Notes on Selected topics to accompany Sakurai's "Modern Quantum Mechanics"

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Properties of a physically acceptible wavefunction

A physically acceptible wavefunction must

1. be square-integrable
2. be single-valued
3. be continuous
4. have its the derivative continuous as long as the potential is finite (even if the potential is discontinuous at some point)

Let's discuss the first three points briefly and elaborate on the fourth point.

Square-integrability

In order for Born's probabilistic interpretation of the wavefunction to hold, the wavefunction must be square-integrable, *i.e.*, the integral $\int_{-\infty}^{+\infty} dx\, |\psi(x)|^2$ must be finite. It is in connection to this condition, we say that a wavefunction must vanish at $\pm\infty$.

Single-valued

Again, it is due to the probabilistic interpretation of the wavefunction, we want $\psi(x)$ to be single-valued. The quantity $\int_a^b dx\, |\psi(x)|^2$ is the probability for locating a particle between the locations a and b. We want this value to be a real number, and we do not want two (or more) values for this quantity. In general, probability distribution functions or probability density functions (in our case, $|\psi(x)|^2$) are supposed to be single-valued.

Continuity

We have

$$\psi^{(2)}(x) = \frac{2m}{\hbar^2}\,(V(x) - E)\,\psi(x)$$

If $V(x)$ is finite, $\psi(x)$ is also finite (according to point-1 discussed above), and since we are also considering a system with finite energy, E, the L.H.S., $\psi^{(2)}(x)$ is also finite.

For $\psi^{(2)}(x)$ to exist, $\psi^{(1)}(x)$ must exist in the first place (and be finite) and it has to be differentiable, hence continuous. This, in turn, means that $\psi(x)$ is also differentiable and continuous.

Derivative continuity/discontinuity

To show that $\psi^{(1)}(x)$ is continuous at some point, x_0, we have to show that the left and right limits of $\psi^{(1)}(x)$ at x_0 are same

$$\begin{aligned} \lim_{\epsilon\to 0} \psi^{(1)}(x)\Big|_{x_0-\epsilon} &= \lim_{\epsilon\to 0} \psi^{(1)}(x)\Big|_{x_0+\epsilon} \\ \Rightarrow \lim_{\epsilon\to 0} \left[\psi^{(1)}(x)\right]_{x_0-\epsilon}^{x_0+\epsilon} &= 0 \end{aligned}$$

Let's introduce $\int_a^b df(x) = |f(x)|_a^b$ in the above equation.

$$\begin{aligned} \lim_{\epsilon\to 0} \int_{x_0-\epsilon}^{x_0+\epsilon} d\left[\psi^{(1)}(x)\right] &= 0 \\ \Rightarrow \lim_{\epsilon\to 0} \int_{x_0-\epsilon}^{x_0+\epsilon} dx\,\psi^{(2)}(x) &= 0 \\ \Rightarrow \lim_{\epsilon\to 0} \int_{x_0-\epsilon}^{x_0+\epsilon} dx\,\left[\frac{2m}{\hbar^2}\,(V(x) - E)\right]\psi(x) &= 0 \end{aligned} \quad (1)$$

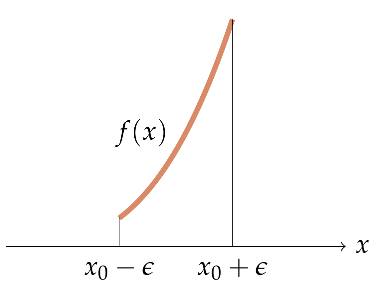

Figure 1: The area under $f(x)$ approaches zero as $\epsilon \to 0$.

Now, in order to show that $\psi^{(1)}(x)$ is continuous at x_0, we have to ensure that the above equation is true. For this, let us try to understand the geometric meaning of the following integral identity for any finite $f(x)$.

$$\lim_{\epsilon\to 0} \int_{x_0-\epsilon}^{x_0+\epsilon} dx\, f(x) \quad (2)$$

The integral denotes the area under the function $f(x)$ between $x_0 - \epsilon$ and $x_0 + \epsilon$. Irrespective of the nature of $f(x)$, the area under the function must approach zero, as the region under the function will become thinner and thinner as ϵ approaches zero (see Figure 1).

Discontinuity of $\psi^{(1)}(x)$

When the potential is not finite, for some values of x, as in the case of Dirac-delta potential

$$V(x) \quad = \quad -A\delta(x - x_0),$$

we have

$$\psi^{(2)}(x_0) = \frac{2m}{\hbar^2}\left[-A\delta(x - x_0) - E\right]\psi(x_0).$$

So, $\psi^{(2)}(x)$ is not defined at $x = x_0$. Hence, we can conclude that $\psi^{(1)}(x)$ is not differentiable/continuous at x_0. We can however find out the value by which the left limit differs from the right limit.

$$\begin{aligned} \lim_{\epsilon \to 0} \psi^{(1)}(x)\Big|_{x_0+\epsilon} - \lim_{\epsilon \to 0} \psi^{(1)}(x)\Big|_{x_0-\epsilon} &= \lim_{\epsilon \to 0}\left[\psi^{(1)}(x)\right]_{x_0-\epsilon}^{x_0+\epsilon} \\ &= \int_{x_0-\epsilon}^{x_0+\epsilon} dx\ \left[-A\delta(x - x_0)\right]\psi(x) \\ &= -A\psi(x_0) \qquad (3) \end{aligned}$$

In the last step, we have used the known property of the Dirac delta function, $\int dx\, f(x)\delta(x - x_0) = f(x_0)$.

You need Eq.(3) for finding the relation between k (as in $e^{\pm ikx}$) and A, when you solve the Dirac delta potential problems.