New mathematical proof of the uncertainty relation

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We present a new proof of the uncertainty relation for wave functions that are absolutely integrable and have absolutely integrable Fourier transforms.

There are two kinds of mathematical argument for the uncertainty relation in many of the quantum-mechanics texts. One is an elegant argument based on the canonical commutation relation (CCR) and the Schwartz inequality, for wave functions in the domain of both of the operators x and p. The other is an intuitively appealing, but hand-waving argument, based on interference.

Although the two arguments are clearly related in content, since they both say something about Fourier transforms, their mathematical contents are not identical. As it is given in Merzbacher's text,[1] for example, the interference argument assumes that, say, the k-space wave packet is appreciably nonzero only in a region of size Δk, and that there it is continuous and has slowly varying phase. Then rapid oscillations in the integrand of the Fourier transform give destructive interference and no appreciable contribution for the x-space wave function outside a region of size roughly $\Delta x \sim 1/\Delta k$, centered near the average position of the x-space wave packet.

In this note, we abstract what we believe to be the mathematical content of this argument, and show that it can be put on a footing of the same generality, rigor, and simplicity as the argument based on the CCR.

Let $f(x)$ be an absolutely integrable function of one real variable; i.e., $\int |f|\, dx < \infty$, where the notation indicates integration from $-\infty$ to $+\infty$; and let

$$\hat{f}(k) = (2\pi)^{-1/2} \int e^{-ikx} f(x)\, dx \qquad (1)$$

be its Fourier transform. We assume that $\hat{f}$ is also absolutely integrable. Although it plays no technical role in our discussion, let us mention that, by the Riemann-Lebesgue lemma,[2] this means that both f and $\hat{f}$ are continuous, uniformly bounded functions that vanish at infinity. We believe the discussion below justifies the assertion that these two properties of a wave packet, that it simultaneously be absolutely integrable and have the smoothness of the Fourier transform of an absolutely integrable function, are the mathematical analogs of the requirements that the wave function be appreciable only in a finite region, say in k space, so that a rough meaning can be given to Δk, and have sufficiently slowly varying phase, so that interference in the Fourier transform produces a roughly defined Δx obeying the uncertainty relation.

As measures of the spreads in the wave packets f and $\hat{f}$, we introduce the following notion. Let B be a region of integration in x space with a finite size Δx, say, an interval or a union of disjoint intervals.[3] Then if we integrate over B, we get a fraction of the integral over the whole real line

$$\int_B |f(x)|\, dx = (1-\epsilon) \int |f(x)|\, dx, \qquad (2)$$

where $0 \le (1-\epsilon) \le 1$. We then say that we have captured a fraction $1-\epsilon$ of the wave packet f within a spread Δx. The extreme value $1-\epsilon = 0$ corresponds to a situation where f vanishes (almost) everywhere in the region of integration B, while the other extreme $1-\epsilon = 1$ corresponds to one where f vanishes almost everywhere outside the region B. As we indicate later, the practical idea is to avoid the extremes and choose the fraction to be some convenient number, such as $1-\epsilon = \frac{1}{2}$ or $\frac{3}{4}$, and then choose a region of integration B that captures $1-\epsilon$ of the wave packet within the smallest possible spread,

$$\Delta x = \int_B dx. \qquad (3)$$

To amplify a bit, as long as we choose a fixed ϵ so that $0 < 1-\epsilon < 1$, there is always at least one finite region of integration B for which Eq. (2) is true; e.g., $\int_{-R}^{R} |f|\, dx$ is a monotone, nondecreasing function of R that takes all values between 0 and $\int |f|\, dx$. It is a fact that there is a minimum value of the spread Δx in Eq. (3) over all regions of integration B (not necessarily simple intervals) that satisfy Eq. (2); and it is a fact that there is at least one region of integration B for which the minimum Δx corresponding to a given ϵ is actually achieved.[4]

We do the same thing in k space, picking a region of integration $\hat{B}$ of finite size Δk that captures $1-\hat{\epsilon}$ of $\hat{f}$:

$$\int_{\hat{B}} |\hat{f}(k)|\, dk = (1-\hat{\epsilon}) \int |\hat{f}(k)|\, dk, \qquad (4)$$

$$\Delta k = \int_{\hat{B}} dk. \qquad (5)$$

The fixed fractions $1-\epsilon$ and $1-\hat{\epsilon}$ may be chosen arbitrarily and independently of each other. Of course, if the wave packet were to be nonvanishing over a large region in x and/or k, we would find that choosing $1-\epsilon$ and/or $1-\hat{\epsilon}$ close to unity forces a large value for Δx and/or Δk. For example, if we choose f to be a finite linear combination of polynomials times Gaussian factors with varying centers and widths, then $\hat{f}$ is a finite linear combination of polynomials times Gaussians times simple phase factors to account for the mean locations in x space; and neither f nor $\hat{f}$ vanishes on any nonempty open set of the real line; for otherwise, as entire functions, they would have to vanish identically. In such a case, both Δx and Δk diverge as ϵ and $\hat{\epsilon}$ become small; and the product $\Delta x \Delta k$ becomes far larger than one would expect for the minimum order of magnitude, unity, for the uncertainty product.

Although we might be able to capture all of one or the other of f and $\hat{f}$ (ϵ or $\hat{\epsilon}$ equal to zero) in a bounded region, it is impossible in principle to capture all of both in bounded regions, because if one of the two functions vanishes outside a bounded region, the other is an entire function, and can vanish only at isolated points of the real axis, unless both functions vanish identically.

Thus, we find it prudent not to be so greedy as to try to capture all of the two wave packets (or at least not all of

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both of them) within a finite spread, but rather to choose some compromise which captures a reasonable fraction within a sensibly small spread. This formulation exhibits the well known, intrinsic imprecision in the *definition* of Δx and Δk, which is inherent in the interference argument, and which is often a source of confusion for beginning quantum-mechanics students.[5]

Having emphasized the element of choice in the definition of the spreads Δx and Δk for given f and $\hat{f}$, we now give a simple proof and mathematical statement of the uncertainty principle, which builds in that freedom of choice. The essential technical assumption is that both f and $\hat{f}$ be absolutely integrable. Then we can write down the two elementary inequalities

$$\int_B |f|\,dx \le \Delta x \sup_x |f| \le \Delta x\,(2\pi)^{-1/2} \int |\hat{f}|dk, \quad (6)$$

$$\int_{\hat{B}} |\hat{f}|\,dk \le \Delta k \sup_k |\hat{f}| \le \Delta k\,(2\pi)^{-1/2} \int |f|dx, \quad (7)$$

Multiplying these together, and using Eqs. (2) and (4), we get

$$2\pi(1-\epsilon)(1-\hat{\epsilon}) \le \Delta x \Delta k. \quad (8)$$

The argument generalizes trivially to functions $f(x_1, x_2, \ldots, x_n)$ which are absolutely integrable in x_1 for fixed $x_2, \ldots, x_n$, and which have one-dimensional Fourier transforms $\hat{f}(k_1, x_2, \ldots, x_n)$ that are absolutely integrable in k_1 for fixed $x_2, \ldots, x_n$, or to the integrals of f and $\hat{f}$ over $x_2, \ldots, x_n$, if one assumes the natural integrability condition.

Another variation of the argument for n dimensions is to assume integrability in both x space and k space with respect to d^nx and d^nk. The sizes of the regions of integration B and $\hat{B}$ become their n-dimensional volumes

$$\Delta V_x = \int_B d^nx,\ \ \Delta V_k = \int_{\hat{B}} d^nk. \quad (9)$$

If we define $1-\epsilon$ and $1-\hat{\epsilon}$ by the n-dimensional analogs of Eqs. (2) and (4), the uncertainty relation reads

$$(2\pi)^n\,(1-\epsilon)(1-\hat{\epsilon}) \le \Delta V_x \Delta V_k. \quad (10)$$

For example, in three dimensions, if B and $\hat{B}$ are spheres with radii Δx and Δk we get

$$[(9/2)\pi(1-\epsilon)(1-\hat{\epsilon})]^{1/3} \le \Delta x \Delta k. \quad (11)$$

To conclude, let us emphasize that we do not in the least claim that our discussion is better than the CCR discussion. It is simply different. One difference is that the CCR argument applies to a smaller class of wave functions, as we show in the Appendix. Nor do we advocate that our discussion replace the intuitively instructive interference argument. We do feel that it is a precise statement of that argument, and that it can claim a certain simplicity.

APPENDIX

Although we feel that the following discussion is too technical to be appropriate as part of a lecture in a typical first year graduate level quantum mechanics course, it is certainly not too sophisticated for such students; and parts of it might be useful as homework exercises on Hilbert spaces and Fourier transforms.

We want to show that the CCR argument assumes a smaller class of wave functions than our abstract interference argument. The CCR argument assumes that f is square integrable, so that it is a physical wave packet, and that xf and $-if'$ are square integrable, so that the expectation values of x^2 and p^2 exist. Thus, $(1+|x|)f$ is square integrable. Since

$$f = (1+|x|)^{-1}(1+|x|)f, \quad (12)$$

and $(1+|x|)^{-1}$ is square integrable (in one dimension), it follows by the Schwartz inequality that f is integrable. We can apply the same argument in k space, because if f is square integrable, so is $\hat{f}$; and the square integrability of $-if'$ means that of $k\hat{f}$. Thus, the hypotheses of the CCR argument imply our hypotheses that f and $\hat{f}$ are integrable.

The converse, however, is false. Even if we make the stronger assumption that f and $\hat{f}$ are not only integrable, but square integrable, which is necessary for f to be a physical wave packet, it is not always true that xf and $k\hat{f}$ are square integrable. A counterexample is the function

$$f = (1+x^2)^{-(1+\epsilon)/2},\ \ 0<\epsilon<1. \quad (13)$$

It is square integrable, so $\hat{f}$ is, too; and it is integrable. Because $\hat{f}$ can be written in terms of a Bessel function,

$$\hat{f} = 2^{(1-\epsilon)/2}\,\Gamma[(1+\epsilon)/2]^{-1}|k|^{\epsilon/2}K_{\epsilon/2}(|k|), \quad (14)$$

which is continuous and exponentially decreasing, it is also integrable. Now $-if'$ is square integrable, but xf is not.

Thus, the one-dimensional wave functions such that f, xf, and $-if'$ are normalizable form a smaller class than those for which f and $\hat{f}$ are both integrable and square integrable.

[1] E. Merzbacher, *Quantum Mechanics*, 2nd ed. (Wiley, New York, 1970), pp. 17–22 and 24.

[2] The proof of the Riemann-Lebesgue lemma is nontrivial, and there is no reason why most of us, as physicists and physics teachers, should feel an obligation to be familiar with it. As people who operate with mathematical ideas, however, we should feel no reluctance to understand what it states and to exploit its consequences, as does, to cite a conspicuous example, the aeronautical engineer M. J. Lighthill in his chapter on "The asymptotic estimation of Fourier transforms" in *Fourier Analysis and Generalized Functions* (Cambridge University, London, 1960).

[3] To put it in precise language, B is a Borel set with finite Lebesgue measure.

[4] There may in principle be several regions of integration that give the same minimum spread for a fixed ϵ.

[5] There is an analogous imprecision in the CCR argument, having to do with the arbitrary choice of the root-mean-square deviation rather than some other positive moment as the measure of spread.