Quantum Mechanics

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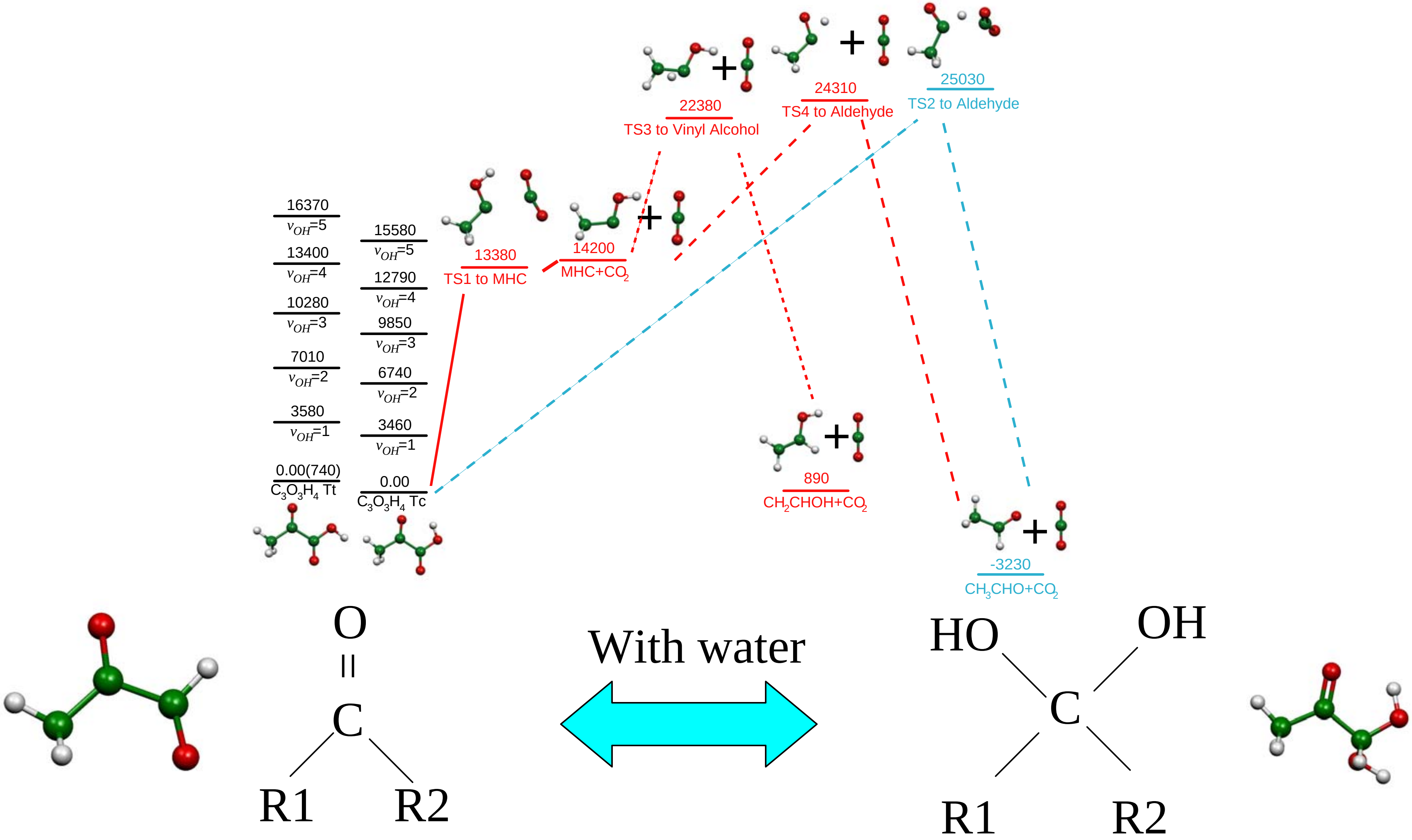
Theoretical Reaction Dynamics Calculations



Classical Mechanics Review

- Dynamical variables that are function of time

$q(t), p(t), l(t),$ $\quad L(q,\dot{q},t)$ $\quad H(q,p,t)$

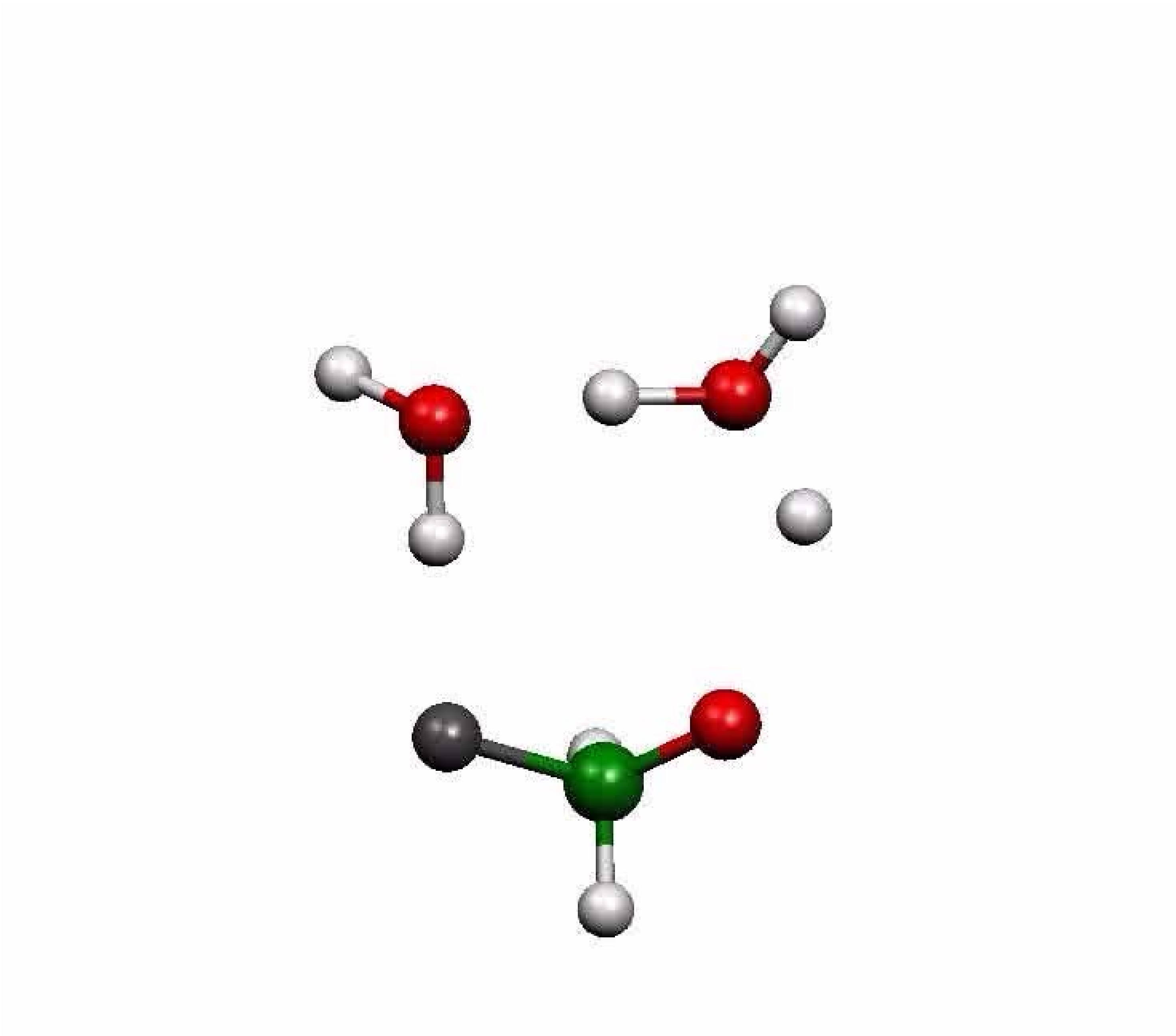
Goal: find the trajectory (what happens to the system

Position and momentum at each time

Use following three forms

- Newton's Law
- Hamilton's equation
- Lagrange equation

Example of Trajectory

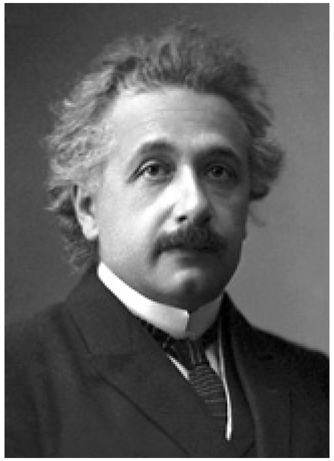


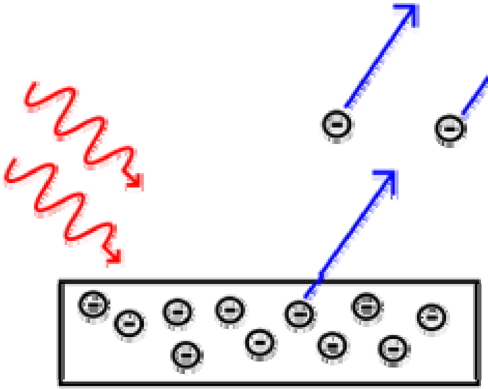
Break down of Classial Mechanics

Early twentieth century experimental results that can not be explained by classical mechanics start to appear

Light show particle like characteristic: Photoelectric effect

1921 Nobel Prize





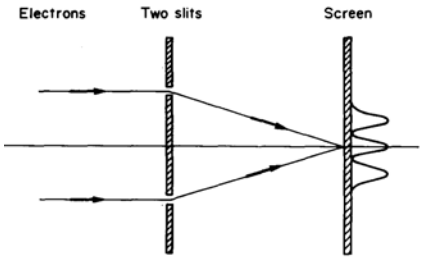
Electron show particle like character

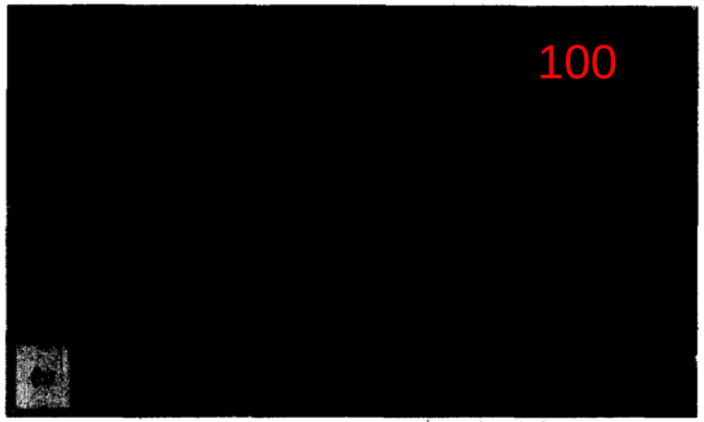
1906 Negative Charge Particle in atom

Electron show wave like character

1937 Diffraction of electrons by crystal

Electron Through a Slit





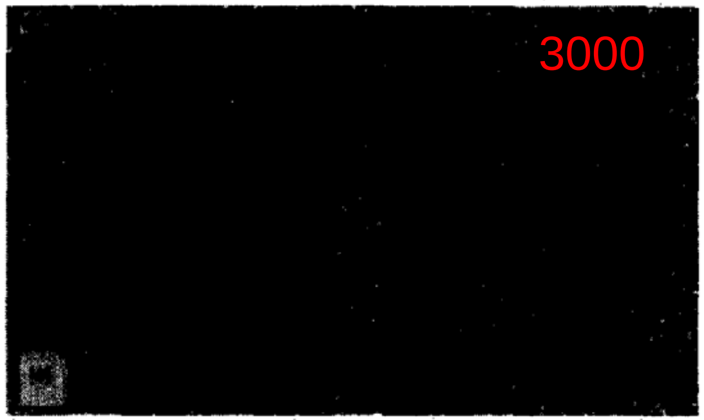


Fig. 5. Buildup of the electron interference pattern. The central field of view, $\frac{1}{3}$ width and $\frac{1}{2}$ length, of the whole field of the detector plane is shown here. The picture extends similarly to the whole field: (a) Number of electrons = 10; (b) Number of electrons = 100; (c) Number of electrons = 3000; (d) Number of electrons = 20 000; and (e) Number of electrons = 70 000.

Quantum Mechanics

State is defined by Wavefunction $\psi(q_1, q_2, \ldots q_n, t)$

The wavefunction follows the Schrodinger Equation

$$\hat{H}\psi(q_1, q_2, \ldots q_n, t) = i\eta \frac{\partial \psi(q_1, q_2, \ldots q_n, t)}{\partial t}$$

$$\hat{H}\psi(q_1, q_2, \ldots q_n) = E\psi(q_1, q_2, \ldots q_n)$$

Probability of observables are given from the expectation value of the corresponding Hermite operator

Basic Mathematical tools

- Linear operators
- Eigenfunction Eigenvalue
- Hermite Operators

Basic Quantum Mechanics

- Schrodinger Equation
- Wavefunctions characteristic
- Born Interpretation

Linear Operators

Actions that work on functions are called operators

Linear operators follow the following relationship

$$\hat{A}(af + bg) = a\hat{A}f + b\hat{A}g$$

$\hat{A}$ Operator A a, b constants f, g functions

Which of the following are linear operators?

$$\frac{d}{dq}$$

$$\int_{-\infty}^{+\infty} \quad dq$$

$$(\quad)^2$$

Eigenfunction Eigenvalue

Usually operation on a function gives a different function

BUT CERTAIN CASES OUTCOME OF OPERATION IS THE ORIGINAL FUNCTION TIMES A CONSTANT

$$\hat{A} f_a = a f_a$$

Which are the eigenfunctions of the operator $\frac{d^2}{dq^2}$

And what are their eigenvalues

$$q^3$$

$$\sin(q)$$

$$\sin(3q)$$

$$\exp(-kq)$$

$$\exp(-ikq)$$

Commutator Relationship

Commutator Relationship $\left[\hat{A}, \hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}$

When you think about opperators and commutators always think that a function follows

If $\left[\hat{A}, \hat{B}\right] = 0$ Two operators commute

Which of the following commute?

$\frac{d^2}{dq^2} \quad \frac{d}{dq}$

$\frac{d}{dq} \quad q$

$\frac{d}{dx} \quad \frac{d}{dy}$

Hermite Operators

If operator satisfies

$$\int g(q)^* \hat{A} f(q) dq = \left(\int f(q)^* \hat{A} g(q) dq \right)^* = \int \left(\hat{A} g(q) \right)^* f(q) dq$$

It is called Hermite

- Hermite Operators Eigenvalue is Real

$$\hat{A} f_a = a f_a \qquad \hat{A} f_b = b f_b$$

$$\int f_a(q)^* \hat{A} f_a(q) dq = \int f_a(q)^* a f_a(q) dq = a \int f_a(q)^* f_a(q) dq$$

$$\int \left(\hat{A} f_a(q) \right)^* f_a(q) dq =$$

Hermite Operators cont

If operator satisfies

$$\int g(q)^* \hat{A} f(q) dq = \left(\int f(q)^* \hat{A} g(q) dq \right)^* = \int \left(\hat{A} g(q) \right)^* f(q) dq$$

It is called Hermite

- Hermite Operators Eigenfunctions are orthogonal

$$\hat{A} f_a = a f_a \qquad \hat{A} f_b = b f_b$$

$$\int f_a(q)^* \hat{A} f_b(q) dq = \int f_a(q)^* b f_b(q) dq = b \int f_a(q)^* f_b(q) dq$$

$$\int \left(\hat{A} f_a(q) \right)^* f_b(q) dq =$$

Basic Mathematical tools

- Linear operators
- Eigenfunction Eigenvalue
- Hermite Operators

Basic Quantum Mechanics

- Wavefunctions characteristic
- Schrodinger Equation
- Observables and Operator

Quantum Mechanics

State is defined by Wavefunction $\psi\left(q_1, q_2, \ldots q_n, t\right)$

The wavefunction follows the Schrodinger Equation

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Probability of observables are given from the expectation value of the corresponding Hermite operator

Wave Functions

Born's Interpretation: probability that a one-dimensional particle will be found in volume dx between x and $x+dx$ is

$$\Psi^*(x,t)\Psi(x,t)dx = |\Psi(x,t)|^2 dx$$

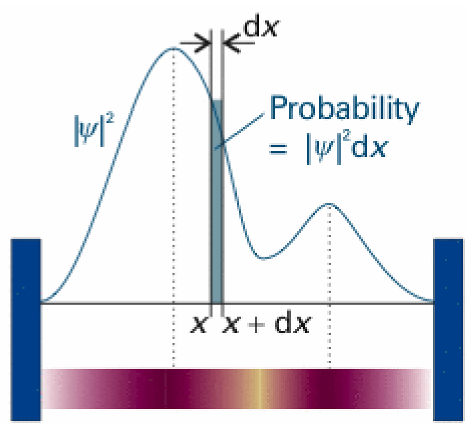
Probability density real and positive

!!! Unlike classical mechanics you can only define probability of finding particle!!!

Normalization of wave function

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$$

The probability of finding a particle in available space should be one



Question p257

P256 text book

Schrodinger Equation

The wavefunction follows the Schrodinger Equation

$$\hat{H}\psi\left(q_1, q_2, \ldots q_n, t\right) = i\eta \frac{\partial \psi\left(q_1, q_2, \ldots q_n, t\right)}{\partial t}$$

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Time independent equation: Wave function is Eigenfunction of Hamiltonian Operator

How to make the Hamiltonian operator?

What is the Hamiltonian in classical mechanics?

$$H = T + V$$

Observables 1

Observable in quantum mechanics described by hermite operators

Why? What are characteristic of hermite operators?

$$\hat{P}_x = \frac{\hbar}{i}\frac{d}{dx}\times \qquad \hat{x} = x\times$$

Interpretation of experimental observation

The result of a single measurement of a mechanical property A can only be an Eigenvalue a_n of the operator $\hat{A}$

What quantum mechanics can say is that the mean value of numerous observations of physical quantity defined by a certain operator can be compared to the expectation value

$$\langle \hat{A} \rangle = \langle \Psi | \hat{A} | \Psi \rangle = \int \Psi^* \hat{A} \Psi d\tau$$

Observables 2

Commutating Observables and Simultaneous Measurement

$$\left[\hat{A},\hat{B}\right]=0$$

Prove that if observables commute you can have same eigen functions

$$\hat{A}f_n = a_n f_n \qquad \hat{B}f_n = b_n f_n$$

However Quantum Mechanics require observables to satisfy

$$\left[\hat{x},\hat{p}_x\right]=i\eta$$

$$\hat{P}_x = \frac{\eta}{i}\frac{d}{dx}\times \qquad \hat{x} = x\times$$

Uncertainty Principle