

Workshop: Momentum of a quantum particle and the Heisenberg uncertainty principle

Quantum aspects of physical chemistry

<http://quantum.bu.edu/courses/PLTL/3/3.pdf>

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In the previous workshop we explored the quantum concept that once we represent a particle by a wavefunction, we can no longer meaningfully represent the particle as "being" at a particular point in space. Rather, we can only work with the *average properties* of the particle, by taking into account how the probability density, $\psi(x)^2$, *changes throughout space*.

In this workshop we will see how to extend these ideas to particle properties that are represented as operators, and then explore the consequences of the position-momentum commutation relation,

$$[x, p] = x\left(-i\hbar \frac{d}{dx}\right) - \left(-i\hbar \frac{d}{dx}\right)x = i\hbar$$

on the simultaneous values of uncertainties of different particle properties. The most famous of these is the position-momentum uncertainty product, $\delta x \delta p$.

■ Review

In the last workshop we introduced several key quantum ideas. Let's begin with a review.

1. What is the difference between wavefunction, probability density, and probability? Be precise in contrasting these terms.
2. What is the quantum concept definition of the average value (the so-called expectation value) of position?

■ Weighted averages

Next, let's explore the concept of weighted average. The key idea of computing the average value of position is that the average is defined in terms of the *relative likelihood of the particle being at each position*. The relative likelihood of a particle being within dx of position x is $w(x) = \psi^2(x) dx$ and so, for example, the average position—the average value of x —is the *weighted average*

$$\langle x \rangle = \sum_{\text{all } x} x w(x) = \int_{-\infty}^{\infty} x \psi^2(x) dx.$$

The terminology "weighted average" means that each position contributes to the sum according to its *relative weight*, $w(x)$.

3. What are the units of the relative weights, $w(x)$?

4. What is the numerical value of the sum of the relative weights, $w(x)$?

5. Assume that the following is the list of scores, out of a possible maximum of 50 points, earned on an exam. Calculate the exam average.

{45, 35, 41, 32, 32, 36, 38, 50, 48, 45, 32, 42, 36, 38, 34, 34, 37, 33,
46, 40, 43, 37, 37, 42, 39, 41, 42, 43, 47, 37, 42, 49, 38, 37, 42, 37}

6. Make a table of scores, s_i , and their corresponding relative weights, w_i . Make sure that your weights add up to 1.

7. Write down an expression for the exam average in terms of the scores, s_i , and their corresponding relative weights, w_i .

8. Use your expression to calculate the exam average. Is your answer the same as the average you computed in question 5? Should it be?

■ Complex-valued wavefunctions

In general wavefunctions can have imaginary components. In this workshop we'll use the same wavefunction as in the previous workshop except that now the wavefunction will contain the factor $i = \sqrt{-1}$. That is, we'll work in one dimension and assume that the wavefunction of a particle confined between $x = 0.0 \text{ \AA}$ and $x = L = 1.0 \text{ \AA}$ is

$$\psi_{2,a}(x) = i \sqrt{2/L} \sin(2\pi x/L).$$

To ensure that quantities calculated from wavefunctions are real numbers, probabilities are computed using a product of wavefunction, ψ , and its complex conjugate, ψ^* , where the $*$ on the wavefunction denotes complex conjugation, that is, to replace everywhere i by $-i$.

9. This means that in general we write probability densities as $|\psi(x)|^2 = \psi(x)^* \psi(x)$ rather than simply as $\psi(x)^2$. Show that the latter rule does not make sense physically but that the former rule does.

10. In the last workshop you determined that the expectation (average) value of position, $\langle x \rangle = \int_0^{1 \text{ \AA}} x \psi_2(x)^2 dx$, was 0.5 \AA . Show that this definition of expectation value used with $\psi_{2,a}(x)$ leads to an unphysical answer.

11. How can we enhance the definition of expectation value of position to make it sensible when used with wavefunctions that contain imaginary factors?

12. Show that your enhanced definition give the same answer for $\langle x \rangle$ for the two wavefunctions, $\psi_2(x)$ and $\psi_{2,a}(x)$.

13. Consider the following statement: In quantum calculations, the overall phase of a wavefunction has no effect on physical quantities calculated with the wavefunction. Assess the correctness of this statement, based on your answers to the previous several questions.

■ Average values of momentum

Now, let's investigate how to compute the average value of momentum. We have learned that, in quantum mechanics, momentum is represented as the operator $p = -i\hbar d/dx$. Since the momentum is expressed in terms of an operator rather than a numerical quantity, we cannot compute the average momentum, $\langle p \rangle$, of a particle in the same way that we used to compute its average position, $\langle x \rangle$.

Here is how we extend the recipe for average values to handle cases where the physical quantity is represented as an operator. The first step is to determine the effect of the operator on the wavefunction. For the case of momentum, this means we need to evaluate the expression

$$g(x) \equiv p \psi(x) = -i\hbar \frac{d}{dx} \psi(x).$$

It is very helpful to interpret this expression as follows: The effect of the momentum operator on a wavefunction is a *new function*, $g(x)$, that is, something that has a *numerical value* at each value of x . That is, in this first step we have gone from operator to numbers.

The second step is to evaluate the product

$$\psi(x)^* g(x) = \psi(x)^* p \psi(x) \equiv -i\hbar \psi(x)^* \frac{d}{dx} \psi(x)$$

at each value of x .

14. Show that, for any wavefunction, $\psi(x)$, the units of $\psi(x)^* p \psi(x)$ are momentum per unit length.

15. In three dimensions the expression in the previous question is replaced by $\psi(x, y, z)^* p_x \psi(x, y, z)$, where now we use p_x to indicate the operator for the x component of the momentum. What would the units of the expression $\psi(x, y, z)^* p_x \psi(x, y, z)$ be? Does it make sense to interpret this expression as a momentum density, $\rho_{p_x}(x, y, z)$? (ρ is the Greek letter rho.)

16. Is this interpretation analogous to interpreting $\psi(x, y, z)^* \psi(x, y, z)$ as a probability density? Can we interpret $\psi(x)^* p \psi(x)$ as a one-dimensional momentum density, $\rho_p(x)$?

A way to estimate the average momentum of the particle, $\langle p \rangle$, is to evaluate the contribution to the momentum for adjacent regions of space and then to sum up these contributions.

17. With respect to the values of the wavefunction $\psi_{2a}(x)$ at the 21 evenly spaced points between 0 and 1 Å, given below, write an equation in terms of the momentum density, $\rho_p(x)$, that corresponds to this definition of average momentum.

In calculus we learn that the derivative of a function, $f(x)$, at a point is the slope of the function at that point,

$$\frac{df}{dx} = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x)}{(x + \Delta x) - x}.$$

An approximation to the derivative is to *not take the limit*, $\Delta x \rightarrow 0$.

18. Use this idea to show that your scheme to evaluate the average momentum is equivalent to

$$\langle p \rangle \simeq -i \hbar \sum_{i=1}^{20} \psi(x_i)^* (\psi(x_{i+1}) - \psi(x_i)).$$

19. Use this scheme to evaluate this approximation to the average momentum. Here are the wavefunction values.

x (Å)	ψ_{2a} (Å ^{-1/2})
0	0
0.05	0.437 i
0.1	0.831 i
0.15	1.14 i
0.2	1.34 i
0.25	1.41 i
0.3	1.34 i
0.35	1.14 i
0.4	0.831 i
0.45	0.437 i
0.5	0
0.55	-0.437 i
0.6	-0.831 i
0.65	-1.14 i
0.7	-1.34 i
0.75	-1.41 i
0.8	-1.34 i
0.85	-1.14 i
0.9	-0.831 i
0.95	-0.437 i
1.	0

20. Do your value and units for the average momentum make sense? Could you have anticipated your value, without doing any calculations? Hint: Analyze your computation pictorially.

21. How could you improve your value for the average momentum?

22. Write the mathematical equation that corresponds to exact value of the average momentum.

23. Write the mathematical equation that corresponds to exact value of the average of any quantity represented by an operator. Does your expression also work for cases where the quantity is not an operator (such as average values of position)?

■ Average values of squared momentum

24. With respect to the values of the wavefunction $\psi_{2,a}(x)$ at the 21 evenly spaced points between 0 and 1 Å used in the previous workshop, show that an approximate scheme to evaluate the squared momentum density is

$$\langle p^2 \rangle \approx -\hbar^2 \sum_{i=2}^{20} \psi(x_i)^* \frac{\psi(x_{i+1}) - 2\psi(x_i) + \psi(x_{i-1}))}{\Delta x},$$

where Δx is the constant spacing between adjacent positions.

25. Use the scheme to evaluate this approximation to the average squared momentum.

26. Do your value and units for the average squared momentum make sense? Could you have anticipated your value, without doing any calculations?

27. How could you improve your value for the average squared momentum?

28 Write the mathematical equation that corresponds to exact value of the average squared momentum.

■ Testing the Heisenberg uncertainty principle

29. Use your results for $\langle p \rangle$ and $\langle p^2 \rangle$ for a particle described by the wavefunction ψ_2 to compute the momentum uncertainty, δp .

30. The values of $\langle x \rangle$ and $\langle x^2 \rangle$ for a particle described by the wavefunction $\psi_{2a}(x)$ are 0.50 \AA and 0.32 \AA^2 . Do you see why these are the same values you get for the wavefunction $\psi_2(x)$?

31 Use your results to evaluate the uncertainty product, $\delta x \delta p$. Are the units of your answer correct?

32. The Heisenberg uncertainty principle applied to position and momentum states that, $\delta x \delta p \geq \hbar/2$. Is the Heisenberg uncertainty principle satisfied in this case? Should it be?