BORN'S CONDITIONS ON THE WAVE FUNCTION

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Max Born's best known contribution to quantum mechanics was his proposal that the wave function, or rather its square modulus, should be interpreted as the probability density for finding the system in a given state at a given time. However, he also proposed four conditions on the wave function which are used in finding many solutions of the Schrödinger equation. Remarkably few textbooks refer to these conditions, or at least, if they do, they don't credit Born as their originator.

As always, it's useful to write down the Schrödinger equation (in one dimension) so we can see how Born's conditions fit in.

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V(x,t)\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{1}$$

Born's conditions to be imposed on the wave function $\Psi(x,t)$ are:

(1) The wave function must be single valued. This means that for any given values of x and t, $\Psi(x,t)$ must have a unique value. This is a way of guaranteeing that there is only a single value for the probability of the system being in a given state. Actually, if Ψ is a proper mathematical function, it will satisfy this requirement automatically, since one condition all functions must satisfy is that they are single-valued. The most common example of a 'function' (that isn't really a function) encountered by most undergraduate math students is the inverse sine (or arcsin), which gives the angle corresponding to a particular value. Thus any multiple of π has a sine of 0, so in principle, the inverse sine could give any multiple of π as its value and thus it seems this is a multi-valued function. However, in practice, only the range from 0 (inclusive) to π (exclusive) is used in the 'proper' arcsin function.

(2) The wave function must be square-integrable. In other words, the integral of $|\Psi|^2$ over all space must be finite. This is another way of saying that it must be possible to use $|\Psi|^2$ as a probability density, since any probability density must integrate over all space to give a value of 1, which is clearly not possible if the integral of $|\Psi|^2$ is

infinite or zero. One consequence of this proposal is that Ψ must tend to 0 for infinite distances.

(3) The wave function must be continuous everywhere. That is, there are no sudden jumps in the probability density when moving through space. If a function has a discontinuity such as a sharp step upwards or downwards, this can be seen as a limiting case of a very rapid change in the function. Such a rapid change would mean that the derivative of the function was very large (either a very large positive or negative number). In the limit of a step function, this would imply an infinite derivative. Since the momentum of the system is found using the momentum operator, which is a first order derivative, this would imply an infinite momentum, which is not possible in a physically realistic system. Such an infinite derivative would also violate condition 4.

(4) All first-order derivatives of the wave function must be continuous. Following the same reasoning as in condition 3, a discontinuous first derivative would imply an infinite second derivative, and since the energy of the system is found using the second derivative, a discontinuous first derivative would imply an infinite energy, which again is not physically realistic.

Having stated Born's conditions, however, we need to note that several systems commonly studied in introductory quantum mechanics courses do violate one or more of them. For example, the 'particle in a box' system is composed of a particle moving in a box with infinitely high sides, represented by a potential function that is zero in a limited area, and infinite outside this area. In such a system, the third condition (continuity of the wave function) is imposed to find a solution, but the solution so found violates the fourth condition, in that the derivative of the wave function is *not* continuous at the boundary of the box.

The particle in a box is clearly not a physically realistic system, however, since there is no known physical mechanism which can generate an infinitely deep potential well. Despite that, the system is still useful as a model of some real-life situations in which a particle is found in a very deep well. And of course the particle in a box provides a relatively painless way of introducing many of the concepts of quantum mechanics, so is useful heuristically, even if it's not entirely realistic.

It's rather odd that most textbooks gloss over these conditions (well, they usually mention the square integrable one since it's essential for using the wave function as a probability density) by simply stating that the wave function and its derivatives are required to be continuous, without explaining why.

In the online MIT course, Barton 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:

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

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 2 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 2 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 2, 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.

REFERENCES AND FURTHER READING

(1) Griffiths, David J. (2005), *Introduction to Quantum Mechanics*, 2nd Edition; Pearson Education, Chapter 2. (Doesn't mention Born by name, but does use some of the conditions.)
(2) Zwiebach, Barton, Online course *Mastering Quantum Mechanics Part 1: Wave Mechanics*. Archive available here.

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