Four Conditions that a Physically Meaningful Spatial Wavefunction must Satisfy—C.E. Mungan, Fall 2018

FIRST PAIR OF CONDITIONS

The wavefunction must be **normalizable**,

$$\int_{-\infty}^{\infty} \left|\psi(x)\right|^2 dx = 1 .$$

This has two implications:

1. The wavefunction $\psi(x)$ must be finite everywhere. Normally a wave cannot have infinite amplitude!

Rare exception: A wavefunction is sometimes represented by a Dirac delta function, particularly for a plane wave in the momentum representation. However, a Dirac delta is actually a *distribution* not a *function*: it represents a very sharp peak with infinitesimal width and arbitrarily large height such that its area remains unity, and so this exception is not really physical.

2. The wavefunction must go to zero fast enough as $x \to \pm\infty$. Specifically, faster than $|x|^{-1/2}$ as $|x| \to \infty$. For example, $A/\ln(kx)$ is not an acceptable wavefunction over all $x > k^{-1}$ (LogIntegral[x] in Mathematica *diverges* for large x) whereas $A\text{sinc}(kx)$ is acceptable (SinIntegral[x] levels off to $\pi/2$ for large x).

Special exception: A harmonic plane wave has constant amplitude for all x. But in reality all particles are confined (if nothing else in a box the size of the universe) and hence must eventually cut off.

SECOND PAIR OF CONDITIONS

The wavefunction must be **smooth**. This again has two implications:

3. The wavefunction must be continuous everywhere. Trying to fit a jump such as in a Fourier series would require wavelengths down to zero, or equivalently wavenumbers or particle momenta extending up to infinity.

Rare exception: We can write down a Fourier series for say a square pulse which has discontinuities. But that's not actually physically realizable, any more than our Dirac delta function was in case 1. Physicists often adopt such mathematical models for simplicity, but they are only approximations just as are frictionless surfaces, point particles, and the like.

4. The wavefunction must be differentiable everywhere. There can be no cusps; its slope must be continuous. Otherwise the second derivative would be infinite at that point, which corresponds to infinite kinetic energy of the particle!

Important exception: If the potential energy jumps up to positive infinity in some region of space, then the particle's kinetic energy would have to become negative infinity in that region, which is impossible. The only way to prevent that from happening is to exclude the particle from that region by making its probability density and hence its wavefunction equal to zero. Although infinite potential energy is physically unachievable, it is a common approximation used for example in the "particle in a box" model and so it is best to modify condition 4 as follows:

4. The derivative $d\psi/dx$ must be continuous anywhere that U is finite, whereas ψ must equal zero anywhere that U is infinite (even if that requires a sudden discontinuity in $d\psi/dx$).