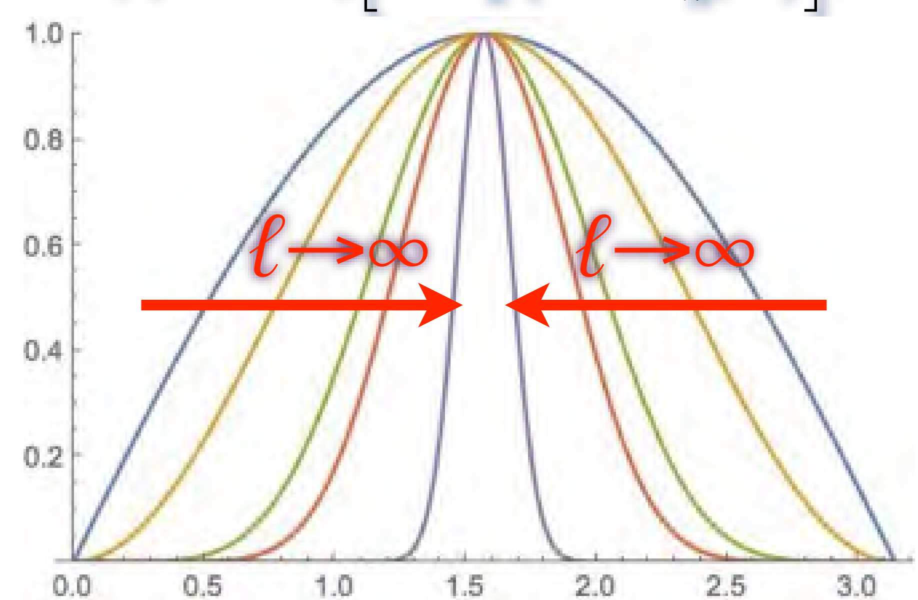
$$\langle r^2\rangle - \langle r\rangle^2 \xrightarrow{\ell \to n-1} \left(\frac{a_0}{2}\right)^2 n^2(1+2n)$$

$$\frac{\langle r^2\rangle - \langle r\rangle^2}{\langle r^2\rangle} \xrightarrow{\ell \to n-1} \frac{1}{2}\,\frac{1}{1+n} \xrightarrow{n\to\infty} 0$$

$$\langle r^2\rangle = n^4 a_0^2\left[1 + \tfrac{3}{2}\left(1 - \tfrac{\ell(\ell+1)-\frac{1}{3}}{n^2}\right)\right],$$

$$\langle r\rangle = n^2 a_0\left[1 + \tfrac{1}{2}\left(1 - \tfrac{\ell(\ell+1)}{n^2}\right)\right],$$

  - Angular dependence: $\left|Y^\ell_\ell(\theta,\phi)\right|^2 \propto \sin^{2\ell}(\theta)$
  - peaks @ $\theta = \pi/2$ → equatorial orbits



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The Phase→Hamilton-Jacobi Theorem

- Inspired by the WKB approximation, consider

$$\Psi(\vec{r},t) = A(\vec{r},t)\, e^{iS(\vec{r},t)/\hbar}$$

  - for which the Schrödinger equation produces

$$-\frac{\partial S}{\partial t} = \frac{(\vec{\nabla} S)^2}{2M} + W - \frac{\hbar^2}{2M}\frac{\vec{\nabla}^2 A}{A}$$

$$\frac{\partial A}{\partial t} = -\frac{1}{2M}\big[\vec{\nabla}\cdot(A\vec{\nabla}S) + (\vec{\nabla}A)\cdot(\vec{\nabla}S)\big]$$

$$W_Q := -\frac{\hbar^2}{2M}\frac{\vec{\nabla}^2 A}{A}$$

Does **NOT** always vanish for $\hbar \to 0$

- Defining $P := A^2$, this becomes:

$$0 = \frac{\partial S}{\partial t} + \frac{(\vec{\nabla} S)^2}{2M} + (W + W_Q)$$

Hamilton-Jacobi equation, with $W \to W + W_Q$

$$0 = \frac{\partial P}{\partial t} + \frac{1}{M}\vec{\nabla}\cdot(P\vec{\nabla}S) \qquad \vec{J} := (P\vec{\nabla}S)/M$$

probability density continuity equation

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Now, go forth and calculate!!

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