(3) The Wavefunction

1 So far

on left front board

- if classical mechanics were right, we couldn't exist (no atoms, no Sun, no smart phones, ...)
- EM radiation is quantized in units of $E_\nu = h\nu$
- photons have momentum $p = E_\nu/c = h/\lambda$

  oh, and they are a wave too!
- electron orbits have quantized angular momentum $L = n\hbar$
- electron behave like waves with $\lambda = h/p$

  oh, and they are particles too!
- Randomness and uncertainty have crept in...

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2 This Time

- Rewriting the rules: Wavefunctions
- Superposition of waves
- from de Broglie to wave packets (Fourier analysis)

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3 Wavefunctions as System Configuration

- Gr. 1.(1,2,4), Sc. 3.1, Ga. 2.(1-3), E&R 3.4, Li. 2.8, Sh. 4.(1,2)

In order to create a new theory which will allow us to get some clarity on this wave-particle thing, we will need to start from the very bottom and work our way up. In classical mechanics we use $\vec{x}_n$ and $\vec{p}_n$ of each mass to define the configuration of our system, and everything else is determined by this configuration and the laws of motion.

(left back board)

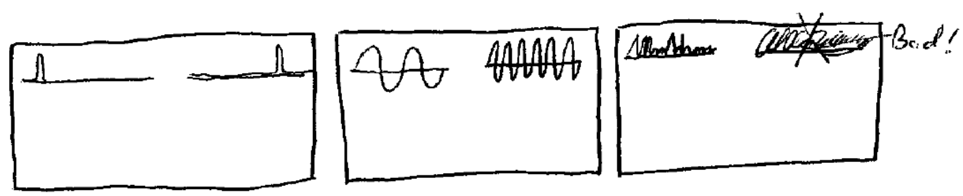
- Classical Configuration: $\vec{x}_n$ and $\vec{p}_n$ of all masses
- Deterministic Evolution: $\vec{F} = \frac{\partial \vec{p}}{\partial t}$, $E = \frac{p^2}{2m} + U(\vec{x})$
- In REALITY we have Randomness and Waves!

We need something new, and without dragging you through the history of it all, I can tell you that what we need is called a “wavefunction“.

(middle back board)

- In QM the system configuration is determined by $\psi(\vec{x})$
- WF is complex $\quad \psi(\vec{x}) \in \mathbb{C}$
- WF has a value at all $\vec{x}$
- WF is a “nice” function (single valued, continuous, ...)

Wavefunctions (all front boards)



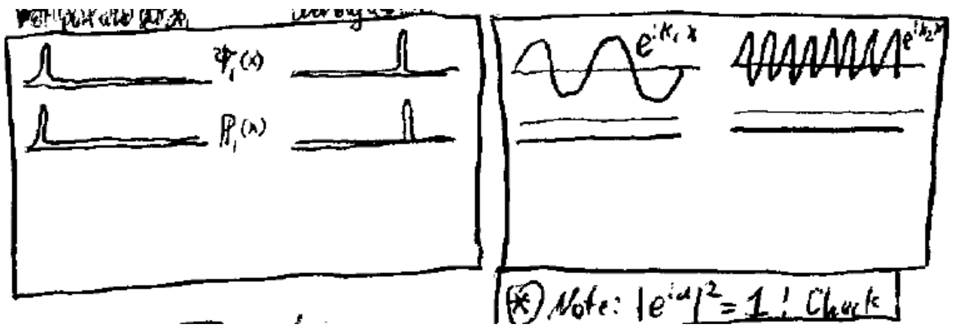
I can only draw the real part!

To get the randomness we are looking for, the interpretation of the WF is a probabilistic one. Recall that the dual slit interference patterns we build with many little flashes on the screen, with each one happening randomly, but with the final result being the expected intensity pattern.

(top of right back board, compress!)

$\mathbb{P}(x) = |\psi(x)|^2$ is the probability (density) of finding our particle at x (Born)

Wavefunctions and Probabilities (left-middle front boards)



$\mathbb{P}$ is always real! Note the similarity with E-field and intensity.

If we are going to use these WFs to make probability density functions we need to be able to normalize them.

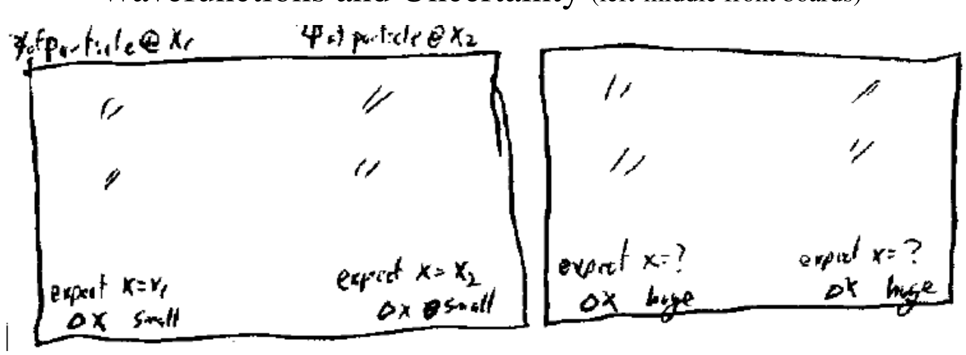
(rest of right back board) Our particle must be *somewhere*, so

- $\int \mathbb{P}(x)\, dx = 1 \qquad \Rightarrow \qquad \int |\psi(x)|^2\, dx = 1$
- Dimensions? $\quad [\mathbb{P}(x)\, dx] = [1]$

$$\Rightarrow\ [\mathbb{P}(x)] = [1/\mathrm{m}]\ \Rightarrow\ [\psi(x)] = [1/\sqrt{\mathrm{m}}]$$

Where do we expect to find our particle? For the narrow WFs, we have some idea, but for the e^{ikx} WF we have no information!

Wavefunctions and Uncertainty (left-middle front boards)

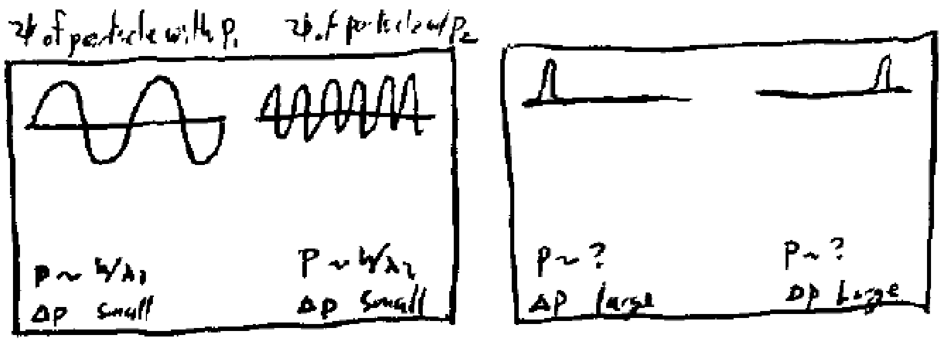


Ok, the e^{ikx} WFs look worthless. They don't tell us anything about our particle... or do they? Recall that de Broglie told us $\lambda = h/p$; this is where that takes shape in our new theory.

(top of right front board, erase bad WFs)

- Wave with $\lambda = h/p$ means particle with momentum p
- $p = h/\lambda = \hbar k$ just like $E = h\nu = \hbar\omega$

Wavefunctions and Momentum (left-middle front boards, swapped!)



(rest of right front board)

NOTE: small Δx goes with large Δp and vice versa.

We will come back to precise definitions of Δx and Δp in a bit

Ok, that is enough to get us started, but we still don't really have any clear way to represent particles with WFs. We need to be able to make something that is localized, and has momentum, analogous to our dear x and p.

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4 Superposition and Wavepackets

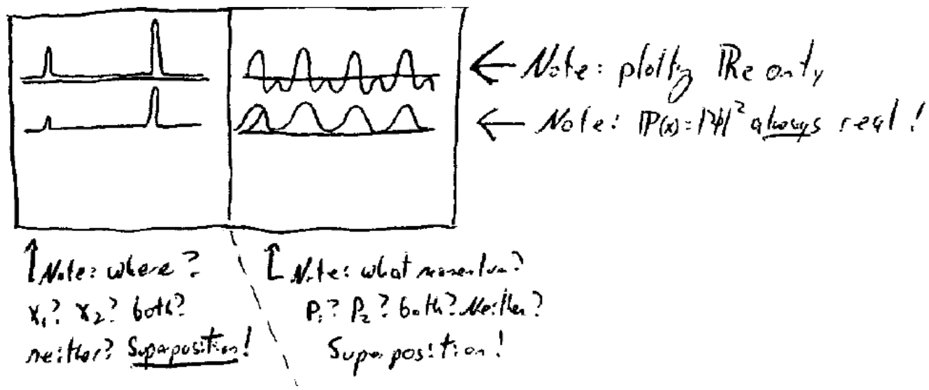
- Ga. 2.(2, 3), E&R 3.4, Li. 2.8, Sh. 4.(1,2)

One of the key features of WFs is that you can combine any two valid WFs to make another WF.

(left back board) **Superposition**

$\psi(x) = \alpha\psi_1(x) + \beta\psi_2(x)$ with α and $\beta \in \mathbb{C}$

Superposition (retake left-middle front boards)



With superposition, we can make all kinds of WFs from other WFs. In particular, given a complete set of basis WFs, we can make *any* WF. Not only that, with superposition, we can get *interference*, which we have seen to be key to this weird wave-particle problem.

Superposition is the key to QM! Superposition gives rise to interference!

(middle-right back boards) **Interference**

$$\mathbb{P}(x) = |\alpha\psi_1(x) + \beta\psi_2(x)|^2 \tag{1}$$

$$= |\alpha|^2 |\psi_1(x)|^2 + |\beta|^2 |\psi_2(x)|^2 + \alpha^*\psi_1^*(x)\beta\psi_2(x) + \alpha\psi_1(x)\beta^*\psi_2^*(x)$$

$$= |\alpha|^2 \mathbb{P}_1(x) + |\beta|^2 \mathbb{P}_2(x) + \text{Interference} \tag{2}$$

$$\text{If } \psi_1(x)\,\psi_2(x) = 0 \;\forall\, x \quad \mathbb{P}(x) = |\alpha|^2 \mathbb{P}_1(x) + |\beta|^2 \mathbb{P}_2(x) \tag{3}$$

$$\text{If } \psi_1(x) = e^{ik_1 x} \text{ and } \psi_2(x) = e^{ik_2 x} \tag{4}$$

$$\mathbb{P}(x) = |\alpha|^2 + |\beta|^2 + \underbrace{2\,|\alpha\beta|\cos((k_1 - k_2)x + \phi)}_{\text{Interference}} \tag{5}$$

and that last bit is interference, like what we got in the 2 slit experiment!

In fact, for $\alpha = \beta = 1/\sqrt{2}$, this becomes

$$\mathbb{P}(x) = 1 + \cos((k_1 - k_2)x) \tag{6}$$

which is a perfect match to the form of the intensity in the 2-slit experiment.

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5 Fourier Analysis: building $\psi(x)$ from plane waves

Let's look harder at the second example of adding plane-waves which gave rise to this interference term. We started with 2 WF each of which had definite momentum (the k in e^{ikx} since $p = \hbar k$) and no information about the position of our particle (same $\mathbb{P}$ at all x). Then we added them to get a WF which had some information about position due to the $\cos((k_1 - k_2)x)$ term.

Summing many plane waves can localize our particle. Like

$$\psi(x) = c_1 e^{ik_1 x} + c_2 e^{ik_2 x} + c_3 e^{ik_3 x} \tag{7}$$

or better, summing over N plane waves

$$\psi(x) = \sum_n c_n e^{ik_n x} \tag{8}$$

MATHEMATICA SLIDES (wavepacket.nb, discrete)

Moving to the limit of summing over a continuum of oscillating complex functions of the form e^{ikx} allows us construct any WF we like! For each value of k we need a coefficient, like c_n, but continuous, so $c(k)$ (though we will not call it that). This is known mathematically from the Fourier Transform, as described by

Fourier Transform:

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \tag{9}$$

and there is a corresponding inverse transform.

Inverse Fourier Transform:

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) e^{ikx} dk \tag{10}$$

We will use this on our wavefunctions to define

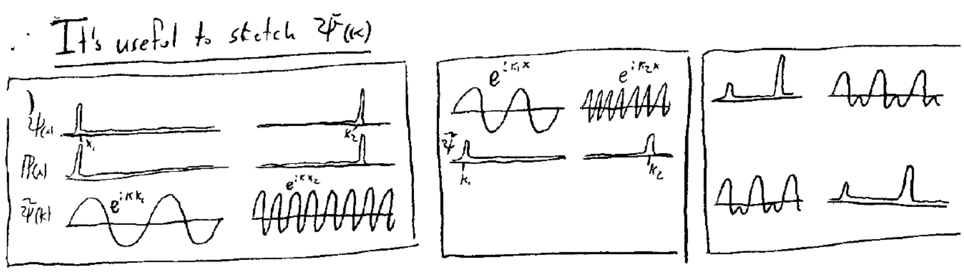
FT and IFT for WFs

$$\begin{aligned} \tilde{\psi}(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x) e^{-ikx}\, dx \\ \psi(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\psi}(k) e^{ikx}\, dk \end{aligned}$$

Note: $\psi(x)$ determines $\tilde{\psi}(k)$ and *vice versa*.
Note 2: you integrate over x or k to eliminate it!

MATHEMATICA SLIDES (continuous)

$\psi(x)$ and $\tilde{\psi}(k)$



Compare the sum of discrete plane waves with *definite momentum* to the continuous FT

Discrete vs. Continuous

$$\psi_1(x) = \sum_n c_n e^{ik_n x}$$

$$\psi_2(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\psi}(k) e^{ikx}\, dk$$

Note: $\tilde{\psi}(k)$ plays the role of c_n telling you how much of each momentum you have.

Which leads us to the probability density for momentum

$$\mathbb{P}(k) = \left|\tilde{\psi}(k)\right|^2 \tag{11}$$

MATHEMATIC SLIDES (Gaussian wave packet, in wavepacket.nb)

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6 Chopped Sine Example

An interesting example of a FT can be found in the "chopped sine wave"

Chopped Sine

$$\psi(x) = \begin{cases} A\sin(k_0 x) & -L < x < L \text{ where } L = \frac{n\pi}{k_0},\ n \in \mathbb{Z} \\ 0 & \text{otherwise} \end{cases} \tag{12}$$

Normalization of Chopped Sine

$$
\begin{aligned}
1 &= \int_{-L}^{L} |A\sin(k_0 x)|^2 \; dx \\
&= |A|^2 \underbrace{\int_{-L}^{L} \sin^2(k_0 x) \; dx}_{=\frac{1}{2}(2L)=L} \\
\Rightarrow A &= e^{i\phi}\frac{1}{\sqrt{L}} \quad \text{note phase and units}
\end{aligned}
$$

FT of Chopped Sine

$$
\begin{aligned}
\tilde{\psi}(k) &= \frac{A}{\sqrt{2\pi}} \int_{-L}^{L} \sin(k_0 x)\, e^{-ikx} \, dx \\
&\propto \underbrace{\int_{-L}^{L}}_{\text{even}} \underbrace{\sin(k_0 x)}_{\text{odd}} \left(\underbrace{\cos(kx)}_{\text{even}} - \underbrace{i\sin(kx)}_{\text{odd}} \right) \, dx \\
&\propto \int_{-L}^{L} \sin(k_0 x) \sin(kx) \; dx \\
&\propto \frac{\sin(Lk)}{k_0^2 - k^2} = \frac{\sin(n\pi k/k_0)}{k_0^2 - k^2} \\
&\quad \text{note} \;\; \sin(n\pi k/k_0) = 0 \;\; \text{for} \;\; k = k_0
\end{aligned}
$$

MATHEMATIC SLIDES (chopped_sine.nb)

7 Delta Functions

This is a bit of a mathematical aside, but I would like to introduce you all to delta functions. You might have asked yourself what mathematical expression I would use for the narrow WFs I have been drawing. For the wide ones, I wrote the infinitely wide e^{ikx}. For the narrow ones, I could be using any narrow function, like the Gaussian wavepackets we have seen in the slides, but taking this to the limit of infinitely narrow gives a delta function.

The Dirac delta function, $\delta(x)$, is defined by the condition

Delta Function

$$\int_a^b \delta(x)\ f(x)\ dx = \begin{cases} f(0) & 0 \in [a,b] \\ 0 & \text{otherwise} \end{cases} \tag{13}$$

with the immediate implication that

$$\delta(x) = \begin{cases} 0 & x \neq 0 \\ \infty & x = 0 \end{cases} \tag{14}$$

which I like to think of as an infinitely narrow Gaussian.

Examples of how you might use a delta function are

$$\begin{aligned} \int_{-\infty}^{\infty} \delta(x) x^2\ dx &= 0 \\ \int_{-\infty}^{\infty} \delta(x - x_0) x^2\ dx &= x_0^2 \\ \int_{-\infty}^{\infty} \delta(x) e^{ik(x-x_0)}\ dx &= e^{-ikx_0} \end{aligned}$$

Delta functions, like plane waves, will play an important role in this class.

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8 Next Time

Next time we'll learn how to quantify what the WF tells us about the position and momentum of our particle.