Ψ as an aid in finding "most probable" values of QM variables.

Expectation Values of QM Variables

Re the "unfinished business" on p. Sch. 6, we have dealt with point Ⓐ, by showing [in Eqs. (14)-(22)] that -- for Schrödinger's Ψ (free particle) -- $|\Psi|^2$ can indeed be interpreted as a probability density. We still have to deal with point Ⓑ, viz: how do external forces enter Schrödinger's Eqtn?

Before we look at this last question, we will develop some QM formalism that will help us to understand: (A) how the notion of $|\Psi|^2$ as a probability distribution leads to the idea of "most probable" values of QM variables, and (B) how QM variables are connected with operators -- e.g., as at bottom of p. Sch. 9 preceding: momentum $\mathbf{p} \rightarrow \mathbf{p}_{op} = (\hbar/i)\nabla$. These points will aid us in putting external forces into the theory, and altogether they will make us feel better about QM. The formalism is that of "expectation values."

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1) Start from the packet representation of a wavefcn Ψ at time $t=0$...

$$\rightarrow \underline{\underline{\Psi(x,0) = (1/\sqrt{2\pi}) \int \varphi(k) e^{ikx} dk}}, \text{ at } t=0. \tag{23}$$

We will work in 1D, and $\int$ means $\int_{-\infty}^{\infty}$ unless noted otherwise. We are using a new normalization factor $(1/\sqrt{2\pi})$, so that the Fourier inverse of Eq. (23) is:

$$\rightarrow \underline{\underline{\varphi(k) = (1/\sqrt{2\pi}) \int \Psi(x,0) e^{-ikx} dx}}. \tag{24}$$

This is done so that if we choose a normalization $\int |\Psi|^2 dx = 1$ for Ψ, then φ will have the same norm=n, i.e. $\int |\varphi|^2 dk = 1$ ... we prove this proposition below [see Eq. ( )]. NOTE: from Eqs. (23) & (24), once the spectral fcn $\varphi(k)$ is given, $\Psi(x,0)$ is fixed, and vice-versa.

To see that (23) & (24) are compatible, plug the integral for $\varphi(k)$ back into $\Psi(x,0)$ to obtain...

Fourier consistency. Appearance of the Dirac delta function.

$$\rightarrow \psi(x,0) = \frac{1}{2\pi}\int \overbrace{\left[\int \psi(x',0)\, e^{-ikx'} dx'\right]}^{\varphi(k)} e^{ikx}\, dk$$

$$= \int \underbrace{\left[\frac{1}{2\pi}\int e^{ik(x-x')} dk\right]}_{=\,\delta(x-x'),\ \text{called "Dirac delta function"}} \psi(x',0)\, dx'. \qquad (25)$$

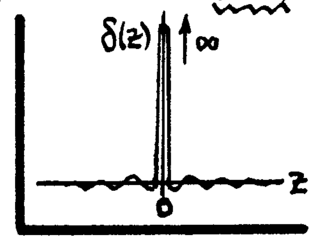
The integral called δ here is not well defined, but can be given a meaning by looking at a limit, viz.

$$\delta(z) = \lim_{K\to\infty} \frac{1}{2\pi}\int_{-K}^{+K} e^{ikz} dk = \lim_{K\to\infty}\left(\frac{\sin Kz}{\pi z}\right). \qquad (26A)$$

NOTES

- For any $z \neq 0$ (and $K \rightarrow$ large), the average value of $\delta(z) = 0$, over finite Δz.
- For $z \rightarrow 0$, however, $\delta(z)$ becomes arbitrarily large...

$$\rightarrow \delta(0) = \lim_{z\to 0}\left[\lim_{K\to\infty}\left(\frac{\sin Kz}{\pi z}\right)\right] = \lim_{K\to\infty}\left[\lim_{z\to 0}\left(\frac{\sin Kz}{\pi z}\right)\right] = \lim_{K\to\infty}\left(\frac{K}{\pi}\right) = \infty. \qquad (26B)$$



In effect, $\delta(z) = 0$ everywhere but at $z = 0$, where it is ∞.

- By direct integration of (26A), we find $\delta(z)$ is normed...

$$\rightarrow \int_{-\infty}^{\infty} \delta(z)\, dz = \lim_{K\to\infty} \frac{1}{\pi}\int_{-\infty}^{\infty}\left(\frac{\sin Kz}{z}\right) dz = \frac{1}{\pi}\int_{-\infty}^{\infty}\left(\frac{\sin u}{u}\right) du \overset{\text{tabulated}}{=} 1, \qquad (26C)$$

and this normalization is independent of K. So it is indep^{t} of the limit.

- With an appreciable value only at $z = 0$, $\delta(z)$ projects out an integrand value just at that point, i.e.

$$\boxed{\int_{-\infty}^{\infty} \delta(z)\, f(z)\, dz = f(0)}. \qquad (26D)$$

This relation defines $\delta(z)$. That the integral converges is "evident" from the fact that [by Eq. (26C)], we need $\int_{-\infty}^{\infty} \delta(z)\, dz = 1$ for the choice $f(z) = 1$.

When these results are used in Eq. (25) above, it is clear that we have an identity: $\psi(x,0) = \int_{-\infty}^{\infty} \delta(x-x')\, \psi(x',0)\, dx' = \psi(x,0)$. So the transform pair in Eqs. (23) & (24) are self-consistent.

The spectral fcn $\varphi(k)$ as a probability distribution in k-space.

2) The fact that $\Psi(x,0)$ & $\varphi(k)$ are "interchangeable" via the transform pair in Eqs. (23) & (24) suggests that both functions can be used as probability distributions. If $\psi(x,0)$ is used for calculations in position space (i.e. x cds), then $\varphi(k)$ should be useful for calculations in momentum space (i.e. k cds, with $k = p/\hbar$ directly proportional to momentum p). Thus, we are suggesting...

$$\left[\begin{array}{l} \Psi(x,0) \text{ in } x\text{-space} \xleftarrow{\text{(specifies)}}\!\!\rightarrow \varphi(k) \text{ in } k\text{-space}, \\ \text{so, if } |\Psi(x,0)|^2 dx = \text{prob. of finding particle in } dx \text{ @ position } x, \\ \quad \text{then } |\varphi(k)|^2 dk = \text{prob. of finding particle in } dk \text{ w/ momentum } k. \end{array}\right\} \quad (27)$$

If this is to be true, then both Ψ & φ should be normalizable in the same way, i.e. if $\int |\Psi|^2 dx = 1$, then $\int |\varphi|^2 dk = 1$ also. That this is in fact true is a result of Parseval's Theorem, i.e. ...

$\boxed{\text{PARSEVAL'S THEOREM}}$ If $A(x)$ and $B(k)$ are a Fourier transform pair, i.e.

$A(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} B(k) e^{ikx} dk$ & $B(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(x) e^{-ikx} dx$, then the normalization $\int_{-\infty}^{\infty} |A(x)|^2 dx = 1$ implies the norm $\int_{-\infty}^{\infty} |B(k)|^2 dk = 1$ (and vice-versa).

Proof (w/ all $\int = \int_{-\infty}^{\infty}$)

$$\int |B(k)|^2 dk = \frac{1}{2\pi} \int dk \left[\int A(x) e^{-ikx} dx\right]^* \left[\int A(x') e^{-ikx'} dx'\right]$$

$$= \int dx\, A^*(x) \int dx' A(x') \left[\frac{1}{2\pi} \int dk\, e^{ik(x-x')}\right] \quad \text{this [ ] is } \delta(x-x')$$

$$= \int dx\, A^*(x) \underbrace{\int dx' A(x')\, \delta(x-x')}_{= A(x)} = \int dx\, |A(x)|^2$$

so,

$$\int |B(k)|^2 dk = \int |A(x)|^2 dx, \text{ and: } \underline{\underline{\int |B|^2 dk = 1 \text{ iff } \int |A|^2 dx = 1}}. \quad \textbf{QED} \quad (28)$$

Just as the uncertainty relation $\Delta k \Delta x \sim 1$ suggested that momentum k and position x were linked variables on equivalent footing, so now we see that the distributions $\Psi(x,0)$ & $\varphi(k)$ can be treated equivalently (in their own spaces).

Expectation-Value Postulate of QM.

3) We now take a step which constitutes a postulate of QM. It is done so as to give the notion of ψ & φ as "probability distributions" as precise a meaning as possible for the motion of QM particles, and done because we know that (in QM) we cannot determine the particle's position x and momentum k to within tolerances better than $\Delta k \Delta x \sim \hbar$. So, although we cannot specify position x precisely, we can calculate...

$$\rightarrow \langle x(t) \rangle = \int_{-\infty}^{\infty} \psi^*(x,t) \{x\} \psi(x,t)\, dx = \int_{-\infty}^{\infty} x\, |\psi(x,t)|^2\, dx. \qquad (29)$$

$\langle x(t) \rangle$ is the center-of-gravity, or average (mean) position of the distribution $|\psi|^2$ that measures the particle's probable location. Similarly:

$$\rightarrow \langle k \rangle = \int_{-\infty}^{\infty} \varphi^*(k) \{k\} \varphi(k)\, dk = \int_{-\infty}^{\infty} k\, |\varphi(k)|^2\, dk, \qquad (30)$$

is the mean momentum associated with the distribution $|\varphi|^2$ that measures the particle's probable momentum values. In the packet analysis example on pp. Pack 5-6, we would have $\langle x(t) \rangle = v_g t$ specifying the motion of the center of the packet, and $\langle k \rangle = k_0$ = its nominal wave #.

This idea of settling for mean values of dynamical quantities as being the maximum information available in a theory characterized by uncertainties in those quantities, and by probability distributions for them, is now elevated to the following:

> **POSTULATE** For a given QM state or system, specified by a wave fcn $\psi(\mathbf{r},t)$, there corresponds to any observable quantity $f(\mathbf{r})$ -- e.g. position $\mathbf{r}$, potential energy $V(\mathbf{r})$, etc. -- a "most probable value" or "expectation value", defined by: $\langle f \rangle = \int_\infty \psi^*(\mathbf{r},t) \{f(\mathbf{r})\} \psi(\mathbf{r},t)\, d^3r$. Generally, $\langle f \rangle$ is a fcn of time t, and it gives the maximum information possible regarding measurable values of $f(\mathbf{r})$ in the QM system.

Calculation of mean momentum at $t=0$ w.r.t. space wavefcn $\psi(x,0)$.

NOTE: In $\langle f\rangle = \int_\infty \psi^* \{f\} \psi\, d^3r$, f is "sandwiched" between ψ^* & ψ. If f is an ordinary fcn of $\mathbf{r}$ (e.g. $f=\mathbf{r}, \mathbf{r}^2, \ldots$ etc.), the sandwich disappears, and $\langle f\rangle = \int_\infty f|\psi|^2 d^3r$. If, however, f is an operator (say $f = \partial/\partial\mathbf{r} = \nabla$), then clearly $\int_\infty \psi^*\{f\}\psi\, d^3r$ differs from $\int_\infty f|\psi|^2 d^3r$. We go with the definition $\langle f\rangle = \int_\infty \psi^*\{f\}\psi\, d^3r$, and next show why this is useful.

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4) A QM particle described by a wavefcn $\psi(x,t)$ in 1D has -- at time $t=0$ -- a mean position and mean momentum given by (all $\int = \int_{-\infty}^{+\infty}$)...

$$\langle x\rangle_0 = \int \psi_0^*(x)\{x\}\psi_0(x)\,dx, \text{ w/ } \psi_0(x) = \psi(x,0); \tag{31A}$$

$$\langle p\rangle_0 = \int \varphi^*(k)\{\hbar k\}\varphi(k)\,dk, \text{ w/ } p = \hbar k = \text{momentum}. \tag{31B}$$

To get $\langle p\rangle_0$, we have to use the transform $\psi_0(x) \to \varphi(k) = \frac{1}{\sqrt{2\pi}}\int \psi_0(x) e^{-ikx} dx$. It would be convenient if we could calculate both $\langle x\rangle_0$ & $\langle p\rangle_0$ from just $\psi_0(x)$ alone. In fact, this can be done, by transforming (31B) back to x-space, as...

$$\rightarrow \langle p\rangle_0 = \frac{\hbar}{2\pi}\int dk \left[\int \psi_0(x')e^{-ikx'}dx'\right]^* \{k\} \left[\int \psi_0(x) e^{-ikx} dx\right]$$

$$= \frac{\hbar}{2\pi}\int dk \int dx' \psi_0^*(x') e^{ikx'} \underbrace{\int dx\, \psi_0(x)\, k e^{-ikx}}_{F(k)}. \tag{32}$$

Now, perform a trick on $F(k)$...

$$k e^{-ikx} = i\frac{\partial}{\partial x} e^{-ikx} \quad \leftarrow \text{assumes } k \text{ is indept of } x \text{ (true for free particle)}$$

$$\xrightarrow{\text{so}} F(k) = \int dx\, \psi_0(x)\, i\frac{\partial}{\partial x}e^{-ikx} = i\int \psi_0(x)\, d e^{-ikx} \quad \text{do a partial integration} \tag{33}$$

$$= i\left[\psi_0(x)e^{-ikx}\Big|_{x=-\infty}^{x=+\infty} - \int e^{-ikx} d\psi_0(x)\right] = -\int dx\, e^{-ikx}\frac{\partial}{\partial x}\psi_0(x).$$

$\rightarrow 0$ ($\psi_0(x)$ vanishes at $|\infty|$)

So (32) becomes...

$$\rightarrow \langle p\rangle_0 = -\frac{i\hbar}{2\pi}\int dk \int dx' \psi_0^*(x') e^{ikx'} \int dx\, e^{-ikx}\frac{\partial}{\partial x}\psi_0(x) \quad \text{change order of integration}$$

$$= -i\hbar \int dx' \psi_0^*(x') \int dx \frac{\partial}{\partial x}\psi_0(x) \cdot \left[\frac{1}{2\pi}\int dk\, e^{ik(x'-x)}\right] \leftarrow [\;] = \delta(x'-x)$$

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