Quantum Mechanics II

Classical → Quantum Physics

Quantum Mechanics over Phase-Space; Feynman-Hibbs Path-Integrals; Quantization and Anomalies

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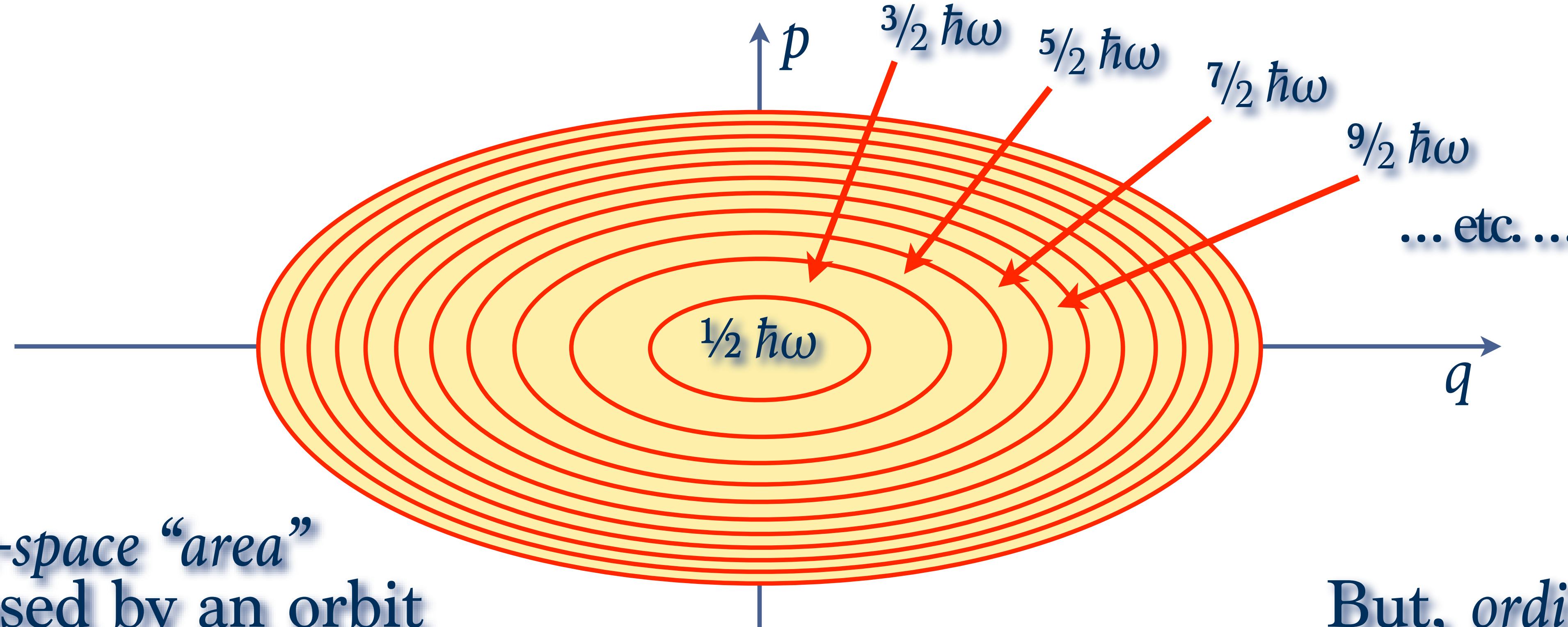
Quantum Mechanics over Phase-Space

- Recall:
  - Heisenberg's indeterminacy relations: $\Delta_{x^i}\Delta_{p_i} > \tfrac{1}{2}\hbar,\ i = x, y, z\ldots$
  - Classical mechanics is defined over phase-space (x^i, p_j)
- Heisenberg relations make phase-space "granular"
  - …albeit *not* as a chess-board with a fixed tiling
  - E.g. the linear harmonic oscillator



Phase-space "area" enclosed by an orbit is an integral multiple of $\hbar$.

But, *ordinary space* remains just as continuous.

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Quantum Mechanics over Phase-Space

- Classical mechanics is defined over phase-space (q^i, p_j)
- All observables are real functions, $F(q^i, p_j)$, over phase-space
- Dynamics is governed by the equations of motion

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

- …which "converts" to the Heisenberg equations of motion

$$\frac{\mathrm{d}\widehat{F}}{\mathrm{d}t} = \frac{\partial \widehat{F}}{\partial t} + \tfrac{1}{i\hbar}[\widehat{H}, \widehat{F}]$$

- But what of the state operator?
- There is no analogous dynamical object in classical physics.
- Also, quantum mechanics results in (amplitudes of) probabilities, not actual orbits, trajectories, positions…

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Quantum Mechanics over Phase-Space

- To reproduce quantum mechanics from classical mechanics on the phase space, we must introduce probability distributions.
- Such a distribution, $\rho_Q(q,p)$, must satisfy

$$\int \mathrm{d}p\, \rho_Q(q,p) = \langle q|\widehat{\rho}|q\rangle \qquad \int \mathrm{d}q\, \rho_Q(q,p) = \langle p|\widehat{\rho}|p\rangle$$

- …as well as

$$\rho^*(q,p) = \rho(q,p) \qquad \int \mathrm{d}q \int \mathrm{d}p\, \rho_Q(q,p) = 1 \qquad \rho(q,p) \geqslant 0$$

- Turns out:
  - For any desired quantum state operator, there are infinitely many functions $\rho_Q(q,p)$ that satisfy the above equations
  - But, there is no uniformly specified choice for all state operators
  - There is no universal "quantization" assignment $\widehat{\rho} \overset{1-1}{\longleftrightarrow} \rho_Q(q,p)$

Two Proof-of-Concept Distributions

Kodi Husimi

Eugene Wigner

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The Wigner Representation

- Consider the function over phase space [Wigner, 1932]

$$\rho_W(q,p) := \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \mathrm{d}y\; e^{ipy/\hbar}\,\langle q-\tfrac{1}{2}y|\hat{\rho}|q+\tfrac{1}{2}y\rangle$$

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \mathrm{d}k\; e^{iqk/\hbar}\,\langle p-\tfrac{1}{2}k|\hat{\rho}|p+\tfrac{1}{2}k\rangle$$

Reverse-engineered! Constructs a classical distribution from a given quantum state operator.

- Then:

$$\int \mathrm{d}p\;\rho_W(q,p) = \overset{1}{\frac{1}{2\pi\hbar}}\int_{-\infty}^{\infty} \mathrm{d}y\;\underbrace{\int \mathrm{d}p\; e^{ipy/\hbar}}_{2\pi\hbar\,\delta(y)}\,\langle q-\tfrac{1}{2}\overset{0}{y}|\hat{\rho}|q+\tfrac{1}{2}\overset{0}{y}\rangle = \langle q|\hat{\rho}|q\rangle$$

- Easy:

$$\iint \mathrm{d}q\,\mathrm{d}p\;\rho_W(q,p) = \int \mathrm{d}q\langle q|\hat{\rho}|q\rangle = \mathrm{Tr}[\,\hat{\rho}\,] = 1$$

$$\hat{\rho}^\dagger = \hat{\rho} \quad\Leftrightarrow\quad \rho^*_W(q,p) = \rho_W(q,p)$$

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The Wigner Representation

- However, for two states to be orthogonal

$$0 \stackrel{!}{=} \mathrm{Tr}[\hat{\rho}_1\,\hat{\rho}_2] \;=\; \iint \mathrm{d}q\,\mathrm{d}p\;\rho_{1\mathrm{W}}(q,p)\,\rho_{2\mathrm{W}}(q,p)$$

$$\mathrm{Tr}[\,\hat{\rho}^2\,] \leqslant 1$$

- Assuming that $0 \le \rho_{\mathrm{W}}(q,p) \le 1$ (appropriate for probabilities)
  - it must be that ρ_1 and ρ_2 have no overlap.
  - Then, N orthogonal states $\Rightarrow$ each $\neq 0$ only over $1/N$ of phase-space
  - When $N \to \infty$ (as typical), the ρ's would have to be δ-function-like
- But, phase-space is granular: distributions cannot be pinpointed better than size-$2\pi\hbar$ "areas" in the phase-space

$$\rho_{i\mathrm{W}}(q,p) = \left\{\begin{array}{ll} 0 & (q,p) \notin A \\ A^{-1} & (q,p) \in A \end{array}\right\} \qquad \iint \mathrm{d}q\,\mathrm{d}p\;\rho_{i\mathrm{W}}(q,p) = 1$$

$$\langle\mathscr{O}\rangle := \iint \mathrm{d}q\,\mathrm{d}p\;\rho_{1\mathrm{W}}\,\mathscr{O}(q,p) \;\to 2\pi\hbar \iint \mathrm{d}q\,\mathrm{d}p\;\rho_{1\mathrm{W}}^2 = \frac{2\pi\hbar}{A} \leqslant 1 \qquad \boxed{A \geqslant 2\pi\hbar}$$

- So, the only way out is to permit $\rho_{\mathrm{W}}(q,p)$ to be negative
  - …and so fail as a probability distribution.

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The Wigner Representation

- Nevertheless…

$$\psi(q) = \langle q|\psi\rangle = \frac{1}{\sqrt{\sqrt{2\pi}a}} e^{-q^2/4a^2} \qquad \widehat{\rho} = |\psi\rangle\langle\psi|$$

$$\rho_W(q,p) = \frac{1}{\pi\hbar} e^{-q^2/(2\triangle_q{}^2)} e^{-p^2/(2\triangle_p{}^2)} \qquad \triangle_q = a \quad \triangle_p = \hbar/2a$$

- …turns out non-negative. *(Only true for the Gaussian!)*
- Time dependence:

$$\frac{\mathrm{d}\widehat{\rho}}{\mathrm{d}t} = \frac{i}{\hbar}\left[\widehat{H},\widehat{\rho}\right] = \frac{i}{2M\hbar}\left[\widehat{P}^2,\widehat{\rho}\right] + \frac{i}{\hbar}\left[\widehat{W},\widehat{\rho}\right]$$

  - Calculate the 1st term in momentum rep., 2nd in coordinate rep.,
  - …then transform into the Wigner representation

$$\frac{\partial\rho_W}{\partial t} = \frac{p}{M}\frac{\partial\rho_W}{\partial q} + \sum_{n=\text{odd}} \frac{1}{q!}\left(-\tfrac{1}{2}i\hbar\right)^{n-1} \frac{\mathrm{d}^n W}{\mathrm{d}q^n}\frac{\partial^n\rho_W}{\partial p^n}$$

  - For the LHO, all ($n \geq 2$)-order derivatives of $W(q)$ vanish
  - …the equation = classical Liouville equation. *(Only true for the LHO!)*

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The Husimi Representation

- Main problem: no simultaneous eigenstates $|\,q,p\rangle$
- K. Husimi: use the next-best-thing, such that

$$\langle x|q,p\rangle = \frac{1}{\sqrt{\sqrt{2\pi}\,\sigma}}\, e^{-\left(\frac{(x-q)}{2\sigma}\right)^2 + ipx/\hbar}$$

  - Gaussian "lump," centered at (q, p) in the phase-space
  - with the complementary half-widths $\Delta_q = \sigma$ and $\Delta_p = \hbar/(2\sigma)$
  - These functions are not orthogonal (all overlaps ≥ 0)
  - …and are over-complete: $\int \mathrm{d}q\,\mathrm{d}p\,|\,q,p\rangle\,\langle q,p\,|\, = 2\pi\hbar$

but…

- Define then

$$\rho_H(q,p) := \frac{1}{2\pi\hbar}\langle q,p|\hat{\rho}|q,p\rangle$$

- This equals to a Gaussian smoothing of $\rho_W(q,p)$
  - Is a true probability density function
  - w/fuzziness controlled by σ, and complementary for q and p

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Feynman-Hibbs Path-Integrals *(Section 4.8)*

- A "triviality":

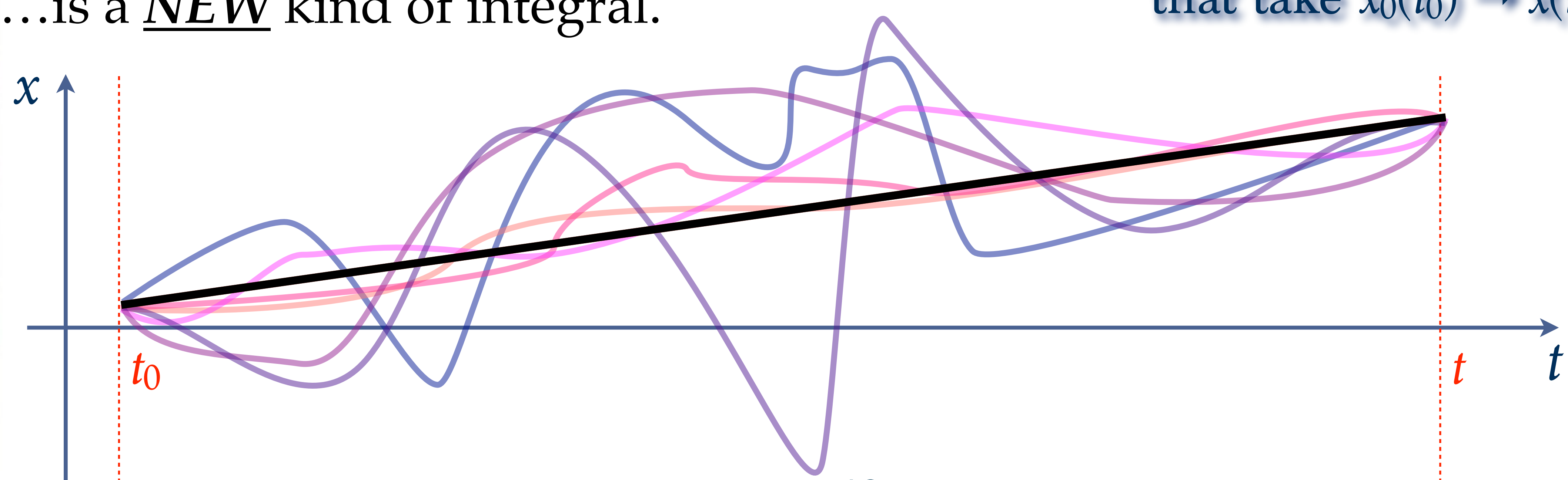
$$\begin{aligned}\Psi(x,t) &:= \langle x|\Psi(t)\rangle = \hat{U}(t,t_0)\langle x|\Psi(t_0)\rangle \quad := \langle x|\hat{U}(t,t_0)|\Psi(t_0)\rangle\\ &= \langle x|\hat{U}(t,t_0)\,\mathbb{1}|\Psi(t_0)\rangle \quad = \int_{x'} \mathrm{d}x'\,\langle x|\hat{U}(t,t_0)|x'\rangle\langle x'|\Psi(t_0)\rangle\\ &= \int_{x'} \mathrm{d}x'\,G(x,t;x',t_0)\Psi(x',t_0)\end{aligned}$$

- …except,

$$= \int \mathrm{D}[x'(t)]\,G(x,t;x',t_0)\Psi(x',t_0)$$

a sum over all possible (unrestricted) paths $x(t)$ that take $x_0(t_0) \to x(t)$.

- …is a ***NEW*** kind of integral.



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Feynman-Hibbs Path-Integrals (Section 4.8)

- The "propagator" $G(x,t;x_0,t_0)$
  - concatenates: $G(x,t;x_0,t_0) = G(x,t;x_1,t_1)\cdot G(x_1,t_1;x_0,t_0)$
    $= G(x,t;x_2,t_2)\cdot G(x_2,t_2;x_1,t_1)\cdot G(x_1,t_1;x_0,t_0)$
    $= \dots$ *etc.*
  - Subdividing until each time-interval $[t_i, t_{i+1}]$ is infinitesimal,

$$G(x_{j+1},t_{j+1};x_j,t_j) \approx \langle x_{j+1}|e^{-i\triangle_j t[\frac{\widehat{P}^2}{2M}+W]/\hbar}|x_j\rangle \qquad \triangle_j t := (t_{j+1}-t_j)$$

$$\approx \langle x_{j+1}|e^{-i\triangle_j t\widehat{P}^2/(2M\hbar)}|x_j\rangle\, e^{-i\triangle_j tW(x_j)/\hbar}$$

$$= \int \mathrm{d}p\ \langle x_{j+1}|e^{-i\triangle_j t\widehat{P}^2/(2M\hbar)}|p\rangle\langle p|x_j\rangle\, e^{-i\triangle_j tW(x_j)/\hbar}$$

$$= e^{-i\triangle_j tW(x_j)/\hbar}\int \mathrm{d}p\ \langle x_{j+1}|p\rangle\langle p|x_j\rangle\, e^{-i\triangle_j tp^2/(2M\hbar)}$$

$$= e^{-i\triangle_j tW(x_j)/\hbar}\,\frac{1}{2\pi\hbar}\int \mathrm{d}p\ e^{ip(x_{j+1}-x_j)}\, e^{-i\triangle_j tp^2/(2M\hbar)}$$

$$= e^{-i\triangle_j tW(x_j)/\hbar}\sqrt{\frac{M}{2i\pi\hbar\triangle_j t}}\ \exp\left\{i\frac{M(x_{j+1}-x_j)^2}{2\hbar\triangle_j t}\right\}$$

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Feynman-Hibbs Path-Integrals

$$= e^{-i\triangle_j t W(x_j)/\hbar} \sqrt{\frac{M}{2i\pi\hbar\triangle_j t}} \exp\left\{ i\frac{M(x_{j+1}-x_j)^2}{2\hbar\triangle_j t} \right\}$$

- So,

$$G(x,t;x_0,t_0) = \lim_{N\to\infty} \int\cdots\int \mathrm{d}x_1\cdots\mathrm{d}x_N \prod_{j=0}^{N} G(x_{j+1},t_{j+1};x_j,t_j)$$

$$= \lim_{N\to\infty} \int \prod_{k=0}^{N} \mathrm{d}x_k \left(\frac{M}{2i\pi\hbar\triangle_k t}\right)^{\frac{N+1}{2}} e^{\frac{i}{\hbar}\sum_{j=0}^{N}\triangle_j t\left\{\frac{M}{2}\left[\frac{x_{j+1}-x_j}{\triangle_j t}\right]^2 - W(x_j)\right\}}$$

- For infinitesimal subdivisions

$$i\frac{M(x_{j+1}-x_j)^2}{2\hbar\triangle_j t} = \frac{i}{\hbar}\triangle_j t\left[\frac{x_{j+1}-x_j}{\triangle_j t}\right]^2 \quad \to \frac{i}{\hbar}\,\mathrm{d}t\left[\frac{\mathrm{d}x}{\mathrm{d}t}\right]^2$$

$$= \int \mathrm{D}[x(t)]\, e^{iS[x(t)]/\hbar} \qquad S[x(t)] := \int \mathrm{d}t\,\left[\frac{m}{2}\dot{x}^2 - W(x)\right]$$

- The classical path minimizes $S[x(t)]$ by definition
  - …and is the dominant single contribution in the integral
  - …nearby paths are sub-dominant, but there is ***many*** of them
  - …even wildly non-classical paths contribute!

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Quantization and Anomalies

Extra!

- In general, "quantization" is a prescription of assigning a quantum theory to a classical one.
- Not unique at all [Pauli, 1930's]:

$$\mathscr{P}\mathscr{Q}^2 \mapsto \widehat{P}\widehat{Q}^2 \quad \text{or} \quad \big[\widehat{Q}\widehat{P}\widehat{Q} = \widehat{P}\widehat{Q}^2 + i\hbar\widehat{Q}\big] \quad \text{or} \quad \big[\widehat{Q}^2\widehat{P} = \widehat{P}\widehat{Q}^2 + 2i\hbar\widehat{Q}\big]$$

- Denote by "π" the chosen prescription:

$$\widehat{P} = \pi(\mathscr{P}), \quad \widehat{Q} = \pi(\mathscr{Q}), \quad \widehat{F} = \pi(\mathscr{F}(\mathscr{Q},\mathscr{P}))$$

- But, classical observables are not independent.
- So, compute:

$$\tfrac{i}{\hbar}\big[\,\pi(\mathscr{A})\,,\,\pi(\mathscr{B})\,\big] \;-\pi\Big(\{\,\mathscr{A}\,,\,\mathscr{B}\,\}_{PB}\Big) \;= \text{anomaly}(\widehat{A},\widehat{B})$$

  - for all Poisson brackets/commutators in a theory
  - and redefine the prescription π until all anomalies cancel—if possible
  - ***especially*** for the cases representing symmetries and conservation laws!

Quantum Mechanics II

Now, go forth and calculate!!

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