8/26/2024

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  - Applying operators
  - Commutation
  - Linear operators
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    - Eigenfunctions and eigenvalues
    - Complex conjugates
    - Dirac Bra-ket Notation
    - Definition of a Hermitian operator

- This lecture is designed to help you achieve the following learning objectives
  - Define operators and apply them to functions
  - Evaluate commutators
  - Write mathematical expressions in Dirac Bra-Ket notation

Syllabus

https://daveminh.github.io/Chem550-2024F/

Introductions

About me: work

Biographical

Professional History

2020 – present	**Robert E. Frey, Jr. Endowed Faculty in Chemistry**, Illinois Institute of Technology (Illinois Tech), Chicago, IL
2019 – present	**Associate Professor** (tenured), Department of Chemistry, Illinois Tech
2018 – present	**Associate Director**, Center for Interdisciplinary Scientific Computation, Illinois Tech
2013 – 2019	**Assistant Professor** (tenure-track), Department of Chemistry, Illinois Tech
2011 – 2013	**Postdoctoral Research Associate**, Duke University, Durham, NC
2009 – 2011	**Director's Postdoctoral Fellow**, Argonne National Laboratory, Argonne, IL
2007 – 2009	**Postdoctoral Trainee**, National Institutes of Health, Bethesda, MD

Education

2004 – 2007	**Ph.D. in Physical Chemistry**, University of California, San Diego. Thesis Title: Free Energy Reconstruction from Irreversible Single-Molecule Pulling Experiments. Recipient of Molecular Biophysics Training Grant and Aguoron Kamen and Kaplan Fellowship.
2000 – 2003	**B.A. in Chemistry**, University of California, Berkeley. Recipient of Chancellor's Scholarship (Berkeley's most prestigious scholarship) and National Merit Scholarship.

Awards

2020	College of Letters and Science Nominee, Michael J. Graf IIT Teaching and Advising Innovation Award.
2019	40 under 40 Chicago Scientists. Selected by Halo Cures.
2019	Sigma Xi Junior Faculty Award, in recognition of Outstanding Accomplishments in Research and Scholarship. Awarded by the Illinois Tech chapter of the scientific research honor society, Sigma Xi.
2018	College of Science Dean's Excellence Award in Research, at the Junior Level
2012	OpenMM Visiting Scholar (at Stanford)
2009 – 2011	Director's Postdoctoral Fellowship
2007 – 2009	Postdoctoral Intramural Research Training Award
2005 – 2007	NIH Molecular Biophysics Training Grant
2004 – 2005	Aguoron Kamen and Kaplan Fellowship
2000 – 2003	UC Berkeley Chancellor's Scholarship

- Coauthored 56 peer-reviewed journal articles
- Cited over 1500 times with an h-index of 22, according to Google scholar.
- Current research in computational chemistry
  - Developing methods related to structure-based drug design
    - predicting binding affinities and ligand efficacy
    - simulating biological macromolecules
  - Involved in antibiotic drug discovery
  - research has been funded by NIH and NSF

Full curriculum vitae: https://ccbatiit.github.io/downloads/DavidMinh_CV.pdf

About me: beyond work

- Outside of work, I like to
  - play sports, especially Taekwondo, tennis, and basketball.
  - listen to podcasts and audiobooks. Some of my favorite podcasts are Hidden Brain and Planet Money from NPR.
  - play board games, especially strategy and word games.
  - sometimes play music, especially classical piano. Sometimes I also play guitar and bass.
  - read news and sometimes books
  - play video games
  - exercise, especially weights, swimming, biking, and skiing
  - travel. I’ve been to 6 continents
- I am
  - Australian-born and American-raised by Vietnamese parents of Vietnamese and Chinese descent
  - married, with 2 children
  - Christian
  - incredibly blessed!

[Introduce yourself]

- What is your full name? What do you like to be called?
- Which degree program are you in?
- What are you hoping to learn in this class?
- How will this help you achieve your goals?
- Share something interesting about yourself

Operators

- This lecture is intended to help you achieve the following learning objectives:
  - Define operators and apply them to functions
  - Evaluate commutators
  - Write mathematical expressions in Dirac Bra-ket notation
- At the end of this lecture, you should be able to
  - answer the following questions:
    - What are operators and how are they useful in quantum mechanics?
    - What does it mean for an operator to commute? What is a commutator?
    - What is an eigenfunction and an eigenvalue?
    - What are some properties of quantum mechanical operators?
  - apply a series of operators to a function
  - evaluate a commutator
  - determine whether a function is an eigenfunction of an operator and its eigenvalue
  - write mathematical expressions in Dirac Bra-ket notation
  - determine whether an operator is linear and Hermitian

Operators

- Observable - any dynamical variable that can be measured
  - e.g. position or momentum
  - All quantum observables have corresponding operators
- Operator - a symbol for an instruction to carry out an ``operation'' on a function
  - e.g. multiplication or differentiation
  - For a general operator, we will use the hat symbol $\hat{\mathbf{A}}$

- If $f = 3x + 10$ and $\hat{\mathbf{A}}f = 5f$, then what is $\hat{\mathbf{A}}f$ in terms of x?
  - $\hat{\mathbf{A}}f = 15x + 50$
- If $f = 3x + 10$ and $\hat{\mathbf{A}}f = |\sqrt{f}|$, then what is $\hat{\mathbf{A}}f$ in terms of x?
  - $\hat{\mathbf{A}}f = |\sqrt{3x + 10}|$

Applying Multiple Operators

- Operators are always applied from the right to the left
- Does it matter what order operators are applied?

- Suppose that $f = 3x + 10$ and $\hat{\mathbf{A}}f = f^2$ and $\hat{\mathbf{B}}f = \dfrac{\partial}{\partial x}f$
- What is $\hat{\mathbf{A}}\hat{\mathbf{B}}f$ in terms of x?
  - $\hat{\mathbf{A}}\hat{\mathbf{B}}f = \hat{\mathbf{A}}(3) = 9$
- What is $\hat{\mathbf{B}}\hat{\mathbf{A}}f$ in terms of x?
  - $\hat{\mathbf{B}}\hat{\mathbf{A}}f = \hat{\mathbf{B}}(9x^2 + 60x + 100) = 18x + 60$

Commutation

- $[\hat{\mathbf{A}}, \hat{\mathbf{B}}] = \hat{\mathbf{A}}\hat{\mathbf{B}} - \hat{\mathbf{B}}\hat{\mathbf{A}}$ is commutation
- If $[\hat{\mathbf{A}}, \hat{\mathbf{B}}] = 0$, the operators $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$ are said to *commute*
- Evaluate the commutator $\left[x, \dfrac{d}{dx}\right]$. Do the operators commute?
  - $\left[x, \dfrac{d}{dx}\right] f = x\dfrac{df}{dx} - \dfrac{d}{dx}(xf) = x\dfrac{df}{dx} - f - x\dfrac{df}{dx} = -f$
  - $\left[x, \dfrac{d}{dx}\right] = -1$. Since this is not zero, the operators do not commute.

Operators for QM observables are *linear* and *Hermitian*

What does this mean?

Linear Operators

- Linear operators satisfy the following criterion
  - $\hat{\mathbf{A}}(af) = a\hat{\mathbf{A}}f$, where a is a constant and f is a function
  - $\hat{\mathbf{A}}(f + g) = \hat{\mathbf{A}}f + \hat{\mathbf{A}}g$, where a is a constant and f and g are functions

- Which of the following operators are linear?
  - Integration, $\hat{\mathbf{A}}f = \int_a^b f dx$
  - Multiplication, $\hat{\mathbf{A}}f = af$
  - Logarithm, $\hat{\mathbf{A}}f = \ln(f)$
  - Square root, $\hat{\mathbf{A}}f = \sqrt{f}$

- Integration and multiplication are linear

Hermitian Operators

- To understand a Hermitian operator, you need to understand
  - eigenfunctions and eigenvalues
  - complex conjugates
  - quantum mechanical integrals
- We will also introduce Dirac Bra-ket notation, a simplification that will be used throughout the course

Eigenfunctions and eigenvalues

- Applying an operator to an *eigenfunction* will yield a constant, the *eigenvalue*, times the original eigenfunction, such that $\hat{\mathbf{A}}f = af$.
  - e.g. for the operator $\hat{\mathbf{A}}f = \dfrac{d^2}{dx^2}f$, an eigenfunction is $f = \sin(ax)$.
- What is the eigenvalue?
  - $\hat{\mathbf{A}}f = \dfrac{d^2}{dx^2}\sin(ax) = a\dfrac{d}{dx}\cos(ax) = -a^2\sin(ax)$
  - The eigenvalue is $-a^2$
- Is $f = \sin(ax)$ an eigenfunction of $\hat{\mathbf{A}}f = \dfrac{d}{dx}f$?
  - No, the function changes upon applying the operator

Eigenfunction Self-Test

- Which of the following are eigenfunctions of $\hat{\mathbf{A}}f = \frac{d}{dx}f$? For the eigenfunctions, what are the eigenvalues?
  - $f = x^2$
  - $f = e^{4x}$
  - $f = \sin(2x)$
  - $f = ax + b$
- The only eigenfunction is $f = e^{4x}$. Its eigenvalue is 4.

Complex Conjugate

- Let f^* denote the complex conjugate of f
- In a complex conjugate of a complex number
  - the real part is the same
  - the imaginary part has the same magnitude but the opposite sign
- If $f = 3 + 9i$, what is f^*?
  - $f^* = 3 - 9i$

Quantum Mechanical Integral Notation

- Integrals of the form $I = \int f_m^* \hat{\mathbf{A}} f_n d\tau$ are common in quantum mechanics
  - the integral is over all space
  - $d\tau$ is the volume element
  - n and m are indices for functions
- Dirac Bra-ket notation simplifies this type of integral to $\left\langle m \middle| \hat{\mathbf{A}} \middle| n \right\rangle$
  - $\langle m| = f_m^*$ is known as the *bra*
  - $|n\rangle = f_n$ is known as the *ket*
  - The operator $\hat{\mathbf{A}}$ is applied on the *ket*
  - If $\hat{\mathbf{A}}f = f$, then the bra-ket is $\langle m|n\rangle$; the middle is omitted
- An even shorter notation for the same integral is the matrix element, A_{mn}

Dirac Bra-ket Notation Practice

- In Dirac Bra-ket notation, $\int f_m^* \hat{\mathbf{A}} f_n d\tau = \left\langle m \,|\, \hat{\mathbf{A}} \,|\, n \right\rangle$
- Write the following in bra-ket notation
  - $\int f_n^* x^2 f_m d\tau \qquad = \langle n \,|\, x^2 \,|\, m \rangle$
  - $\int f_1^* \frac{d}{dx} f_3 d\tau \qquad = \left\langle 1 \,\middle|\, \frac{d}{dx} \,\middle|\, 3 \right\rangle$
  - $\int \Psi_1^* \Psi_2 d\tau \qquad = \langle 1 \,|\, 2 \rangle$

Hermitian Operators

- For a Hermitian operator, $\int f_m^* \hat{\mathbf{A}} f_n d\tau = \left\{ \int f_n^* \hat{\mathbf{A}} f_m d\tau \right\}^* = \int (\hat{\mathbf{A}} f_m)^* f_n d\tau$
- Write the first equality in Dirac Bra-ket notation
  - $\left\langle m \middle| \hat{\mathbf{A}} \middle| n \right\rangle = \left\langle n \middle| \hat{\mathbf{A}} \middle| m \right\rangle^*$

Properties of Hermitian Operators

- For a Hermitian operator, $\int f_m^* \hat{\mathbf{A}} f_n d\tau = \left\{ \int f_n^* \hat{\mathbf{A}} f_m d\tau \right\}^* = \int (\hat{\mathbf{A}} f_m)^* f_n d\tau$
- Properties
  - The eigenvalues of Hermitian operators are real
  - Eigenfunctions corresponding to different eigenvalues of a Hermitian operator are *orthogonal*, such that $S = \int f_m^* f_n d\tau = 0$

Review on Operators

- Ask yourself whether you can
  - answer the following questions:
    - What are operators and how are they useful in quantum mechanics?
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    - What is an eigenfunction and an eigenvalue?
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  - apply a series of operators to a function
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  - determine whether a function is an eigenfunction of an operator and its eigenvalue
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