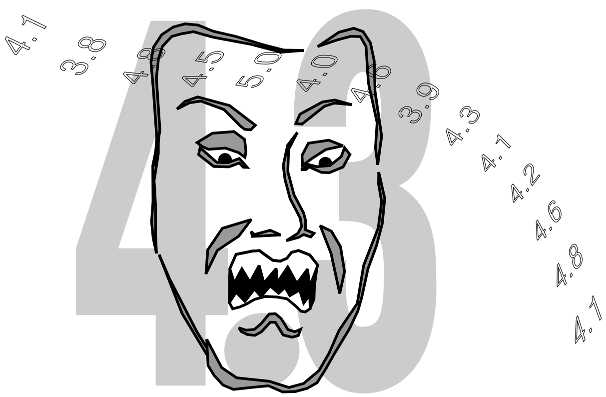
PHYSNET

MISN-0-243

WAVE FUNCTIONS, PROBABILITY, AND MEAN VALUES



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Project PHYSNET Physics Bldg. Michigan State University East Lansing, MI

WAVE FUNCTIONS, PROBABILITY, AND MEAN VALUES

by

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Title: **Wave Functions, Probability, and Mean Values**

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Input Skills:

1. State the relation of wave functions to probability density (MISN-0-242).
2. Describe the harmonic oscillator wave functions (MISN-0-242).
3. Interpret momentum as a derivative operator (MISN-0-242).
4. Define complex conjugation of a complex number (MISN-0-59).

Output Skills (Knowledge):

K1. Define quantum mechanical uncertainty in position and momentum in terms of RMS deviation from the mean.

K2. Show how a system's quantum mechanical uncertainties in position and momentum are obtained from its wave function.

Output Skills (Rule Application):

S1. Given a system's wave function, find the position and momentum uncertainty product for the system.

Post-Options:

1. "Numerical Solution of the Schrödinger Equation for the Hydrogen Atom" (MISN-0-245).
2. "The Time-Dependent Schrödinger Equation: Derivation of Newton's Second Law" (MISN-0-248).

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New authors, reviewers and field testers are welcome.

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1. Definition of Uncertainty

Heisenberg's Uncertainty Relation is often stated[1] as:

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}. \qquad (1)$$

Since the lower limit of this uncertainty product has a precise value, the uncertainties in position and momentum, Δx and Δp, must have correspondingly precise definitions. How would one precisely define, say, the uncertainty in the position of an atom in a diatomic molecule or of an electron in an atom? Any such specification must begin with a precise knowledge of the spatial probability distribution $P(x)$ for the particle being considered. Suppose we have the probability distribution $P(x) = |\psi(x)|^2$ shown in Fig. 1. The "position" of this particle can be reasonably stated[1] as:

$$\text{"position"} \;= \bar{x} \pm \Delta x, \qquad (2)$$

where $\bar{x}$ is the particle's mean position. One meaning one might try to ascribe to Eq. (2) is that if one determines the position of the particle a large number of times, it will be found to be within the limits in Eq. (2) in 50% of the determinations. We would say "it is within those limits 50% of the time."

[1] See "The Uncertainty Relations" (MISN-0-241).

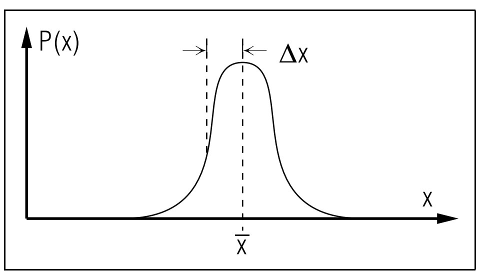

Figure 1. A possible probability density.

However, it has been found that in order to be able to derive and state a universal lower limit to the uncertainty product shown in Eq. (1), one needs a different kind of specification of uncertainty. The one used to derive the limit shown in Eq. (1) is that of "root-mean-square (RMS) deviation from the mean":

$$\Delta x = \sqrt{\overline{(x - \bar{x})^2}}\ .$$

▷ Identify each piece of the above quote with an ever deeper part of the expression on the right hand side of the equation.

The next task is to see how to compute $\bar{x}$ and $\overline{(x-\bar{x})^2}$ from the probability density $P(x)$.

2. Quantum Mechanical Mean Values

2a. Definition of Mean Value. For a set of N identical objects located at positions x_n ($n = 1, 2, \ldots, m$) the mean value of, say, x^4 for these objects would be (Appendix A):

$$\overline{x^4} = \sum_{n=1}^{m} x^4 P(x_n)\,.$$

where $P(x_n)$ is the fraction of the objects located at x_n and the bar over x indicates its mean value. Equally, $P(x_n)$ is the probability that any one specific object is located at x_n. In general, the mean value of a function $f(x)$ is then (Appendix A):

$$\overline{f(x)} = \sum_{n=1}^{m} f(x_n) P(x_n).$$

Generalizing to a continuum of locations x,

$$\overline{f(x)} = \int_{-\infty}^{+\infty} f(x) P(x)\, dx, \qquad (3)$$

where $P(x)$ is now the *probability density* at the point x. This mean value equation is used throughout statistical physics.[2]

[2] See, for example, "Energy Distribution Functions" (MISN1-0-159).

2b. Mean Value and Probability Density in Quantum Physics. For quantum physics, the mean position of an object described by the wave function $\psi(x)$ is:

$$\bar{x} = \int_{-\infty}^{+\infty} xP(x)\,dx = \int_{-\infty}^{+\infty} x|\psi(x)|^2\,dx,$$

since the quantum mechanical probability density[3] is $|\psi|^2$. Thus, given any $\psi(x)$ representing the state of a particle, we can perform the above integral and obtain the mean value of the particle's position.[4] Similarly, the particle's mean square position can be calculated from its wave function:

$$\overline{x^2} = \int_{-\infty}^{+\infty} x^2 P(x)\,dx = \int_{-\infty}^{+\infty} x^2|\psi(x)|^2\,dx,$$

For example, one can straightforwardly find that the mean square position for the ground state of a simple harmonic oscillator is (Appendix B):

$$\overline{x^2} = \int_{-\infty}^{+\infty} x^2 \left(a^{1/4}\pi^{-1/4}e^{-ax^2/2}\right)^2\,dx = \frac{1}{2a}\,,$$

where the harmonic oscillator parameters are related to a by:

$$a = \sqrt{km}/\hbar.$$

3. The General Rule for Mean Values

3a. Mean Value of Momentum. In the preceding section we obtained the rule for computing mean values of functions of the coordinate parameter x:

$$\overline{f(x)} = \int_{-\infty}^{+\infty} f(x)|\psi(x)|^2\,dx.$$

Suppose, however, that we wish to find the mean value of a function of momentum. The problem that arises can be illustrated with the momentum itself. Suppose we were to try:

$$\bar{p} = ?\int_{-\infty}^{+\infty} p\,|\psi(x)|^2\,dx. \qquad (4)$$

[3]In "Numerical Solution of the Schrodinger Equation for the Hydrogen Atom" (MISN-0-245), quantization of energy is seen to be due to the requirement that the probability of finding the hydrogen atom's electron somewhere in space is unity.

[4]In "The Time-Dependent Schrödinger Equation: Derivation of Newton's Second Law" (MISN-0-248), it is found that Newton's Second Law is exactly valid only for free particles, particles experiencing constant forces, and Simple Harmonic Oscillators.

Replacing p by its *derivative operator*[5] and then taking the complex conjugate of the entire equation, one finds: [S-1][6]

$$\bar{p}^* = -\bar{p} \qquad \text{(assuming equation (4),}$$

which means that the mean momentum of any object is an imaginary number. This is ridiculous so Eq. (4) is ruled out. The rule that works is:

$$\bar{p} = \int_{-\infty}^{+\infty} \psi^*(x)\;p\;\psi(x)\,dx = \int_{-\infty}^{+\infty} \psi^*(x)\left(-i\hbar\frac{d}{dx}\right)\psi(x)\,dx.$$

After an integration by parts, one finds that the mean momentum is now a real number with the restriction that: [S-2]

$$|\psi(+\infty)|^2 = |\psi(-\infty)|^2.$$

This condition turns out to be obeyed for those wave functions that are of practical use.

3b. Mean Value of Functions of Position and Momentum. The general rule, then, is to sandwich a function between * and in order to find its mean value:

$$\overline{f(x,p)} = \int_{-\infty}^{+\infty} \psi^*(x)\;f\left(x,\;-i\hbar\frac{d}{dx}\right)\;\psi(x)\,dx. \qquad (5)$$

For example, one can straightforwardly find the mean square momentum for the ground state of the simple harmonic oscillator: [S-3]

$$\overline{p^2} = \frac{\hbar^2 a}{2} \qquad \text{(SHO, ground state).}$$

4. Mean Values and Rms Deviations

4a. Uncertainty in Position. The quantum mechanical uncertainty in position, Δx, is defined to be the root-mean-square (RMS) deviation from the mean position:

$$\Delta x \equiv \sqrt{\;\overline{(x-\bar{x})^2}\;}\;.$$

[5]See "The Schrodinger Equation in One Dimension" (MISN-0-242).

[6]See this module's Special Assistance Supplement.

Carrying out the square and using the mean value equation, Eq. (3):

$$(\Delta x)^2 = \int_{-\infty}^{+\infty} (x^2 - 2x\bar{x} + \bar{x}^2)\, P(x)\, dx = \overline{x^2} - 2\bar{x}^2 + \bar{x}^2 = \overline{x^2} - \bar{x}^2.$$

Then:

$$\Delta x = \sqrt{\overline{x^2} - \bar{x}^2}\,.$$

4b. Uncertainty in Momentum. Similarly, the RMS uncertainty in momentum is:

$$\Delta p = \sqrt{\overline{(p - \bar{p})^2}} = \sqrt{\overline{p^2} - \bar{p}^2}.$$

Is the mean of a sum equal to the sum of the means? Is the mean of a product or quotient equal to the product or quotient of the means? Does this answer depend on whether all factors but one are constant?

5. The SHO Uncertainty Product

5a. Mean Position for the Harmonic Oscillator. We will illustrate the calculation of uncertainties with the ground state of a simple harmonic oscillator (SHO). The SH0 is an interesting case because, for example, the atoms in diatomic molecules exhibit radial harmonic oscillations about the molecular center of mass for small displacements from equilibrium. The SHO ground state wave function is:[7]

$$\psi(x) = (a/\pi)^{1/4} e^{-ax^2/2}, \qquad a \equiv \sqrt{km}/\hbar. \qquad (6)$$

where the potential and total energies are:

$$V(x) = \frac{1}{2}kx^2; \qquad E_0 = \frac{\hbar^2 a}{2m} = \frac{\hbar}{2}\sqrt{k/m}.$$

Here $\psi(x)$ has been normalized to unit probability of finding the oscillator somewhere in all of space:

$$1 = \int_{-\infty}^{+\infty} P(x)\, dx = \int_{-\infty}^{+\infty} |\psi(x)|^2\, dx.$$

Since our wave function is symmetrical about the origin, the mean position is zero [S-4]:

$$\bar{x} = \int_{-\infty}^{+\infty} x\, |\psi(x)|^2\, dx = \sqrt{a/\pi} \int_{-\infty}^{+\infty} x e^{-ax^2}\, dx = 0.$$

[7]See “The Schrodinger Equation in One Dimension” (MISN-0-242).

One can immediately see that the integral is zero by noting that the integrand is antisymmetrical about the origin while the limits are symmetrical.

5b. Mean Square Position and Momentum. The mean square position is not zero and can be directly found by integration (Appendix B):

$$\overline{x^2} = \frac{1}{2a},$$

and so the position uncertainty is:

$$\Delta x = 1/\sqrt{2a}.$$

The square of the momentum is given by:

$$p^2\psi = 2m[E - V(x)]\psi = \hbar^2(a - a^2x^2)\psi.$$

The mean square momentum follows immediately:

$$\overline{p^2} = \hbar^2 a/2.$$

Since the mean momentum is zero [S-5], the uncertainty in momentum is [S-6]:

$$\Delta p = \hbar\sqrt{a/2}.$$

5c. Product of Uncertainties in Position and Momentum. The product of the uncertainties in position and momentum for the ground state of the SHO turns out to be the minimum allowed by the Uncertainty Relation![8]

Acknowledgments

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[8]See “The Uncertainty Relations” (MISN-0-241).

A. Mean Values

Let $N(x_n)$ represent the numbers of objects at various positions x_n. The mean (average) value of x^4 for those objects is:

$$\overline{x^4} = \frac{1}{N}\sum_{n=1}^{m} x^4 N(x_n),$$

where the N objects are distributed among m positions. The fraction $F(x_n)$ of the N objects which are located at x_n is:

$$F(x_n) = \frac{N(x_n)}{N}.$$

We can rewrite the mean value in terms of this fraction:

$$x = \overline{x^4} = \sum_{n=1}^{m} x^4 F(x_n),$$

However, the fraction of the objects at x_n can be reinterpreted as the probability $P(x_n)$ that any one of them is there:

$$F(x_n) = P(x_n),$$

and hence:

$$\overline{x^4} = \sum_{n=1}^{m} x^4 P(x_n),$$

For a continuum of locations x:

$$\overline{x^4} = \int_{-\infty}^{+\infty} x^4 P(x)\,dx.$$

where $P(x)$ is now a probability density, not the probability of x. Note that just as the sum of all fractions of the whole is unity, so also the probability of finding one object somewhere is unity:

$$1 = \sum_{n=1}^{m} F(x_n) = \sum_{n=1}^{m} P(x_n) = 1,$$

or:

$$1 = \int_{-\infty}^{+\infty} P(x)\,dx.$$

B. Solving Gaussian Integrals

The function e^{-ax^2} is-called a *Gaussian* function. It is frequently met in physics and in statistics so the method of solution of its integral is worthwhile knowing.

Method 1

Find the appropriate form in a Table of Integrals.[9] For example, in *A Short Table of Integrals*, B. O. Peirce, Ginn & Co. (Xerox Corporation), Boston (1929), one finds on page 63:

491. $\int_0 \sqrt{x} \quad \int_0 \sqrt{\pi}$

492. $\int_0^\infty e^{-a^2x^2}dx = \frac{1}{2a}\sqrt{\pi} = \frac{1}{2a}\Gamma(\tfrac{1}{2}).\ a>0$

493. $\int_0^\infty x^n e^{-ax}dx = \frac{\Gamma(n+1)}{a^{n+1}}.\ n>-1$ and $a>0$

494. $\int_0^\infty x^{2n} e^{-ax^2}dx = \frac{1\cdot 3\cdot 5\cdots(2n-1)}{2^{n+1}a^n}\sqrt{\frac{\pi}{a}}.$

495. $\int_0^\infty e^{-x^2-\frac{a^2}{x^2}}dx \quad e^{-2a}\sqrt{\pi}$

Hence:

$$\overline{x^2} = \sqrt{a/\pi}\int_{-\infty}^{+\infty} x^2 e^{-ax^2}\,dx.$$

Because the integrand is symmetric, this can be written:

$$\overline{x^2} = \sqrt{a/\pi}\,2\int_{0}^{+\infty} x^2 e^{-ax^2}\,dx.$$

Now by No. 494 in Peirce's book this becomes:

$$\overline{x^2} = \sqrt{a/\pi}\;2\,\frac{1}{4a}\sqrt{\pi/a} = \frac{1}{2a}.$$

[9] We recommend that you own a table of integrals, such as that above, or: *Table of Integrals, Series and Products*, I. S. Gradshteyn and I. M. Ryzhik, Academic Press, New York and London (1965); or *Mathematical Tables from the Handbook of Chemistry and Physics*, Charles Hougman, Chemical Rubber Publishing Co. (1931 and later dates).

Method 2

$$\int_{-\infty}^{+\infty} e^{-ax^2}\,dx = \sqrt{\int_{-\infty}^{+\infty} e^{-ax^2}\,dx \int_{-\infty}^{+\infty} e^{-ay^2}\,dy}$$
$$= \sqrt{\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} e^{-a(x^2+y^2)}\,dx\,dy}$$
$$= \sqrt{\int_0^{+\infty} e^{-ar^2}\,2\pi r\,dr}\,.$$

where the planar area integration has been re-expressed in polar coordinates. Now let $z \equiv r^2$ so that $dz = 2rdr$:

$$\int_{-\infty}^{+\infty} e^{-ax^2}\,dx = \sqrt{\pi \int_0^{+\infty} e^{-az}\,dz} = \sqrt{\pi/a}.$$

$$\overline{x^2} = \int_{-\infty}^{+\infty} x^2 e^{-ax^2}\,dx$$
$$= -\frac{d}{da}\int_{-\infty}^{+\infty} e^{-ax^2}\,dx$$
$$= -\frac{d}{da}\sqrt{\pi/a} = \frac{1}{2a}\sqrt{\pi/a}\,.$$

SPECIAL ASSISTANCE SUPPLEMENT

S-1 *(from TX-3a)*

Imaginary Mean Momentum from Wrong Definition

Try:

$$\bar{p} = ?\int_{-\infty}^{+\infty}\left(-i\hbar\frac{d}{dx}\right)\psi^*(x)\psi(x)\,dx = -i\hbar\int_{-\infty}^{+\infty}\left(\psi^{*\prime}\psi + \psi^*\psi^\prime\right)dx.$$

Take the complex conjugate[a] of all terms, including the number $\bar{p}$:

$$\bar{p}^* = ?i\hbar\int_{-\infty}^{+\infty}\left(\psi^\prime\psi^* + \psi\psi^{*\prime}\right)dx.$$

Now the right hand side is just the negative of the right hand side of $\bar{p}$ hence:

$$\bar{p}^* = ? - \bar{p}\,.$$

This can only be true for an imaginary number, which $\bar{p}$ certainly is not.

[a] See "Some Simple Functions in the Complex Plane" (MISN-0-59).

S-2 *(from TX-3a)*

Real Momentum from Correct Definition

$$\bar{p} = \int_{-\infty}^{+\infty} \psi^*(x) \left(-i\hbar \frac{d}{dx}\right) \psi(x)\, dx = -i\hbar \int_{-\infty}^{+\infty} \psi^* \psi')\, dx.$$

$$\begin{aligned}\bar{p}^* &= i\hbar \int_{-\infty}^{+\infty} \psi \psi^{*\prime}\, dx = i\hbar \int_{-\infty}^{+\infty} \left[\frac{d}{dx}(\psi^*\psi) - \psi^*\psi'\right] dx \\ &= i\hbar \int_{-\infty}^{+\infty} \frac{d}{dx}(\psi^*\psi)\, dx - i\hbar \int_{-\infty}^{+\infty} \psi^*\psi'\, dx \\ &= i\hbar \left[\, |\psi(+\infty)|^2 - |\psi(-\infty)|^2 \,\right] + \bar{p}.\end{aligned}$$

Now assume that $P(+\infty) = P(-\infty)$, which is virtually always true, hence:

$$\bar{p}^* = \bar{p},$$

as it should be.

S-3 *(from TX-3b)*

Calculation of SHO $\bar{p}^2$

Method 1

$$\begin{aligned}p^2\psi &= \left(-i\hbar \frac{d}{dx}\right)\left(-i\hbar \frac{d}{dx}\right)\psi = -\hbar^2\psi'' \\ &= -\hbar^2 \left[(a/\pi)^{1/4}(-a + a^2x^2)e^{-ax^2}\right] \\ &= -\hbar^2(-a + a^2x^2)\psi.\end{aligned}$$

Then using the fact that the mean value of a constant is just the constant itself (why?), and using Appendix B:

$$\begin{aligned}\overline{p^2} &= \overline{\hbar^2(a - a^2x^2)} = \hbar^2 a - \hbar^2 a^2 \overline{x^2} \\ &= \hbar^2 a - \hbar^2 a^2 \frac{1}{2a} = \frac{\hbar^2 a}{2}.\end{aligned}$$

Method 2

$$\frac{p^2}{2m}\psi + V\psi = E\psi$$

$$\begin{aligned}p^2\psi &= 2m(E - V)\psi = 2m\left(E - \frac{1}{2}kx^2\right)\psi \\ &= 2m\left(\frac{\hbar^2 a}{2m} - \frac{1}{2}\frac{a^2\hbar^2}{m}x^2\right)\psi \\ &= \hbar^2(a - a^2x^2)\psi\,,\end{aligned}$$

etc.

S-4 *(from TX-5a)*

Calculation of SHO $\bar{x}$

Method 1

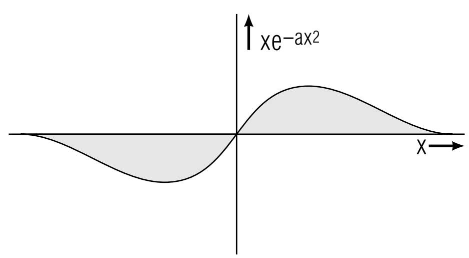
In the following we define (y) as $(-x)$ and then switch the limits on the integral:

$$\begin{aligned}\int_{-\infty}^{+\infty} xe^{-ax^2}\,dx &= \int_{-\infty}^{0} xe^{-ax^2}\,dx + \int_{0}^{\infty} xe^{-ax^2}\,dx \\ &= \int_{\infty}^{0}(-y)e^{-ay^2}\,(-dy) + \int_{0}^{\infty} xe^{-ax^2}\,dx \\ &= -\int_{0}^{\infty}(-y)e^{-ay^2}\,(-dy) + \int_{0}^{\infty} xe^{-ax^2}\,dx \\ &= -\int_{0}^{\infty} ye^{-ay^2}\,dy + \int_{0}^{\infty} xe^{-ax^2}\,dx \\ &= -f(a) + f(a) = 0.\end{aligned}$$

where $f(a)$ is either of the integrals.

Method 2

$$\int_{-\infty}^{+\infty} xe^{-ax^2}\,dx = ?$$



First note that e^{-ax^2} is symmetric with respect to the origin: if we substitute $(-x)$ for (x) the function does not change sign. However, x is antisymmetrical; it does change sign. The product of a symmetric and an antisymmetric function is an antisymmetric one so the integrand is antisymmetric. This can also be seen by direct substitution. We now sketch this antisymmetric function, whose graphical area is the integral, and we see there is as much area below the x-axis as above it so the net area (the integral) is zero.

S-5 *(from TX-5b)*

Calculation of SHO $\bar{p}$

Method 1

The mean momentum is zero because a particle undergoing simple harmonic motion spends as much time going one direction as the other. That is, its momentum is negative as much as it is positive. The same type of argument can be used to show that $\bar{x} = 0$.

Method 2

$$p\psi = -i\hbar\frac{d\psi}{dx} = -ax\psi,$$

hence:

$$\bar{p} = -a\bar{x} = 0.$$

S-6 *(from TX-5b)*

Calculation of SHO Δp

$$\Delta p = \sqrt{\overline{(p-\bar{p})^2}} = \overline{p^2} - \bar{p}^2,$$

but $\bar{p} = 0$. Then:

$$\Delta p = \sqrt{\overline{p^2}} = \sqrt{\frac{\hbar^2 a}{2}} = \hbar\sqrt{a/2}.$$