

Summary of Quantum Mechanical Formalism

Chemistry BC3253x

Lecture

McQuarrie

Part I.

Operators

linear operators: definition

operators for position and momentum

Postulate 2

Operator equations

meaning of operator multiplication

Commutators: definition

Eigenvalue equations (eigenfunction, eigenvalue)

The Schrodinger equation: solutions called wavefunctions

Properties of wavefunctions

Well behaved: single-valued, continuous, square-integrable, and $\partial^2 f / \partial x \partial y = \partial^2 f / \partial y \partial x$

Normalization

Probability interpretation

Postulate 1

Expectation values

Postulate 4

Part II.

Hermitian operators: definition

All QM operators are Hermitian

Theorem: eigenfunctions of Hermitian operators are real

Orthogonal sets of functions: definition

Expanding arbitrary functions in a complete orthonormal set

Recipe for finding expansion coefficients

example: Legendre Polynomials on interval $[-1, 1]$

Theorem: Eigenfunctions of hermitian operators form a complete orthogonal set

→ arbitrary wavefunctions can be expanded in eigenfunctions of \hat{H}

Theorem: Commuting hermitian operators have simultaneous eigenfunctions

variables whose operator commutes with the Hamiltonian \hat{H} can have a well-defined value

variables whose operators do not commute with \hat{H} have a distribution of possible values

Measurement: Schrodinger's cat

a single measurement gives an eigenvalue of the corresponding operator

Postulate 3

Time dependence

Time dependent Schrodinger equation

Postulate 5

time dependent part of wavefunction: $\exp(iEt/\hbar)$ where E is eigenvalue of \hat{H}