# Quantum mechanics notes

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## 1 • Wave functions

Consider a (classical) monochromatic plane electromagnetic wave in vacuum, with amplitude $E_0$. The average power per unit area transported by this wave is the *intensity* and is given by

$$I = \frac{1}{2} c \varepsilon_0 E_0^2.$$

If the wave is incident on a screen and $\mathrm{d}A$ denotes the area of an infinitesimal patch $M$ of this screen, then the average power transferred to this patch is $I \,\mathrm{d}A$. Turning down the intensity until individual photons are emitted, the position of a photon on the screen is a random variable[1] $\mathsf{X}$ with values in $\mathbb{R}^2$, and whose distribution $P_{\mathsf{X}}$ has a density $f$ with respect to the Lebesgue measure on $\mathbb{R}^2$. Clearly $I \,\mathrm{d}A$ is proportional to the probability $P_{\mathsf{X}}(M) = f \,\mathrm{d}A$, and hence $I$ is proportional to $f$. It follows that $f$ is proportional to $E_0^2$.

Recall that the electric field (and the magnetic field) constitutes the wave function for electromagnetic waves, so we see that the density $f$ is proportional to the *square* of the wave function. Writing $f = |\psi|^2$, we call $\psi$ the *probability amplitude* for $\mathsf{X}$. (Here we normalise the wave function to obtain $\psi$ such that $|\psi|^2$ becomes a density.) We take the modulus of $\psi$ to allow for the possibility that $\psi$ be complex-valued.

As an example, consider a photon passing through a double slit. Let $\psi_1$ and $\psi_2$ be the contributions to $\psi$ from each of the two slits, such that $\psi = \psi_1 + \psi_2$. If the second slit is closed, then $\psi_2 = 0$, and similarly if the first slit is closed. If both slits are open, then we might expect that $P_{\mathsf{X}}(M) = (|\psi_1|^2 + |\psi_2|^2) \,\mathrm{d}A$. However, the probability that the photon hits the patch $M$ is instead

$$P_{\mathsf{X}}(M) = |\psi|^2 \,\mathrm{d}A = |\psi_1 + \psi_2|^2 \,\mathrm{d}A$$

[1] We are not appealing to any intrinsic randomness in quantum mechanics, only the experimental fact that photons appear seemingly randomly on the screen.

by the principle of superposition.

# 2 • The Schrödinger equation

## *2.1. Unitary time evolution*

Let $|\psi(t)\rangle$ denote the state of a quantum mechanical system at time $t$. We say that the time evolution of the system is *unitary* if there is a two-parameter family of unitary operators $\mathsf{U}(s,t)$, where $s$ and $t$ are real parameters (and $\mathsf{U}(s,t)$ is suitably smooth in $s$ and $t$), such that

$$|\psi(t_2)\rangle = \mathsf{U}(t_2,t_1)|\psi(t_1)\rangle$$

for all appropriate $t_1, t_2$. Note that if a system has unitary time evolution, then the entire evolution of the system (both in the future and in the past) is determined by the state of the system at a single point in time.

## *2.2. Derivation of the Schrödinger equation*

Assume that the time evolution of the system in question is unitary. Further assume that the Hilbert space $\mathcal{H}$ of states of the system is finite-dimensional. Let $I \subseteq \mathbb{R}$ be an open interval, and consider the evolution of the system in this interval. Define a map $\Psi\colon I \to \mathcal{H}$ by $\Psi(t) = |\psi(t)\rangle$.

For $t \in I$ also define a map $\mathsf{G}(t)\colon \mathcal{H} \to \mathcal{H}$ by $\Psi(t) \mapsto \Psi'(t)$.[2] Notice that, since the time evolution is unitary, it is deterministic. The state $\Psi(t)$ of the system thus determines its entire time evolution, hence determines $\Psi'(t)$, so $\mathsf{G}(t)$ is well-defined. Furthermore, if $\Phi\colon I \to \mathcal{H}$ is another possible time-evolution and $\beta \in \mathbb{C}$, then

$$\begin{aligned}\mathsf{G}(t)[\beta\Psi(t) + \Phi(t)] &= \mathsf{G}(t)[(\beta\Psi + \Phi)(t)] = (\beta\Psi + \Phi)'(t)\\ &= \beta\Psi'(t) + \Phi'(t) = \beta\mathsf{G}(t)[\Psi(t)] + \mathsf{G}(t)[\Phi'(t)],\end{aligned}$$

so $\mathsf{G}(t)$ is linear for each fixed $t \in I$, so we denote application of $\mathsf{G}(t)$ by juxtaposition.[3]

[2] Since $\mathcal{H}$ is finite-dimensional, the derivative of $\Psi$ is well-defined and lies in $\mathcal{H}$.

[3] There seems to be a subtlety here, in that it should be possible to obtain any state in $\mathcal{H}$ for $\mathsf{G}(t)$ to make sense.

Next, unitary evolution implies that normalised states remain normalised. Denoting the inner product on $\mathcal{H}$ by $\langle\cdot,\cdot\rangle$, for $t \in I$ it follows that

$$\begin{aligned} 0 &= \left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=t} \langle\Psi(s),\Psi(s)\rangle \\ &= \langle\Psi'(t),\Psi(t)\rangle + \langle\Psi(t),\Psi'(t)\rangle \\ &= \langle \mathsf{G}(t)\Psi(t),\Psi(t)\rangle + \langle\Psi(t),\mathsf{G}(t)\Psi(t)\rangle \\ &= \Big\langle\Psi(t),\Big[\mathsf{G}(t)^\dagger + \mathsf{G}(t)\Big]\Psi(t)\Big\rangle. \end{aligned}$$

Since this holds for all $\Psi(t) \in \mathcal{H}$, it follows that $\mathsf{G}(t)^\dagger + \mathsf{G}(t) = 0$, so $G(t)$ is anti-Hermitian. The Hermitian operator $\mathsf{H}(t) = \mathrm{i}\hbar\mathsf{G}(t)$ is called the *Hamiltonian operator*, and in terms of this we have

$$\mathsf{H}(t)\Psi(t) = \mathrm{i}\hbar\Psi'(t).$$

Or in bra–ket notation,

$$\mathsf{H}(t)|\psi(t)\rangle = \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle.$$

## 2.3. Uniform dynamics

If the dynamics are uniform, then the evolution operators constitute a one-parameter family $t \mapsto \mathsf{U}(t)$ of unitary operators, and the Hamiltonian $\mathsf{H}(t) = \mathsf{H}$ is time-independent. Hence we have $|\psi(t)\rangle = \mathsf{U}(t)|\psi(0)\rangle$, and we can write the Schrödinger equation

$$\mathsf{H}\mathsf{U}(t)|\psi(0)\rangle = \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\mathsf{U}(t)|\psi(0)\rangle.$$

We may also be tempted to write this as

$$\mathsf{H}\mathsf{U}(t) = \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\mathsf{U}(t), \tag{2.1}$$

and while the left-hand side is unproblematic, we have to be careful with the right-hand side. The right-hand denotes the operator which first applies $\mathsf{U}(s)$, with $s$ ranging over $I$, to some vector, and then differentiates the results with respect to $s$ in $s = t$. More precisely we have, for $\psi \in \mathcal{H}$,

$$\left(\frac{\mathrm{d}}{\mathrm{d}t}\mathsf{U}(t)\right)\psi = \left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=t}\mathsf{U}(s)\psi = \lim_{s\to t}\frac{\mathsf{U}(s)\psi - \mathsf{U}(t)\psi}{s-t}.$$

Thus $s \mapsto \mathsf{U}(s)$ need only be strongly differentiable. If $\dim\mathcal{H} < \infty$, then this is the same as it being differentiable with respect to the operator norm (or any norm on $\mathcal{L}(\mathcal{H})$ since they are all equivalent). Furthermore, the derivative of

$s \mapsto \mathsf{U}(s)\psi$ at $s = t$ is just $\mathsf{U}'(t)\psi$. Hence in this case we may indeed interpret (2.1) as a differential equation in an operator-valued variable. This has the solution

$$\mathsf{U}(t) = \exp\left(-\frac{\mathrm{i}}{\hbar}\mathsf{H}t\right).$$