CONTINUITY OF THE WAVE FUNCTION - BORN'S CONDITIONS REVISITED

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Born's conditions on the wave function in one-dimensional quantum mechanics can be a bit mysterious, but in going through the *Mastering Quantum Mechanics* online course from MIT (link here), I came across a very nice discussion of a couple of these conditions, due to Barton Zwiebach. (Incidentally, if you want a bit more background on quantum mechanics, I can highly recommend the trio of courses that make up *Mastering Quantum Mechanics*; Zwiebach's lectures are extremely clear and well-explained, and a joy to listen to. Part 1 of the course reviews a lot of what's in the early chapters of Griffiths's *Introduction to Quantum Mechanics* book that I've covered in my blog, but there are many gems of new insight to be found in the online course. At the time of writing, the course is not in session, but all the course videos and lecture notes are still available. You just won't be able to submit any of the homework answers.)

Zwiebach discusses the requirements that the wave function $\psi(x)$ and its first derivative $\psi'(x)$ are both continuous, and gives examples of when these rules can be violated. We start by looking at the time-independent Schrödinger equation in one dimension:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)=(E-V(x))\psi(x) \tag{1}$$

Basically, the restrictions on ψ arise from restrictions on the types of potential function $V(x)$ that we allow into the theory. We've seen examples in the blog of an unbounded continuous potential (the harmonic oscillator), a potential with finite discontinuities (the finite square well), a potential with an infinite wall (sometimes called a *hard wall*: the infinite square well), and one or more singularities, represented by delta functions. Generally, these are the only types of potential that we will consider, so that, for example, we don't allow derivatives of delta functions or powers of delta functions. We also don't allow pathological potentials (such as the Weierstrass function, which is continuous everywhere, but differentiable nowhere).

These conditions lead to the requirement that $\psi(x)$ must be continuous everywhere, although it may have a few isolated points where it's not differentiable. For example, the wave function for a delta function well has a peak at the location of the delta function where it is not differentiable. We require the first derivative $\psi'(x)$ to be continuous everywhere *except* at points where $\psi(x)$ itself is not differentiable; at these points, $\psi'(x)$ is allowed to have a finite discontinuity (that is, a step up or down). This happens with the delta function potential.

At points where $\psi'(x)$ has a step discontinuity, its derivative $\psi''(x)$ is a delta function, since the derivative of a step function gives rise to a delta function. This behaviour must be allowed in order for 1 to make sense. The second derivative $\frac{d^2}{dx^2}\psi(x)$ must contain the behaviour of the potential due to the presence of $V(x)$ on the RHS of this equation. If the potential contains a delta function then so must $\frac{d^2}{dx^2}\psi(x)$. However, since we're not allowing $V(x)$ to contain *derivatives* of the delta function, then, working backwards from $\psi''(x)$, $\psi'(x)$ cannot contain delta functions which means that $\psi(x)$ cannot contain any step functions (discontinuities). Thus $\psi(x)$ must be continuous.

There are basically four types of potential that we are allowed to consider:

(1) $V(x)$ is continuous everywhere. That means that the RHS of 1 is also continuous everywhere, so $\psi''(x)$ must also be continuous everywhere. Again, working backwards, this means that ψ' and ψ must also be continuous everywhere.
(2) $V(x)$ contains finite discontinuities (jumps or steps). This means that ψ'' contains discontinuities, which in turn means that ψ' must be continuous with a finite number of points where its derivative (ψ'') is discontinuous.
(3) $V(x)$ contains delta functions. This is the case considered above, leading to ψ'' containing delta functions, ψ' containing discontinuities and ψ being continuous.
(4) $V(x)$ contains one or more hard walls, as in the infinite square well. The wave function ψ is zero everywhere the potential is infinite, so $\psi' = 0$ also in this region. However, as in the case of the infinite square well, $\psi' \neq 0$ just inside the wall, so ψ' is discontinuous at the wall boundary. However, ψ itself is still continuous. Looking at 1, it's a bit difficult to interpret what happens to ψ'' outside the wall (where $V = \infty$), since the RHS is the product of ∞ with zero. To be proper about it, we really shouldn't consider what happens outside the wall at all, since there is always zero probability that the particle will ever be found there anyway.

Hopefully this provides a bit more motivation for a couple of Born's conditions on the wave function.

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