1 Telegraphic Intro to QM

These are ad hoc notes used for the Sept. 11 & 18 RIT lectures at UMD, somewhat tidied-up and extended for context and orientation. Tristan Hübsch, thubsch@howard.edu.

1900: Planck's resolution of (what Ehrenfest would in 1911 call the "ultraviolet catastrophe"): Sources (so-called "black-bodies") emit electromagnetic radiation in 2π-integral multiples of (Planck's) constant, $\hbar$, of energy (E) over time (t): $\boxed{\int \mathrm{d}t\; E_\gamma = n(2\pi\hbar),\ n\in\mathbb{N}}$. Note: $\hbar \sim 10^{-34}\,(\frac{\mathrm{kg\,m^2}}{\mathrm{s}} = \mathrm{J\,s})$

1905: Einstein's solution of the photoelectric effect: electromagnetic radiation is absorbed (by charged particles) at energies that are integral multiples of $\hbar\omega$, where $\omega = 2\pi\nu =$ "circular frequency" (=angular velocity) of the radiation: $\boxed{\big(E = n\hbar\omega\big)_\gamma \stackrel{!}{=} \big(KE = \frac{1}{2}m_e v^2\big)_e}$. The linear momentum imparted on the charged particle that absorbed the radiation then must be $\boxed{\big(p{=}E/c{=}\hbar\omega/c{=}2\pi\hbar/\lambda\big)_\gamma \stackrel{!}{=} \big(p{=}m_e v\big)_e}$. Left-hand side is the special case of the general relation $E^2 = p^2c^2 + m^2c^4 \xrightarrow{m_\gamma\to 0} E = pc$.

1913: Bohr's solution to the stability of atoms: the angular momentum of the (*stably*, *non-radiating*) orbiting electron (in his postdoc employer, Ernest Rutherford's, "planetary model of the atom"):[1] $\boxed{\ell = n\hbar}$. (Added bonus: The orbiting electrons have discrete energies, $E_n = -E_0/n^2$, so the hydrogen atom emits radiation from discrete ($n \to n'$) transitions, recovering Balmer's formula "on the nose.")

1924: In his PhD thesis, de Broglie proposed that all forms of matter (radiation included) have both particle-like and wave-like characteristics, so $\boxed{\lambda_{\rm dB} := 2\pi\hbar/p}$, i.e., $\boxed{p = 2\pi\,\hbar/\lambda_{\rm dB}}$ is universal.

The above make statements about *properties* (energy, linear momentum) of the *material things*, not about the *things themselves* — representable by this newfangled "wave." (Start with Ref. [1], perhaps.)

1.1 Waving

This "material wave," $\psi(x,t)$, was *fashioned* with intuition developed from past experience with fluid dynamics and electromagnetism: Maxwell's 1965 unification of electrodynamics laws predicted electromagnetic waves, detected by Herz (1988), where *intensity* ($\propto |\vec{E}|^2, |\vec{B}|^2$) definitely *is* measurable.

$|\psi(x,t)|^2$ is measurable: For a *free* particle, $|\psi(x,t)|^2$ must be x- and t-translationally invariant.

▶ $t = t_0$: $\psi(x+\xi,t_0) \stackrel{!}{=} e^{i\xi\, f(x)}\psi(x,t_0)$.

$$\psi(x+\xi,t_0) = \psi(x+\xi,t_0) = \psi(x,t_0) + \xi\,\psi'(x,t_0) + \tfrac{1}{2}\xi^2\,\psi''(x,t_0) + \dots \tag{1.1}$$
$$e^{i\xi f(x)}\psi(x,t_0) = \big[1 + i\xi f(x) - \tfrac{1}{2}\xi^2 f^2(x) + \dots\big]\psi(x,t_0) \tag{1.2}$$

Comparing order-by-order in ξ:

$$\xi^1: \quad \psi'(x,t_0) \stackrel{!}{=} if(x)\,\psi(x,t_0), \qquad \psi''(x,t_0) \stackrel{!}{=} if'(x)\,\psi(x,t_0) + if(x)\,\psi'(x,t_0); \tag{1.3}$$
$$\xi^2: \quad \psi''(x,t_0) \stackrel{!}{=} -f^2(x)\,\psi(x,t_0). \tag{1.4}$$

$$\Big(\psi''(x,t_0) = -f^2(x)\,\psi(x,t_0)\Big) \stackrel{!}{=} if'(x)\psi(x,t_0) + if(x)\,\Big(\psi'(x,t_0) = if(x)\psi(x,t_0)\Big), \tag{1.5}$$
$$\stackrel{!}{=} \Big(if'(x) - f^2(x)\Big)\psi(x,t_0) \tag{1.6}$$

That is, $f'(x) = \pm k = const.$ (1st sign choice.)

[1] Per https://en.wikipedia.org/wiki/Bohr_model, this is the result of combining a 4th and 5th postulate! Whew.

▶ $x = x_0$: $\psi(x_0, t+\tau) \stackrel{!}{=} e^{i\tau\, g(t)}\psi(x_0, t)$ implies $g(t) = \pm\omega = const.$ (2nd sign choice $\rightsquigarrow$ **relative choice!**)

▶ *Combining:* $\boxed{\psi(x,t) = \psi_0\, e^{i(\pm kx\, -\omega t)}}$ — "plane wave," the simplest kind of wave.
$\psi_0\, e^{i(kx-\omega t)}$ moves to the right ($\Delta x > 0$) as $\Delta t > 0$, $\psi_0\, e^{-i(kx+\omega t)}$ moves to the left ($\Delta x < 0$) as $\Delta t > 0$. In higher dimensions, $kx \to \vec{k}\cdot\vec{r}$, which is a *scalar* product, and invariant with respect to the full orthogonal symmetries of positional- and momentum-space; the sign of $\pm\vec{k}\cdot\vec{r}$ *picks* one of two linearly independent solutions. In fact, the combinations $(\pm\vec{k}\cdot\vec{r} - \omega t)$ are invariant with respect to the larger, Lorentz group of orthogonal transformations in spacetime, $(\vec{r}, t)$, and its dual (wave-vector)-frequency space, $(\vec{k}, \omega)$. Both wave-functions correspond to the same action and Lagrangian. However, incoming and outgoing solutions can correspond to absorption and emission, which need not be symmetric.

—·◆·—

Fixing the signs: using some classical (= pre-quantum) physics, and connecting to it!

▶ *3.39 centuries ago:* $\boxed{F = ma = m\ddot{x}}$ [**Newton, 1686**].
Multiply by $\dot{x}$ and integrate, $t \in [t_a, t_b]$:
Then, $\int_{t_a}^{t_b} \mathrm{d}t\, (F\dot{x} = F\frac{\mathrm{d}x}{\mathrm{d}t}) = \boxed{\int_a^b \mathrm{d}x\, F = W_{a\to b}}$ = work done by the force F over distance $x \in [a, b]$.
By Newton, this equals to $\int_{t_a}^{t_b} \mathrm{d}t\, \big[m\ddot{x}\dot{x} = \frac{\mathrm{d}}{\mathrm{d}t}\big(\frac{1}{2}m\dot{x}^2\big)\big] = \int_{?_a}^{?_b} \mathrm{d}\big(\frac{1}{2}m\dot{x}^2\big)$: define: $\boxed{KE := \frac{1}{2}m\dot{x}^2}$.

So, $W_{a\to b} = KE_b - KE_a$: "work-energy threorem"

For (working *against*) "conservative forces," $\boxed{F = -\frac{\mathrm{d}V}{\mathrm{d}x}}$, so $W_{a\to b} = -(V_b - V_a) = KE_b - KE_a$.

So, total energy, $\boxed{E = KE + V}$, is conserved. ($V = PE$)

▶ *2 centuries ago:* Hamilton (after incremental and meandering development): Find a functional, $\boxed{S[x(t)] := \int \mathrm{d}t\, L\big(x(t), \dot{x}(t), t; \dots\big)}$ such that $\boxed{\big(\delta S[x(t)] = 0\big) \;\Rightarrow\; \big(F = m\ddot{x}\big)}$,
where $\delta x(t)$ is a *variation* of the (*choice* of the) *function* $x(t)$: $x(t) \to x(t) + \delta x(t)$.

$$\delta S[x(t)] = \delta\int_{t_i}^{t_f} \mathrm{d}t\; L = \int_{t_i}^{t_f} \mathrm{d}t\; \Big[\frac{\partial L}{\partial x}\,\delta x + \frac{\partial L}{\partial \dot{x}}\Big(\delta\dot{x} = \delta\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\delta x\Big)\Big] = \int_{t_i}^{t_f} \mathrm{d}t\; \Big[\frac{\partial L}{\partial x}\,\delta x + \frac{\partial L}{\partial \dot{x}}\,\frac{\mathrm{d}}{\mathrm{d}t}\delta x\Big], \tag{1.7}$$

$$= \int_{t_i}^{t_f} \mathrm{d}t\; \Big[\frac{\partial L}{\partial x}\,\delta x - \Big(\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}}\Big)\delta x\Big] + \Big[\Big(\frac{\partial L}{\partial \dot{x}}\,\delta x\Big)_{t_i}^{t_f} = 0: \quad \delta x(t_i) = 0 = \delta x(t_f)\Big] \tag{1.8}$$

$$= \int_{t_i}^{t_f} \mathrm{d}t\; \Big[\frac{\partial L}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}}\Big]\delta x \stackrel{!}{=} 0, \qquad \Rightarrow \qquad \boxed{\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}} \stackrel{!}{=} \frac{\partial L}{\partial x}}. \tag{1.9}$$

Now, *construct* such an "L" from KE and PE: write $L = \alpha\, KE + \beta\, PE$, so

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}} = \alpha\frac{\mathrm{d}}{\mathrm{d}t}\Big[\frac{\partial KE}{\partial \dot{x}} = \frac{\partial}{\partial \dot{x}}\Big(\tfrac{1}{2}m\dot{x}^2\Big) = m\dot{x} =: p\Big] = \alpha\, m\ddot{x}, \tag{1.10}$$

$$\frac{\partial L}{\partial x} = \beta\frac{\partial PE}{\partial x} = \beta\frac{\partial V}{\partial x} = -\beta F. \tag{1.11}$$

$$\alpha\, m\, \ddot{x} = -\beta\, F, \qquad \Rightarrow \qquad \beta = -\alpha, \qquad \boxed{L = KE - PE}. \tag{1.12}$$

Importantly (writing $PE = V(x)$, as usual):

$$\boxed{\big(L := \tfrac{1}{2}m\dot{x}^2 - V(x)\big) \;\neq\; \big(E := \tfrac{1}{2}m\dot{x}^2 + V(x)\big)}, \qquad u[L] = u[E] = \frac{\mathrm{kg\,m^2}}{\mathrm{s^2}}\;!! \tag{1.13}$$

$$\boxed{S[x(t)] := \int \mathrm{d}t\; L(x, \dot{x}, t; \dots)}, \qquad u[S] = \frac{\mathrm{kg\,m^2}}{\mathrm{s}}\;!! \tag{1.14}$$

The Lagrangian function, $L(x,\dot{x};\dots)$, *does* have the units of energy, but differs crucially from *total energy*, $E = KE + PE$, by being *not* the sum but the *difference*, $L = KE - PE$. In turn, Hamilton's "action (functional)" (a.k.a. "Hamilton's principal function"), $S[x(t);\dots]$ is not even an energy of any sort (even Fields- and Abel-laureates' speaking and writing to the contrary) — wrong units, and it is the *time-integral* of the *Lagrangian function* — *not* of the total energy. *Of course,* $[L]_{V=0} = [E]_{V=0}$ — but even so only non-relativistically! In ideal gasses, $iS[x(t)]/\hbar \rightsquigarrow i(E/\hbar)t \rightsquigarrow E/(k_B T)$, where T is the temperature (ensemble-average of the kinetic energy) and k_B the Boltzmann conversion constant: a possible source of the kerfuffle. BTW, $\int \mathrm{d}t(E+L) = \int \mathrm{d}t\, m\dot{x}^2 = \int \mathrm{d}t\, \dot{x}(m\dot{x} = p) = \int \mathrm{d}t\, \dot{x}\pi$, so

$$\int \mathrm{d}t\ (L = KE - PE) = \int \mathrm{d}t\Big(\dot{x}\,p - (E = KE + PE)\Big), \qquad \boxed{L(x,\dot{x}) = \dot{x}\,p - E(x,p)}, \tag{1.15}$$

the last relationship being an example of a *Legendre transformation*.

Back to 1 century ago: (fixing the relative sign choice)
The "free particle wave," $\psi(x,t) = \psi_0\ \exp\{i(\pm kx - \omega t)\}$, where:

$$k\,x = \Big(\int \mathrm{d}x\ p = \int \mathrm{d}t\ \dot{x}\,p\Big)/\hbar, \qquad \text{for } \ p = \hbar k = \textit{const.},\ \tfrac{\partial p}{\partial x} = 0, \tag{1.16}$$

$$\omega\,t = \Big(\int \mathrm{d}t\ E\Big)/\hbar, \qquad \text{for } \ E = \hbar\omega = \textit{const.},\ \tfrac{\partial E}{\partial t} = 0, \tag{1.17}$$

prompts a more general candidate, $\boxed{\psi(x,t) = \psi_0\ \exp\{i\int \mathrm{d}t\,(\dot{x}p - E)/\hbar\} = \psi_0\, e^{i\int \mathrm{d}t\, L/\hbar}}$, even when p, E are not constant. In turn, any less simplistic wave-function can be obtained using these plane waves, by *superposition* — i.e., via the integral Fourier transform, $\psi(x,t) = \int \mathrm{d}k \int \mathrm{d}\omega\ \chi(k,\omega)\, e^{i(kx-\omega t)}$.

Quantum Novelties: (*operators,* values and vectors — oh, my!)
This "matter wave," $\psi(x,t)$ serves nicely:

1. $\frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x,t) = (\hbar k = p)\,\psi(x,t)$: the observable (to be measured) *value*, p, is obtained by *acting* with a differential operator, $p \rightsquigarrow \hat{p} := \frac{\hbar}{i}\frac{\partial}{\partial x}$! This *does not commute* with $\hat{x}$, which in turn is simply *multiplicative*: $\hat{x}\cdot\psi(x,t) = x\,\psi(x,t)$ is ordinary product:

$$[\,\hat{x}\,,\,\hat{p}\,]\,\psi(x,t) = \hat{x}\,\frac{\hbar}{i}\Big(\frac{\partial}{\partial x}\psi(x,t)\Big) - \frac{\hbar}{i}\Big(\frac{\partial}{\partial x}\big(\hat{x}\,\psi(x,t)\big)\Big) = i\hbar\,\psi(x,t) \tag{1.18}$$

   This having to hold on all wave-functions, we obtain the ***canonical commutation relations***:

$$\boxed{[\,\hat{x}\,,\,\hat{p}\,] = i\hbar\,\mathbb{1}}, \tag{1.19}$$

   and the **(1925) Heisenberg & Born (& Jordan):** ***matrix (quantum) mechanics***.
   Physical *observables*, $\hat{\mathcal{O}}$, (such as momentum, energy,..., all stemming from real functions of x,p) are *assigned operators*, the *eigenvalues* of which are being observed in concrete *measurements*. (This is known as the "Born postulate.")

   (a) In classical mechanics (CM), for real functions $\mathcal{A} = \mathcal{A}(x,p)$ and $\mathcal{B} = \mathcal{B}(x,p)$:

$$\{\,\mathcal{A}\,,\,\mathcal{B}\,\}_{PB} := \frac{\partial\mathcal{A}}{\partial x}\frac{\partial\mathcal{B}}{\partial p} - \frac{\partial\mathcal{B}}{\partial x}\frac{\partial\mathcal{A}}{\partial p}. \qquad \text{e.g. } \{x,p\}_{PB} = 1,\ \in\mathbb{R}. \tag{1.20}$$

$\{\ ,\ \}_{PB} \mapsto \frac{1}{i\hbar}[\ ,\ ]$

$$[\,\hat{\mathcal{A}}\,,\,\hat{\mathcal{B}}\,] := \hat{\mathcal{A}}\,\hat{\mathcal{B}} - \hat{\mathcal{B}}\,\hat{\mathcal{A}}. \qquad \text{e.g. } \frac{1}{i\hbar}[\hat{x},\hat{p}] = \mathbb{1},\ \text{Hermitian}. \tag{1.21}$$

So (with $\mathscr{H}(x,p) = KE{+}PE$ the classical Hamiltonian),

$$\frac{\mathrm{d}\mathscr{A}}{\mathrm{d}t} = -\{\mathscr{H}\,,\,\mathscr{A}\}_{PB} + \frac{\partial\mathscr{A}}{\partial t} \quad\mapsto\quad \boxed{\frac{\mathrm{d}\hat{\mathscr{A}}}{\mathrm{d}t} = \frac{i}{\hbar}\big[\,\hat{H}\,,\,\hat{\mathscr{A}}\,\big] + \frac{\partial\hat{\mathscr{A}}}{\partial t}}. \tag{1.22}$$

(b) No "classical-to-quantum" assignment, $\mathscr{O} \to \hat{\mathscr{O}}$, can be unique: it depends (at the very least) on the ordering of $x, \hat{p}$. For example, $px^2 = x^2p$ (in CM) but $\hat{p}\hat{x}^2 = \hat{x}^2\hat{p} - 2i\hbar\,\hat{x}$ (in QM), and (increasingly) higher-power monomials differ (increasingly) more — and are far from "trivial" in any sense; e.g., [2, 3].

The "QM → CM" *limit* is however expected to be unique, although "many-to-one."

(c) Introduce a particular assignment rule ("polarization"): $\mathscr{A} \to \varpi(\mathscr{A}) = \hat{\mathscr{A}}$ [4, 5]. Then,

$$i\hbar\,\varpi\Big(\{\,\mathscr{A}\,,\,\mathscr{B}\,\}_{PB}\Big) - \big[\,\varpi(\mathscr{A})\,,\,\varpi(\mathscr{B})\big] \qquad \forall\mathscr{A},\mathscr{B} \tag{1.23}$$

measures the "anomaly" of the quantum system obtained by the "polarization" ϖ.

2. $i\hbar\frac{\partial}{\partial x}\,\psi(x,t) = (\hbar\omega = E)\psi(x,t)$: $\quad E \rightsquigarrow \hat{H} := i\hbar\frac{\partial}{\partial t}$, producing (**1926**, ***Schrödinger equation***.):

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi(x,t) = \Big[\frac{1}{2m}\hat{p}^2 + V(x)\Big]\psi(x,t), \tag{1.24}$$

$$\boxed{i\hbar\frac{\partial}{\partial t}\psi(x,t) \overset{\#1.}{=} \Big[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\Big]\psi(x,t)}. \tag{1.25}$$

The equation (1.25) (with boundary conditions) is a *linear* PDE, so its solutions form a vector space, $\mathscr{V}_\psi$: if $\psi_1(x,t)$ and $\psi_2(x,t)$ are two solutions, so is their *superposition*, $c_1\psi_1(x,t) + c_2\psi_2(x,t)$, $c_i \in \mathbb{C}$. The $\psi(x,t)$'s are *vectors* in $\mathscr{V}_\psi$. Two solutions, $\psi_1(x,t), \psi_2(x,t)$, are linearly independent precisely if

$$\big(c_1\psi_1(x,t) + c_2\psi_2(x,t) = 0\big) \;\Rightarrow\; \big(c_1 = 0 = c_2\big). \tag{1.26}$$

Then, $\dim(\mathscr{V}_\psi)$ is the smallest number of linearly independent $\psi(x,t)$'s, which may be finite, countably infinite, uncountable or *hybrid* — typically determined by the boundary conditions.

The action $\hat{\mathscr{O}} : \mathscr{V}_\psi \to \mathscr{V}_\psi \;\Rightarrow\;$ *matrix representation* for $\hat{\mathscr{O}}$ in #1. → eigenvalues and eigenvectors.

3. Quantum apocrypha: in 1925, Hilbert explained Heisenberg & Born that they have *matrices* — and told them to look for their generating differential equation. . .

4. Every observable of interest (assigned a Hermitian $\mathscr{A}^\dagger = \mathscr{A}$) operator, has its eigenvectors, which we can label by their eigenvalue: $|a\rangle : \mathscr{A}|a\rangle = a|a\rangle$. The wave-functions, $\psi(x,t)$, are similarly labeled by x, the eigenvalues of their *position* (Hermitian) operator, $\hat{\mathscr{X}}$, so they are also eigenvectors of $\hat{\mathscr{X}}$? Well, not quite: Rather, the eigenvector space, $\mathscr{V}_\mathscr{A} = \big\{|a\rangle : \mathscr{A}|a\rangle = \alpha|a\rangle\big\}$, of every operator, $\hat{\mathscr{A}}$, has its formal dual (antilinear functionals on $\mathscr{V}_\mathscr{A}$), $V^\vee_\mathscr{A} = \big\{\langle a| : \langle a|b\rangle = f(a,b) \in \mathbb{C}\big\}$ and so $\langle a|\mathscr{A} = \alpha\langle a|$, so that the (*literature-standard* [6]) definition is

$$\boxed{\psi(x,t) := \big\langle x\big|\psi(t)\big\rangle}, \qquad \hat{\mathscr{X}}|x\rangle = x|x\rangle; \qquad \boxed{\hat{\mathscr{O}}\cdot\psi(x,t) := \big\langle x\big|\,\hat{\mathscr{O}}\,\big|\psi(t)\big\rangle}. \tag{1.27}$$

This does make $\psi(x,t)$ a $\mathbb{C}$-number-valued function (as it should be), but forces the action of $\hat{\mathscr{O}}$ on $\psi(x,t)$ to be: • *right* on $|\psi\rangle \in \mathscr{V}_\psi$, but • *left* on $\langle x| \in V^\vee_\mathscr{X}$ the positional (or momentum, or. . .) space.

(a) This allows us to re-define $\boxed{\mathscr{V}_\psi = \{\, |\psi(t)\rangle : i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \,\}}$ — *the Hilbert space of "pure" states*. (There is a perfect reason why t *cannot* be the eigenvalue of a "time-operator" and x and t are on completely different footing in QM, but it needs more background… see, e.g., Ref. [6, § 12.3].)

(b) Now can "switch" from the wave-function in the position-representation, $\psi(x,t) = \langle x|\psi(t)\rangle$ to the wave-function in the momentum-representation, $\psi(p,t) = \langle p|\psi(t)\rangle$. (One is the integral Fourier-transform of the other.) … or to any other representation defined by the variable change $(x,p) \to (\mathfrak{x},\mathfrak{p})$, where $\mathfrak{x} = \mathfrak{x}(x,p)$ and $\mathfrak{p}$ must be defined so $[\hat{\mathfrak{x}},\hat{\mathfrak{p}}] = i\hbar$; see [6, § 4.1].
In the momentum representation, $\hat{p} = p$ is multiplicative, while $\hat{x} = i\hbar\frac{\partial}{\partial p}$, to preserve (1.19).

5. The $\psi(x,t)$ of "well localized things" are *square-integrable,* since $\rho(x,t) := |\psi(x,t)|^2$ is the *intensity*, i.e., *probability density* of the wave-function: $\boxed{\int_{-\infty}^{\infty} \mathrm{d}x\, |\psi(x,t)|^2 = 1}$, "the object must be *somewhere*." Also, $\langle\chi|[\cdots] := \int \mathrm{d}x \chi^*(x,t)[\cdots]$, (antilinear functional over $\mathscr{V}_\psi$) so $\langle\chi|\psi\rangle := \int \mathrm{d}x\; \chi^*(x,t)\psi(x,t)$ is a sesquilinear *scalar product*: which turns $\mathscr{V}_\psi$ into a ***Hilbert space***. Observables acting on it are represented by (bounded?,…) operators, $\hat{\mathscr{O}}$, which are supposed to have real eigenvalues — to be measurable in the real world. This is insured by $\hat{\mathscr{O}}$ being Hermitian, but may not be *necessary* [7].

Expectation values: $\hat{\mathscr{O}} \rightsquigarrow \langle\hat{\mathscr{O}}\rangle_\psi := \langle\psi|\hat{\mathscr{O}}|\psi\rangle$. The simplest operator, $\hat{\mathscr{O}} \to \mathbb{1}$ (do nothing, just observe), asks "does the particle even exist?" To which a nonzero $\rho(x,t) := |\psi(x,t)|^2$ provides the *probability distribution/density* (a.k.a. "density matrix") of finding the particle at the location (x,t). Call $\psi(x,t)$ the "wave-function" from now on; it's *square* being a probability density and akin to amplitudes of waves (which *scale* a "waving" functions, such as $\sin(kx+\delta)$), it may also be thought of as a probability *amplitude*.

6. *Entanglement, non-Hermitian observables, "non-Hermitian PT-symmetric QM,"*[2]*… (lots more!!)*

Physics Models, in General:

1. Domain-space, $\mathfrak{D}$: $t \in \mathbb{R}^1$ in CM and QM (string theory: $\mathfrak{D} = \Sigma_g^{1,1}$ — Deligne-Mumford U.C.).
2. Target-space, $\mathfrak{T}$: $x \in \mathbb{R}^1$ for 1d CM and QM, $\vec{r} \in \mathbb{R}^3$ for 1d CM and QM, …
3. A mapping $\mathfrak{D} \to \mathfrak{T}$: in CM and QM, $x(t)$ and $\vec{r}(t)$.
4. An "action functional," $S[x(t); F(t)]$, where $F(t)$ are "external" forces/cources.

#3.+#4. can determine $\mathfrak{T}$ in #2. *dynamically*.

Then, CM: $\delta S[x(t); F(t)] = 0$. However, the same data actually leads to *much* more:

5. The path-integral: $Z[\xi(t); F(t)] := \iint \mathbf{D}[x]\; e^{iS[x(t)+\xi(t);F(t)]/\hbar} =: e^{iS_{\text{eff}}[\xi(t);F(t)]/\hbar}$;

$\frac{\delta}{\delta F(t_1)} \cdots \frac{\delta}{\delta F(t_k)} Z[\xi(t); F(t)] = \langle x(t_1)\cdots x(t_k)\rangle$ **[Dirac, 1933; …** [8–12]]

The functional $Z[\xi(t)]$ includes all possible histories $x(t)$ from known initial to final conditions (emission & detection), and so *a priori* can be used to "extract" any and all information about the full quantum behavior. It also happens to satisfy a Schrödinger equation, so is an *a priori* prescription how to construct a quantum theory out of a classical one [8–12]. It is however not a rigorously well-defined integral.

QM ⇒ EM: Following Schrödinger's unpublished work [12, § 5.1], as only $|\psi(x,t)|^2$ is deemed observable, than the $\psi(x,t) \to e^{i\varphi(x,t)}\psi(x,t)$ change of variables cannot be observable even for *arbitrary* $\varphi(x,t)$.

[2]This particular class of models [7] seems to be very much *en vogue*: one considers an incomplete system, the interaction of which with the "excised/ignored/unknown" complement is modeled by non-Hermitian ("dissipative/decay/lossy") terms in the Hamiltonian (= total energy) and/or other observables of interest.

▶ *Disaster:* But then,

$$i\hbar\frac{\partial}{\partial t}\psi = \Big[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\Big]\psi, \tag{1.28}$$

$\psi(x,t) \to e^{i\varphi(x,t)}\psi(x,t)$

$$i\hbar\frac{\partial}{\partial t}\Big(e^{i\varphi}\psi\Big) = \Big[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\Big]\Big(e^{i\varphi}\psi\Big) \tag{1.29}$$

$$i\hbar\Big(e^{i\varphi}\,i\frac{\partial\varphi}{\partial t}\Big)\psi + i\hbar\,e^{i\varphi}\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial}{\partial x}\bigg(\Big(e^{i\varphi}\,i\frac{\partial\varphi}{\partial x}\Big)\psi + e^{i\varphi}\frac{\partial\psi}{\partial x}\bigg) + V(x,t)\,e^{i\varphi}\psi$$

$$= -\frac{\hbar^2}{2m}\bigg[e^{i\varphi}\Big(i\frac{\partial\varphi}{\partial x}\Big)^2\psi + e^{i\varphi}\Big(i\frac{\partial^2\varphi}{\partial x^2}\Big)\psi + 2e^{i\varphi}\Big(i\frac{\partial\varphi}{\partial x}\Big)\Big(\frac{\partial\psi}{\partial x}\Big) + e^{i\varphi}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}\bigg] + V(x,t)e^{i\varphi}\psi \tag{1.30}$$

so, using the original equation (1.25) and upon dividing by $\psi(x,t)$, we obtain:

$$\frac{\partial\varphi}{\partial t} = \frac{\hbar}{2m}\bigg[i\frac{\partial^2\varphi}{\partial x^2} - \Big(\frac{\partial\varphi}{\partial x}\Big)^2 + 2i\frac{\partial\varphi}{\partial x}\,\frac{\partial\,\ln(\psi)}{\partial x}\bigg]. \tag{1.31}$$

This result is ***absolutely disastrous***! Not only did the (*unmeasurable!*) phase $\varphi(x,t)$ turn out not to be an arbitrarily selectable function of space and time, but it would have to satisfy a differential equation (1.31) which moreover depends on the particular wave-function $\psi(x,t)$!

▶ *Repair:* To "fix" this disaster, we must modify the Schrödinger equation, but in a way that does not obliterate the argumentation that brought us (1.25). To this end we note that the $p \rightsquigarrow \frac{\hbar}{i}\frac{\partial}{\partial x}$ prescription used in (1.18)–(1.19) is *not* the most general one, nor is the assignment (1.24); instead:

$$p \rightsquigarrow \hat{p} := \tfrac{\hbar}{i}\mathscr{D}_x : \quad \text{with} \quad \boxed{\mathscr{D}_x := \tfrac{\partial}{\partial x} + \mathscr{P}(x,t)}, \qquad \big[\,x\,,\,\tfrac{\hbar}{i}\mathscr{D}_x\,\big] = i\hbar\mathbb{1}; \tag{1.32}$$

$$\text{and also} \quad E \rightsquigarrow \hat{H} := i\hbar\mathscr{D}_t : \quad \text{with} \quad \boxed{\mathscr{D}_t := \tfrac{\partial}{\partial t} + \mathscr{E}(x,t)}; \qquad \text{no CCR to check.} \tag{1.33}$$

The newfangled "rate-of-change-operators," $\mathscr{D}_x, \mathscr{D}_t$, are then required to themselves change, $\mathscr{D}_* \to \mathscr{D}'_*$, and simultaneously with $\psi \to e^{i\varphi}\,\psi$, so as to change the Schrödinger equation at most up to an overall nonzero coefficient. This happens when

$$\mathscr{D}'_*\psi' = \mathscr{D}'_*(e^{i\varphi}\,\psi) \overset{!}{=} e^{i\varphi}(\mathscr{D}_*\psi), \qquad \text{i.e.} \quad \mathscr{D}'_* = e^{i\varphi}\mathscr{D}_* e^{-i\varphi}, \tag{1.34}$$

$$\text{so} \quad \mathscr{P}'(x,t) = \mathscr{P}(x,t) - i\frac{\partial\varphi}{\partial x}, \quad \text{and} \quad \mathscr{E}'(x,t) = \mathscr{E}(x,t) - i\frac{\partial\varphi}{\partial t}. \tag{1.35}$$

Comparing with standard texts on electromagnetism [13, 14] lets us identify

$$\mathscr{E} = \tfrac{iq}{\hbar}\Phi, \quad \mathscr{P} = \tfrac{q}{i\hbar}A_x, \quad \varphi = \tfrac{q}{\hbar}\Lambda, \tag{1.36}$$

so that (1.35) reproduce (x-projection of) the standard, $U(1)$ *gauge transformation* of the scalar and vector potentials in electromagnetism

$$\boxed{\Phi \to \Phi' = \Phi - \frac{\partial\Lambda}{\partial t}}, \quad \boxed{\vec{A} \to \vec{A}' = \vec{A} + \vec{\nabla}\Lambda}, \quad \boxed{\psi \to \psi' = e^{i\varphi}\psi}. \tag{1.37}$$

The so-modified Schrödinger equation reads (in 3-dimensions):

$$i\hbar\Big[\mathscr{D}_t := \frac{\partial}{\partial t} + \frac{iq}{\hbar}\Phi\Big]\psi(\vec{r},t) = \Big\{-\frac{\hbar^2}{2m}\Big[\vec{\mathscr{D}} := \vec{\nabla} + \frac{q}{i\hbar}\vec{A}\Big]^2 + V(\vec{r},t)\Big\}\psi(\vec{r},t), \tag{1.38}$$

$$\text{i.e.,}\quad i\hbar\frac{\partial}{\partial t}\psi(\vec r,t) = \Big[-\frac{\hbar^2}{2m}\Big[\vec\nabla+\frac{q}{i\hbar}\vec A\Big]\cdot\Big[\vec\nabla+\frac{q}{i\hbar}\vec A\Big] + \big(V(\vec r,t)+q\Phi\big)\Big]\psi(\vec r,t), \tag{1.39}$$

which couples to the newfangled "rate-of-change-computation corrections," $\mathscr{E} = \frac{iq}{\hbar}\Phi$ and $\vec{\mathscr{P}} = \frac{q}{i\hbar}\vec A$, the electromagnetic potentials, precisely proportionally to the electric charge, q, of the object represented by $\psi(x,t)$. These newfangled, electromagnetic-field-sensing "rate-of-change operators" are

$$\boxed{\mathscr{D}_t := \frac{\partial}{\partial t}+\frac{iq}{\hbar}\Phi(\vec r,t)}\quad\text{and}\quad\boxed{\vec{\mathscr{D}} := \vec\nabla+\frac{q}{i\hbar}\vec A(\vec r,t)},\qquad\text{called } \textit{\textbf{covariant derivatives}}. \tag{1.40}$$

▶ *Curvature:* Since the potentials (1.36) *do change* in gauge transformations (1.37), they must not be observable themselves! (Indeed, one never measures the potential, only ever *potential differences.*)
Owing to the abelian (commutative, $\mathrm{U}(1)$-group action, since $\varphi \simeq \varphi{+}2\pi$) nature of the gauge transformation (1.37), it is easy to see that

$$\vec B := \vec\nabla\times\vec A \quad\text{and}\quad \vec E := -\vec\nabla\Phi - \frac{\partial\vec A}{\partial t} \tag{1.41}$$

remain unchanged by the gauge transformations (1.37), and so *are* observable (consistently measurable).

The same quantities are however also computed "canonically":

$$\big[\,\vec{\mathscr{D}}\,,\,\mathscr{D}_t\,\big] = \Big[\,\vec\nabla - i\frac{q}{\hbar}\vec A,\ \frac{\partial}{\partial t}+i\frac{q}{\hbar}\Phi\,\Big] = i\frac{q}{\hbar}\Big(-\vec\nabla\Phi-\frac{\partial\vec A}{\partial t} = \vec E\Big); \tag{1.42}$$

$$\big[\,\mathscr{D}_x\,,\,\mathscr{D}_y\,\big]\Big[\,\frac{\partial}{\partial x}-i\frac{q}{\hbar}A_x\,,\,\frac{\partial}{\partial y}-i\frac{q}{\hbar}A_y\,\Big] = -i\frac{q}{\hbar}\Big(\frac{\partial A_y}{\partial x}-\frac{\partial A_x}{\partial y} = (\vec B)_z\Big). \tag{1.43}$$

This is straightforward to generalize for non-abelian gauge symmetries [12, § 6.1]. The explicit computation shows that the gauge-invariant $\vec E,\vec B$-fields of electromagnetism are components of *curvature*, the $\mathscr{R}_{ij}$-part of the standard definition, $\boxed{[\mathscr{D}_i,\mathscr{D}_j] =: \mathscr{T}_{ij}{}^k\,\mathscr{D}_k+\mathscr{R}_{ij}}$, and explicitly verifies that covariant derivatives (1.40) of electromagnetism have no (geometric) torsion, $\mathscr{T}_{ij}{}^k$. Electromagnetism is thus *induced* by QM, and could have been discovered by it, had it not been already well known for half a century:

> **Corollary 1.1:** *The only dynamical equation of QM,* (1.25)*, forces the use of complex functions of which the (overall) phase-factor is not observable; maintaining its unobservability introduces the gauge interactions, i.e., curves the spacetime for so-charged objects.*

▶ *WKBJ:* The computation (1.28)–(1.31) reveals an avenue of solving the Schrödinger equation differently: Setting $\psi\to 1$ in (1.30) effectively makes the nonlinear change of variables $\psi(x,t)\to e^{i\varphi(x,t)}$:

$$\frac{\partial\varphi}{\partial t} = \frac{\hbar}{2m}\bigg(i\frac{\partial^2\varphi}{\partial x^2}-\Big(\frac{\partial\varphi}{\partial x}\Big)^2\bigg)-\frac{1}{\hbar}V(x,t), \tag{1.44}$$

which may be solved iteratively in a few different schemes. One of those produces, after the first iteration, the so-called Wentzel–Kramers–Brillouin–Jeffreys (a.k.a. "semi-classical") approximation,

$$\boxed{\psi_{\text{WKBJ}}(x,t) := \frac{C_\pm}{\sqrt{p(x)}}\exp\Big\{i\int \mathrm{d}t\Big(\pm\dot x\,p(x)/\hbar-(E/\hbar)\Big)\Big\},\quad p(x) = \sqrt{2m\big(E-V(x)\big)} = \sqrt{2m\,KE}}, \tag{1.45}$$

where the right-hand side is entirely classical, and E is constant. This is very much akin to the guess after (1.16)–(1.17) — except for the $\frac{1}{\sqrt{p(x)}}$-normalization, which causes the probability density, $|\psi_{\text{WKBJ}}(x,t)|^2$, to have poles at the $(V(x){=}E)$ "turning points," the x-boundaries of the "classically permitted regions," where a classical particle slows about to turn back.

References

[1] X.-B. Yan, "The physical origin of schrödinger equation," *European Journal of Physics* **42** no. 4, (May, 2021) 045402, arXiv:2106.01312 [physics.gen-ph].

[2] H. S. Sahota, "Imprints of the operator ordering ambiguity on the dynamics of perfect fluid dominated quantum Universe," *Class. Quant. Grav.* **41** no. 17, (2024) 175006, arXiv:2310.09905 [gr-qc].

[3] P. Dorlis, N. E. Mavromatos, and S.-N. Vlachos, "Quantum-Ordering Ambiguities in Weak Chern—Simons 4D Gravity and Metastability of the Condensate-Induced Inflation," *Universe* **11** no. 1, (2025) 15, arXiv:2411.12519 [gr-qc].

[4] N. E. Hurt, *Geometric Quantization in Action*. D. Reidel Publishing Company, 1983.

[5] N. M. J. Woodhouse, *Geometric Quantization*. Oxford University Press, 2nd ed., 1997.

[6] L. E. Ballentine, *Quantum Mechanics*. World Scientific Publishing Co. Inc., 2nd ed., 2015. (annotated extension of the 1998 1st ed., with Ch. 21 on Quantum Information).

[7] C. M. Bender and S. Boettcher, "Real spectra in nonHermitian Hamiltonians having PT symmetry," *Phys. Rev. Lett.* **80** (1998) 5243–5246, arXiv:physics/9712001.

[8] P. A. M. Dirac, "The Lagrangian in quantum mechanics," *Phys. Z. Sowjetunion* **2** (1933) 64–72.

[9] N. D. Hari Dass, "Dirac and the Path Integral," arXiv:2003.12683 [physics.hist-ph].

[10] R. P. Feynman, A. R. Hibbs, and D. F. Styer, *Quantum Mechanics and Path Integrals*. Dover Publications Inc, New York, emended ed., 2005.

[11] H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets*. World Scientific Publishing Company, 5th ed., 2009.

[12] T. Hübsch, *Advanced Concepts in Particle and Field Theory*. Cambridge University Press, 2015. http://www.cambridge.org/9781107097483. Since 2022 freely available in Open Access Cambridge Core and @ inSPIREhep.

[13] D. J. Griffiths, *Introduction to Electrodynamics*. Addison-Wesley, 4th ed., 2012.

[14] J. D. Jackson, *Classical Electrodynamics*. John Wiley & Sons Inc., 3rd ed., 1999.