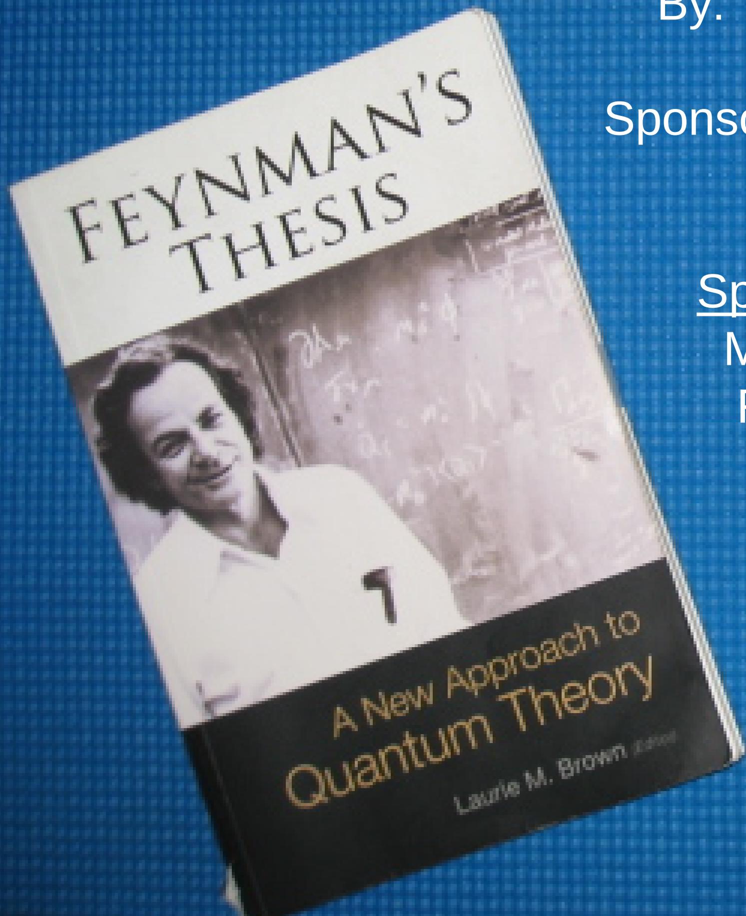
"Applying the Scientific Method to Understanding Anomalous Heat Effects: Opportunities and Challenges"

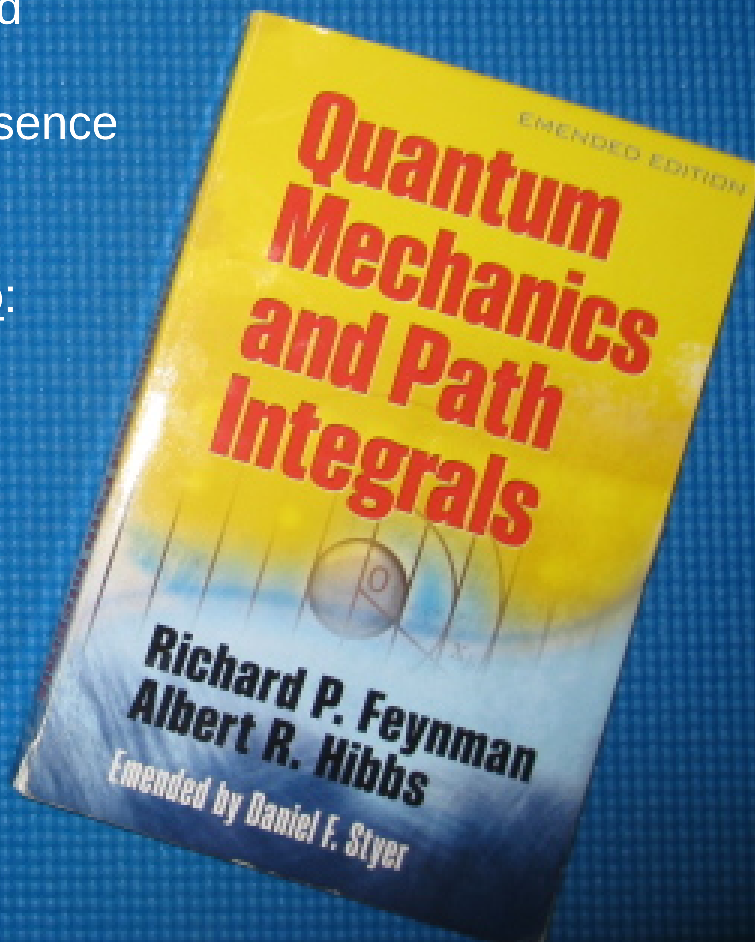
High Energy D_2 Bond from Feynman's Integral Wave Equation

By: Thomas Barnard

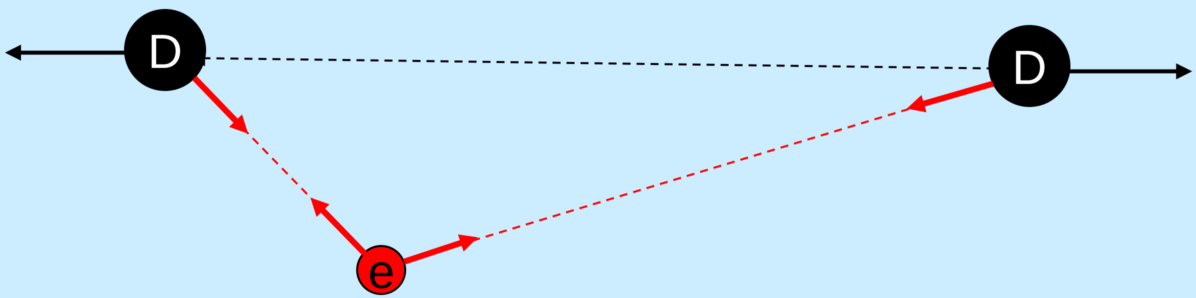
Sponsored by: Coolesence

Special Thanks to:
Mat McConnell
Rick Cantwell
Jim Barnard





Molecular Deuterium



Behavior Determined by
Electro-Static Forces

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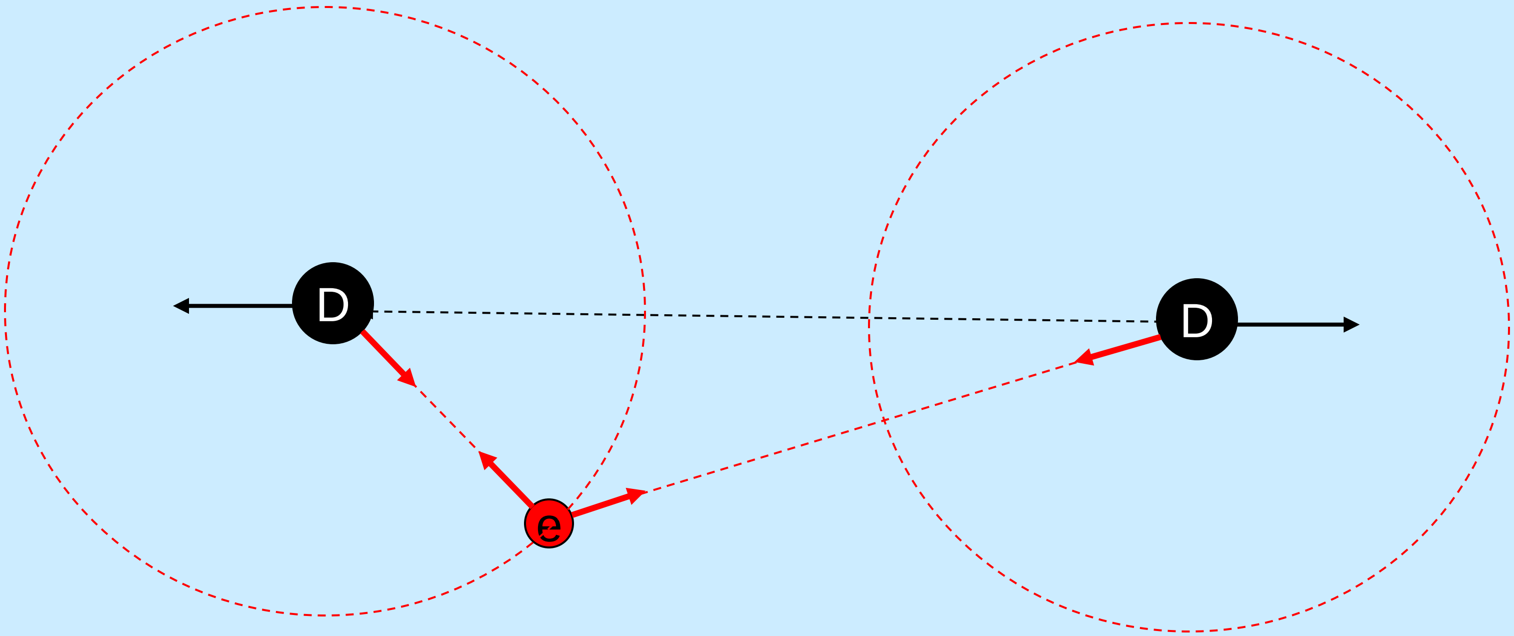
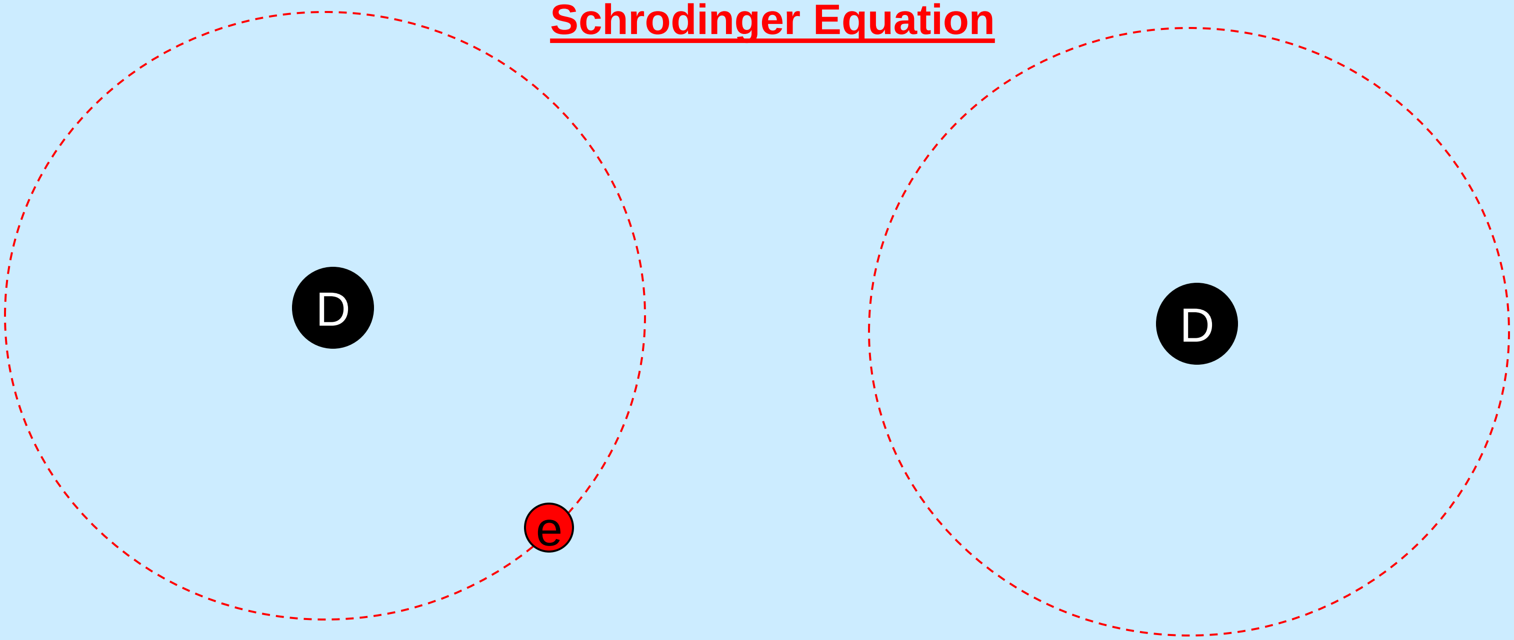


Behavior Determined by
Electro-Static Forces
and
Described by
Quantum Mechanics

Molecular Deuterium

All Properties predicted by the
Schrodinger Equation



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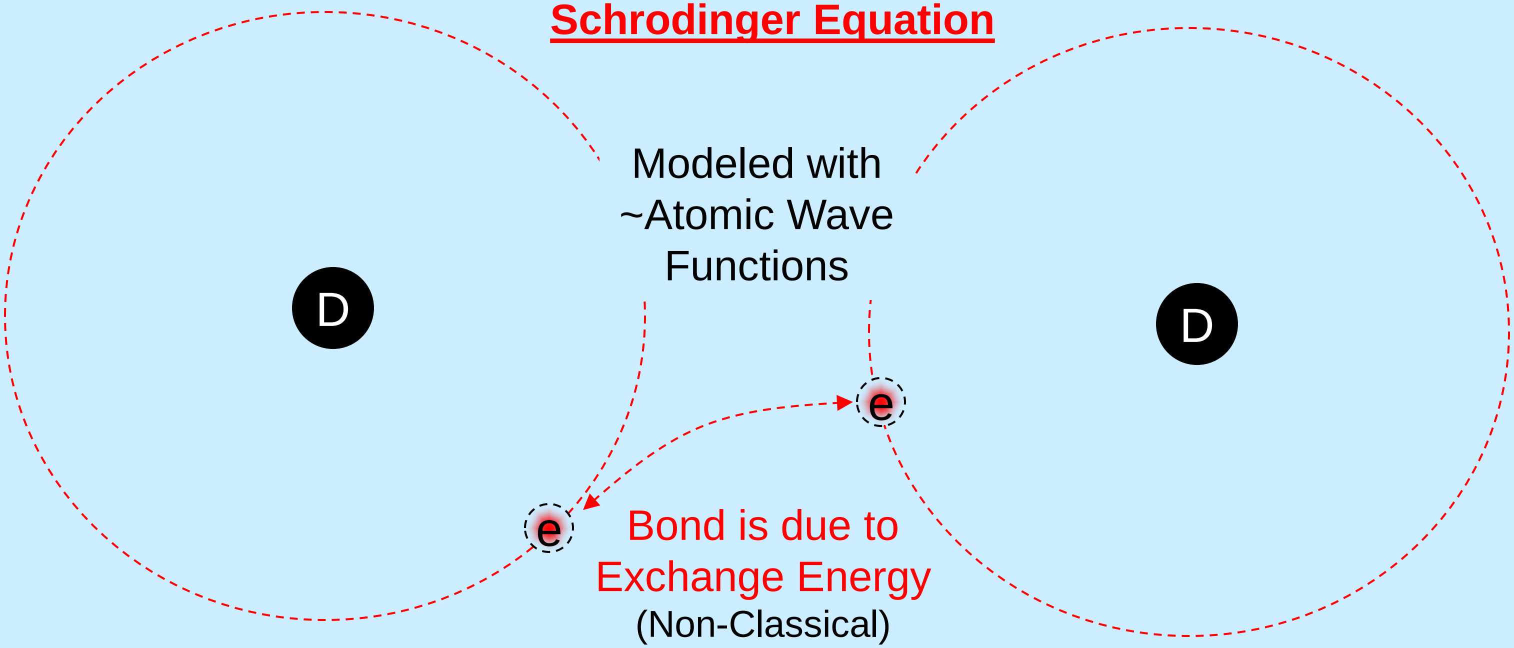

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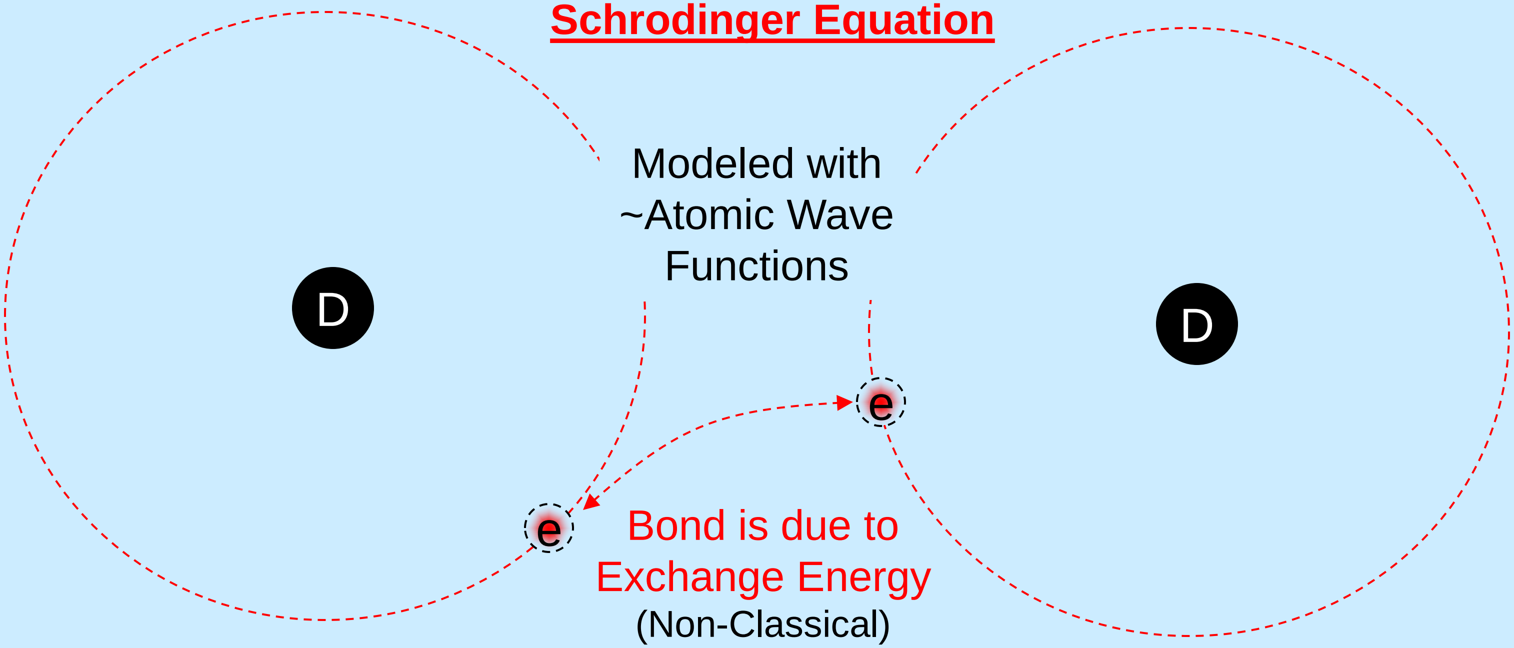

Born-Oppenheimer Approximation

Nuclei are held Stationary while calculating the Electron Wave Function

Good Place to Start?

All Chemistry is Based on this!!

Molecular Deuterium

All Properties predicted by the
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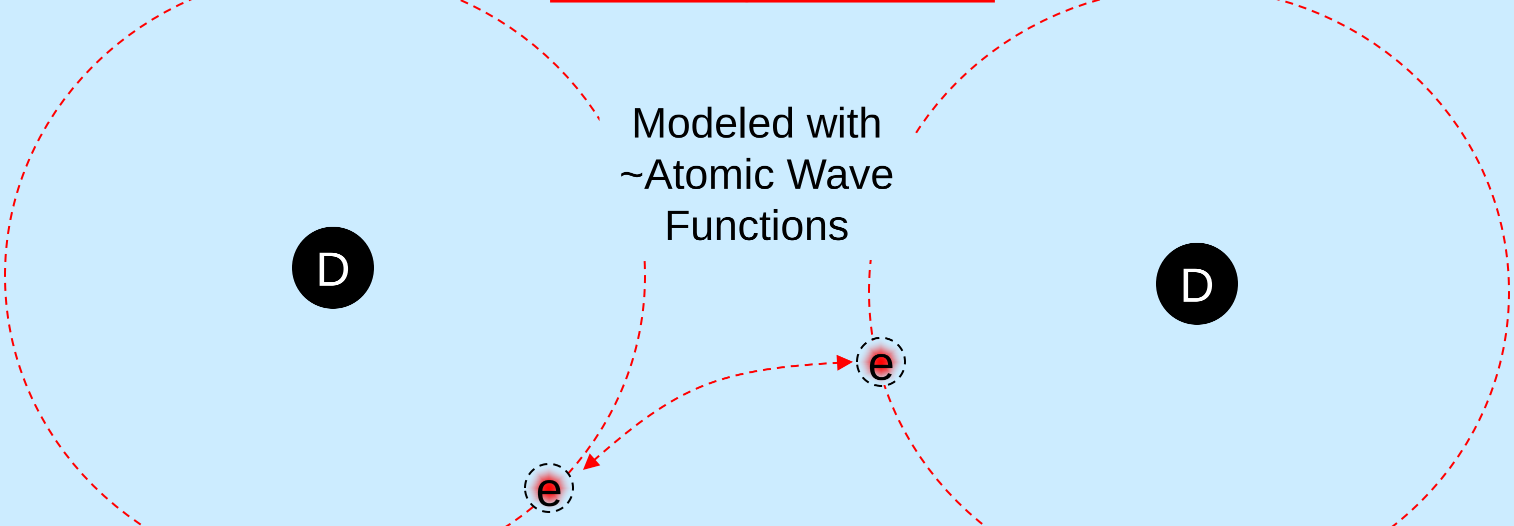


Fleischman-Pons affect would seem to require
High K.E. Deuterons (not stationary):

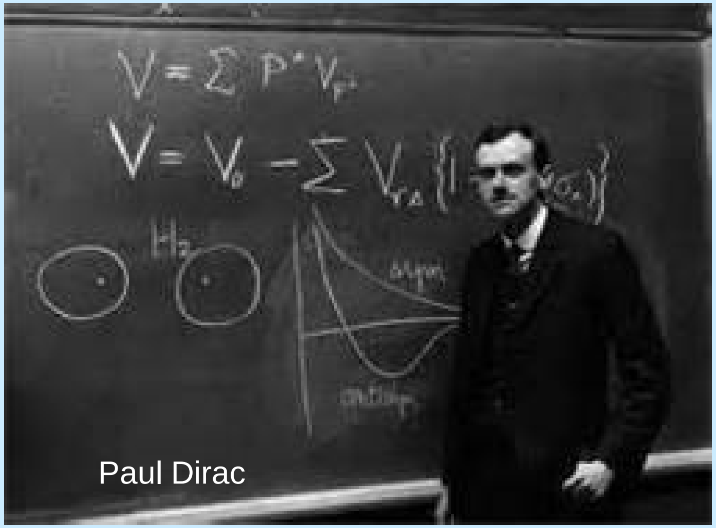
1. To Localize ➔ Uncertainty Principle $\left(\Delta x \geq \frac{\hbar}{2\{2mE_k\}^{1/2}}\right)$
2. To Overcome ➔ Coulomb Repulsion
3. Similar Deuteron - Electron Energies ➔ Coupling

- ➔ **Can not** use Born-Oppenheimer **Approximation**

Paul Dirac's, "The Lagrangian in Quantum Mechanics" : 1932

(The paper that *inspired Feynman's Path Integral Approach ~1942*)

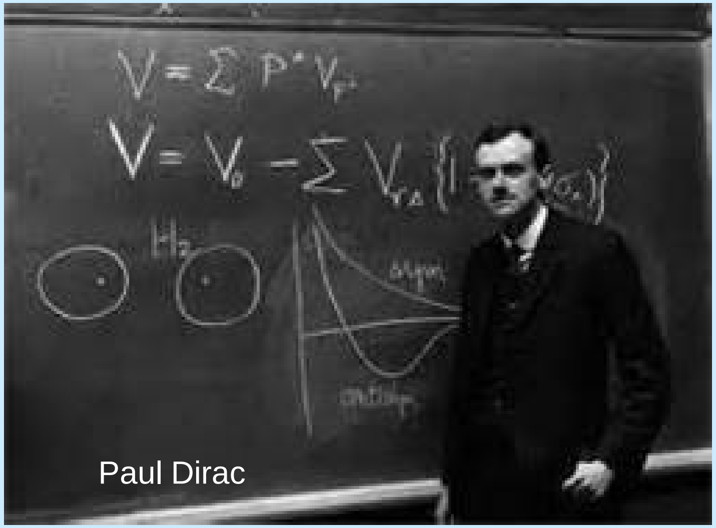
"…Now there is an alternative formulation for classical dynamics provided by the Lagrangian… **there are *reasons for believing that the Lagrangian one is the more fundamental...***"



Paul Dirac

[Paul Dirac, “The Lagrangian in Quantum Mechanics” : 1932]

“…the Lagrangian method allows one to collect together **all the equations of motion and express them as the stationary property of a certain action function.** (This **action function** is just the time integral of the **Lagrangian**). There is no corresponding action principle in terms of the coordinates and momenta of the Hamiltonian theory…”



Paul Dirac

What Does That Mean?

The "Action" integral accounts for particle behavior over the time, or period of an Observation

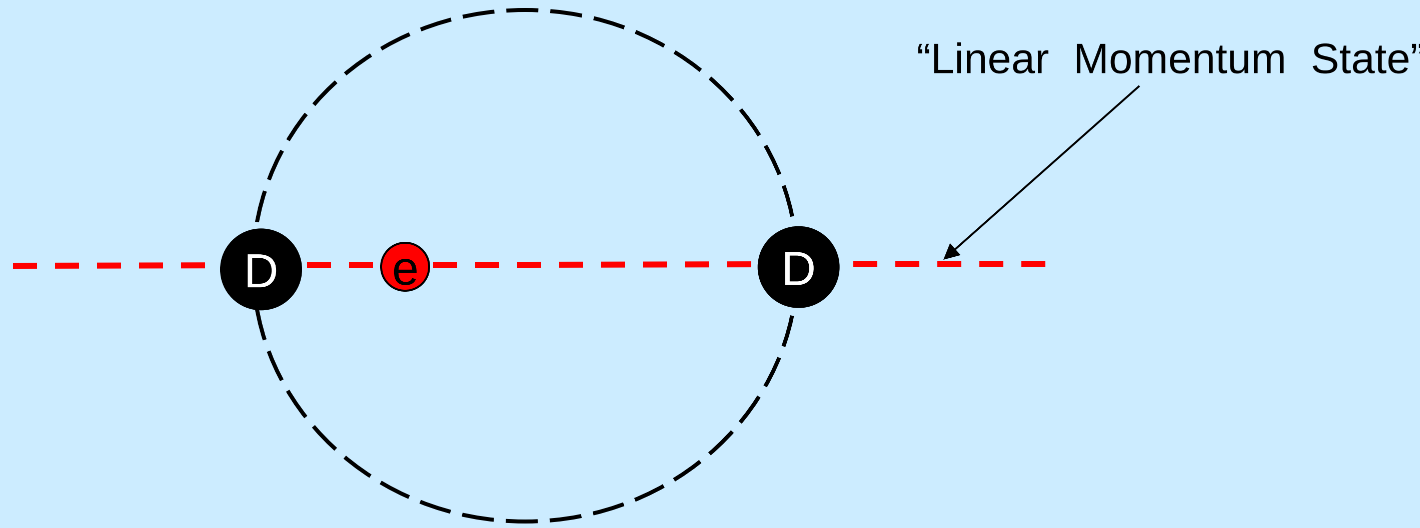
The Differential Hamiltonian (Schrodinger Eq.) can not easily model correlated interference affects over periods of time and space

i.e. Should not use Born-Oppenheimer with High K.E. Deuterons + Electrons

Could there be **<u>Another Form</u>** of **D_2** ?

<u>Hypothesis</u>: A correlated state of 2 Deuterons and an Electron: the **"<u>Linear</u> <u>Momentum</u> <u>State</u>"**

D_2^* ?



A **<u>Dynamic</u> <u>Correlation</u>** ***obscured*** by the

<u>Born-Oppenheimer</u> <u>Approximation</u>

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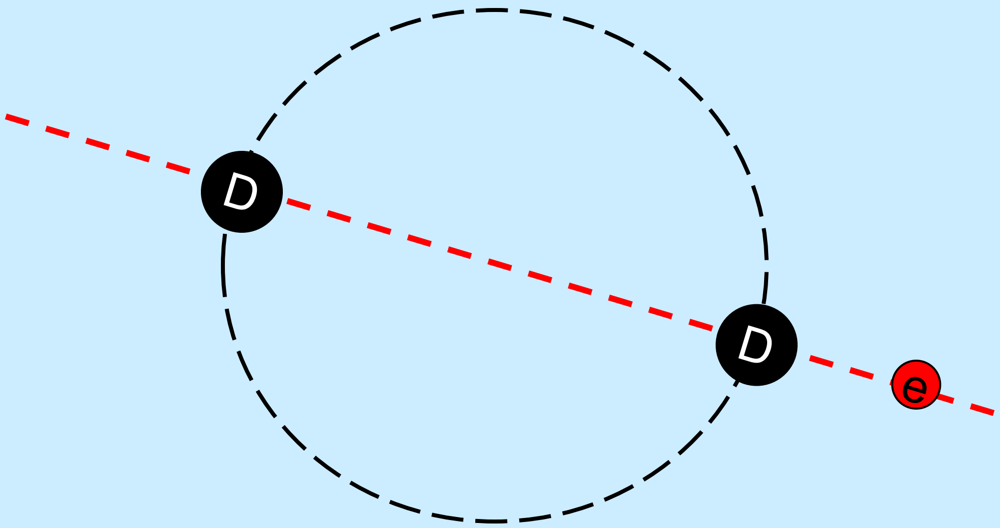

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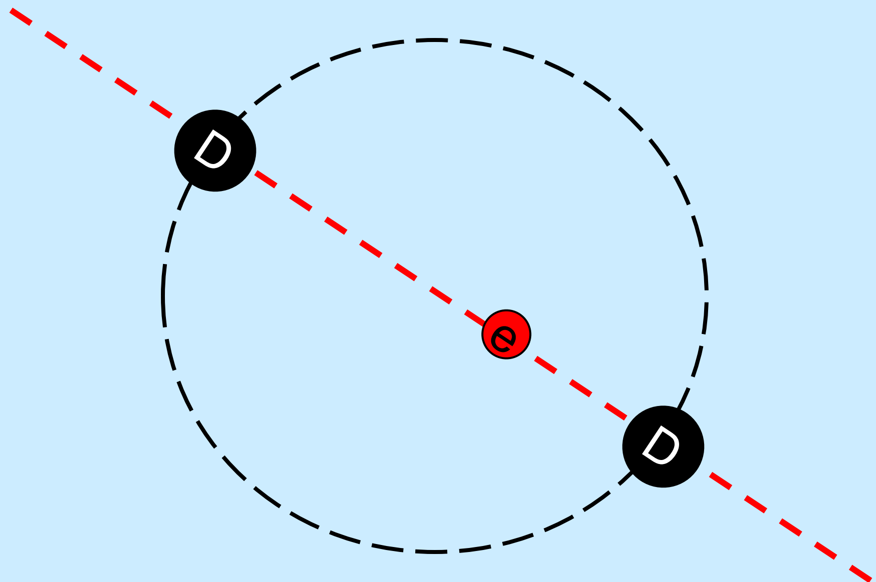

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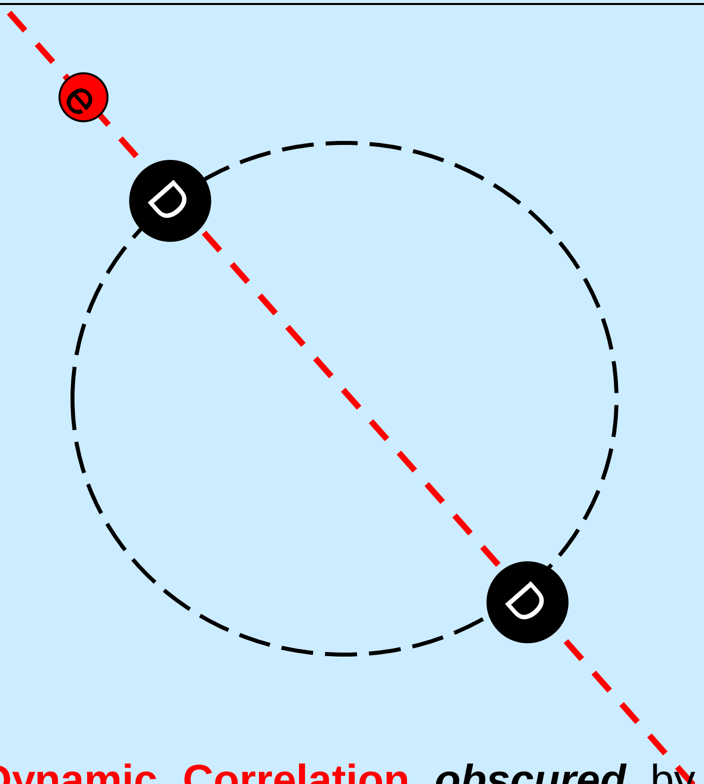

A **Dynamic Correlation** ***obscured*** by the

Born-Oppenheimer Approximation

If the **Linear Momentum State** ***Does*** Exist,

it Leads to the **3 Miracles:**

1- Coulomb Barrier Penetration (~30 keV bond)

2- No Neutrons (coupled Electron - Nuclei)

- Text Book Time-Dependent Coupled Two-State Problem
- Also ppm tritium to ^{4}He ratio

3- No Gammas (coupled Electron - Nuclei)

– Also orders of magnitude effective bonding:

- **~Angstrom to Fermi ➔ Chemical Mechanism**

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<u>**Nagging Question**</u>

Can the <u>Linear Momentum State</u> be derived from **'accepted' Q.M. principles??!!**

Conceptual Understanding

of the Linear Momentum State

We Need 3 Basic Concepts :

1) The 'Action' from the Lagrangian
2) Path Amplitude Summation
3) Stationary State Requirements

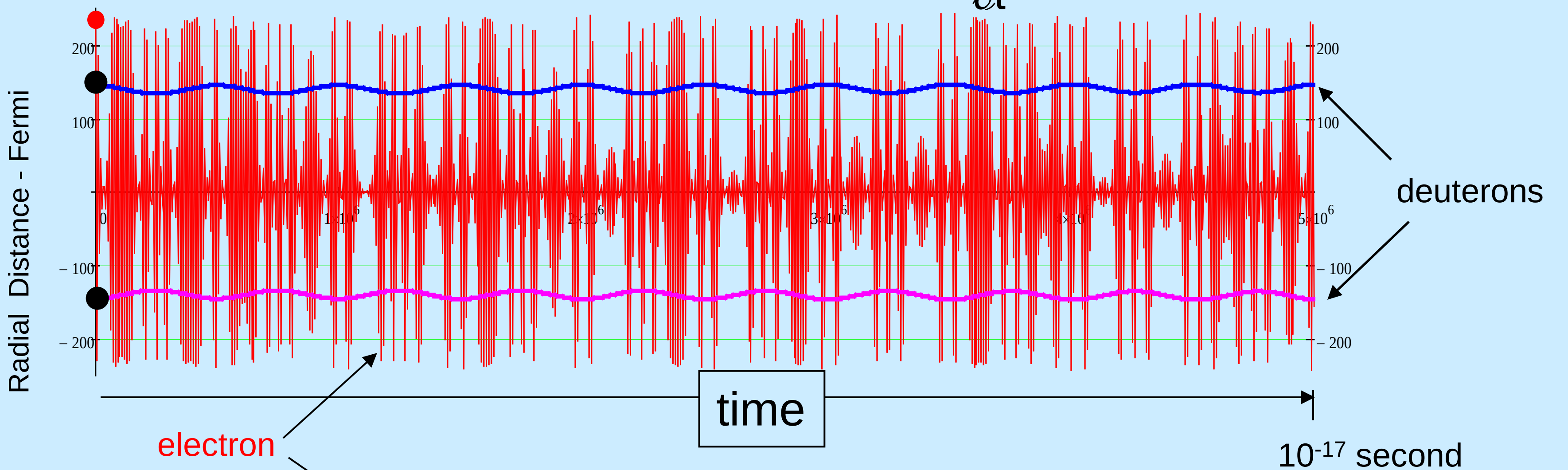
Outline

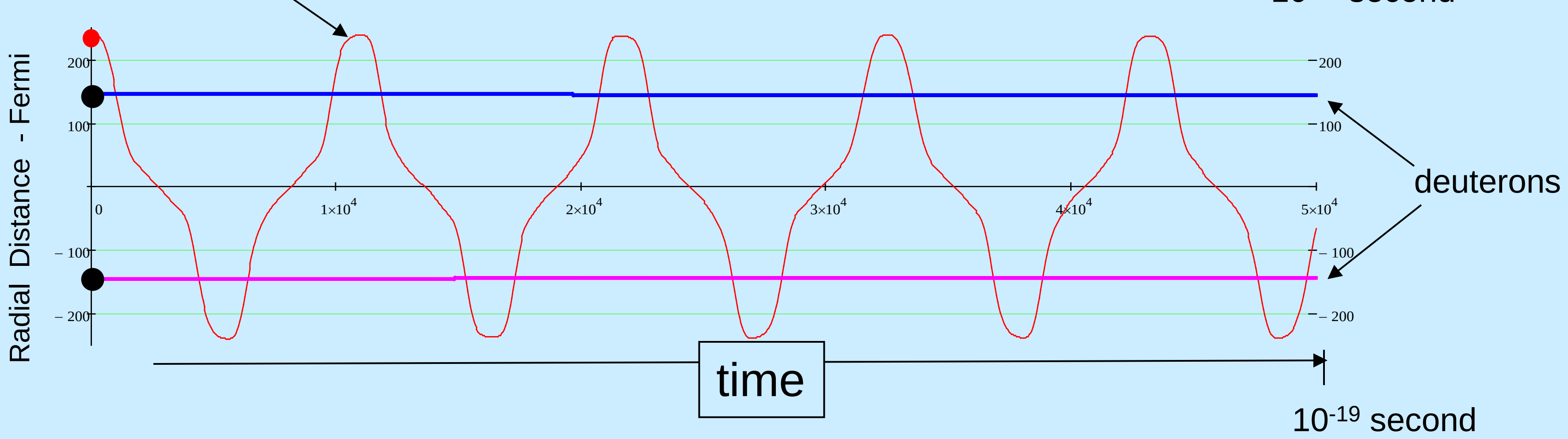
- D_2^* as a Classical Bond
- Review Double Slit Interference
- Dirac's Path Amplitude
- Principle of least Action
- Summing Complex Amplitudes
- Stationary State Requirement
- Conclusion:
  - Semi-Classical "Linear Momentum State"

D_2^* Classical Bond Simulation

-Radial Position vs. Time-

3 coupled 2nd order Differential Eq. using ➔ $F = m \cdot a = m \frac{\partial^2 x}{\partial t^2}$ Initial velocity: $V(t=0) = 0$

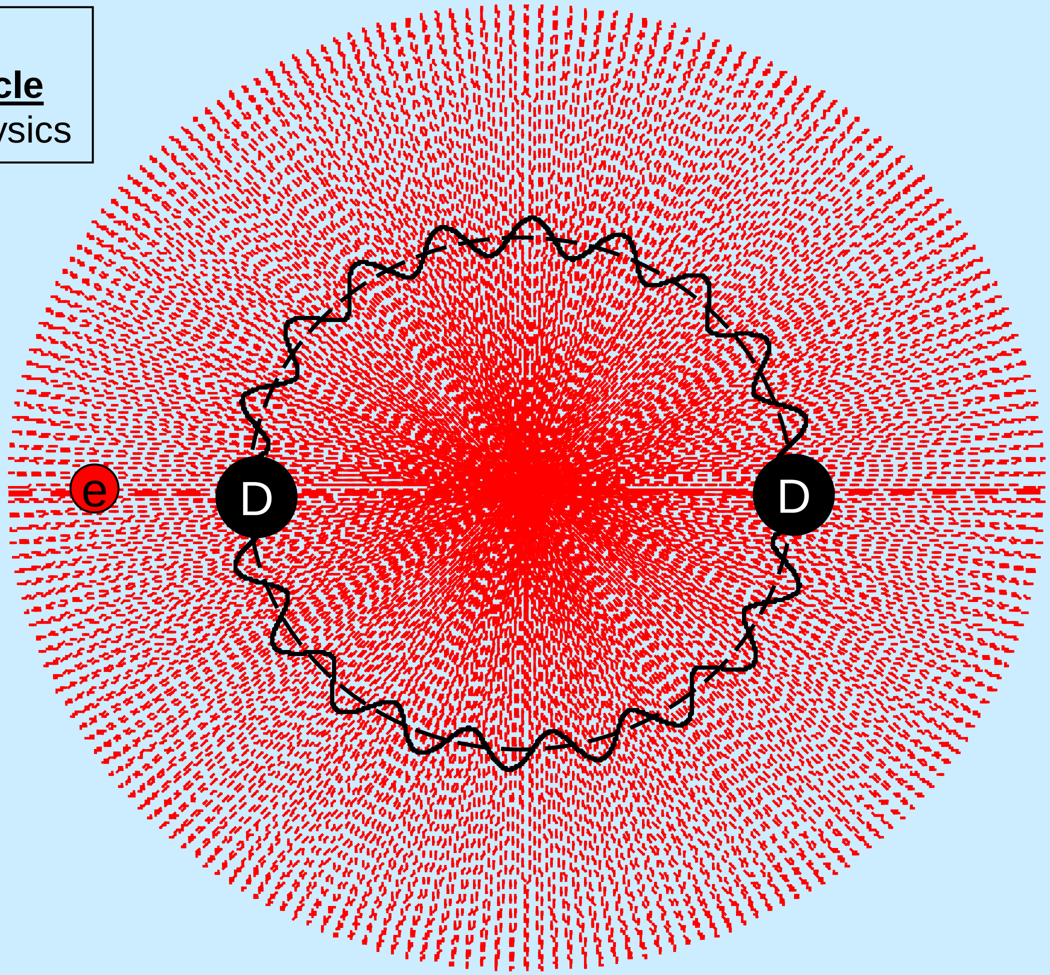




Classical "Orbit" of D_2^*

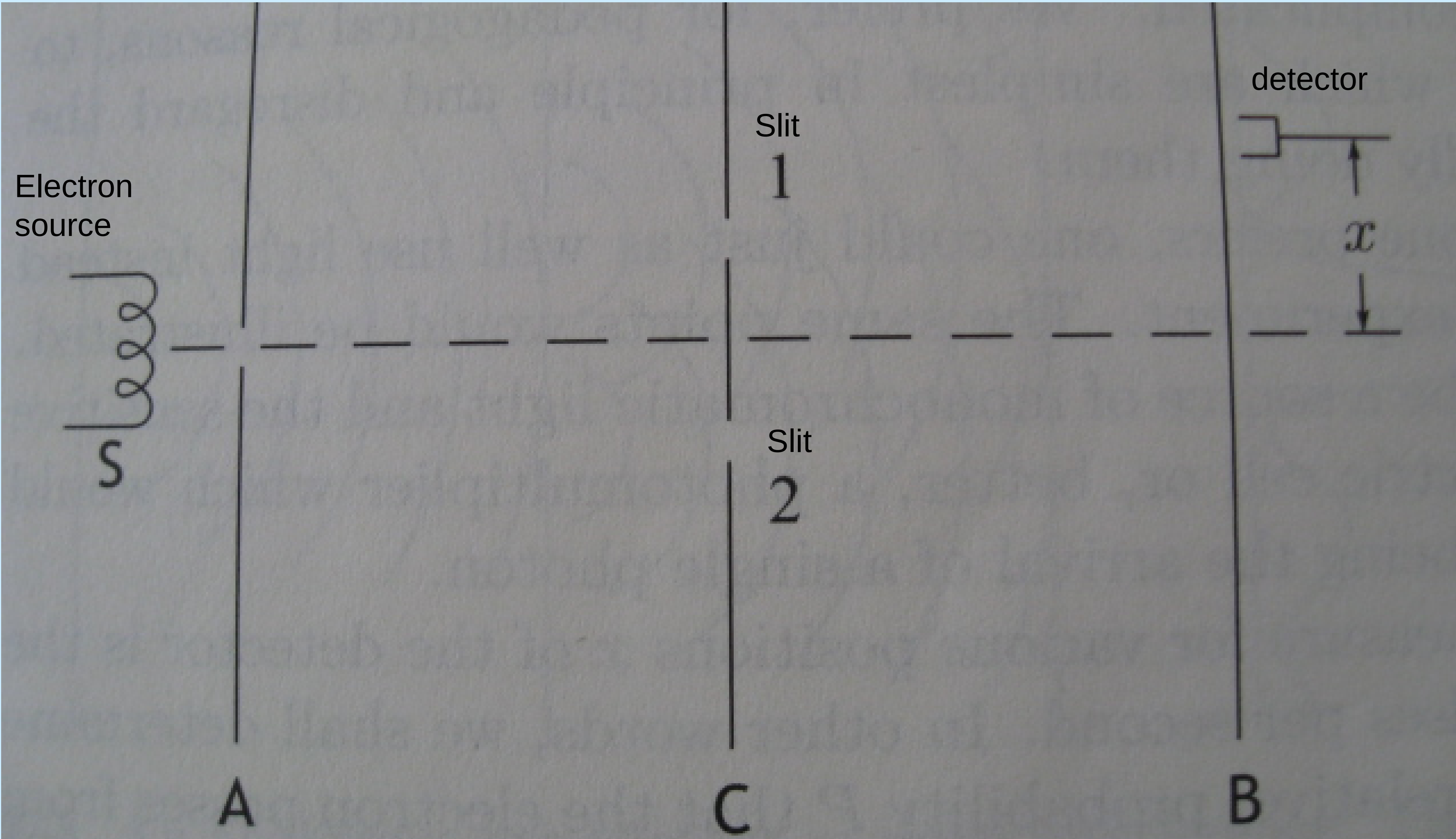
Dimensions determined by Q.M.
just like the Hydrogen atom

Electron acting like a
Force Carrying Particle
familiar to nuclear physics



Double Slit Experiment with Electrons

Feynman and Hibbs , "Quantum Mechanics and Path Integrals" pg. 3



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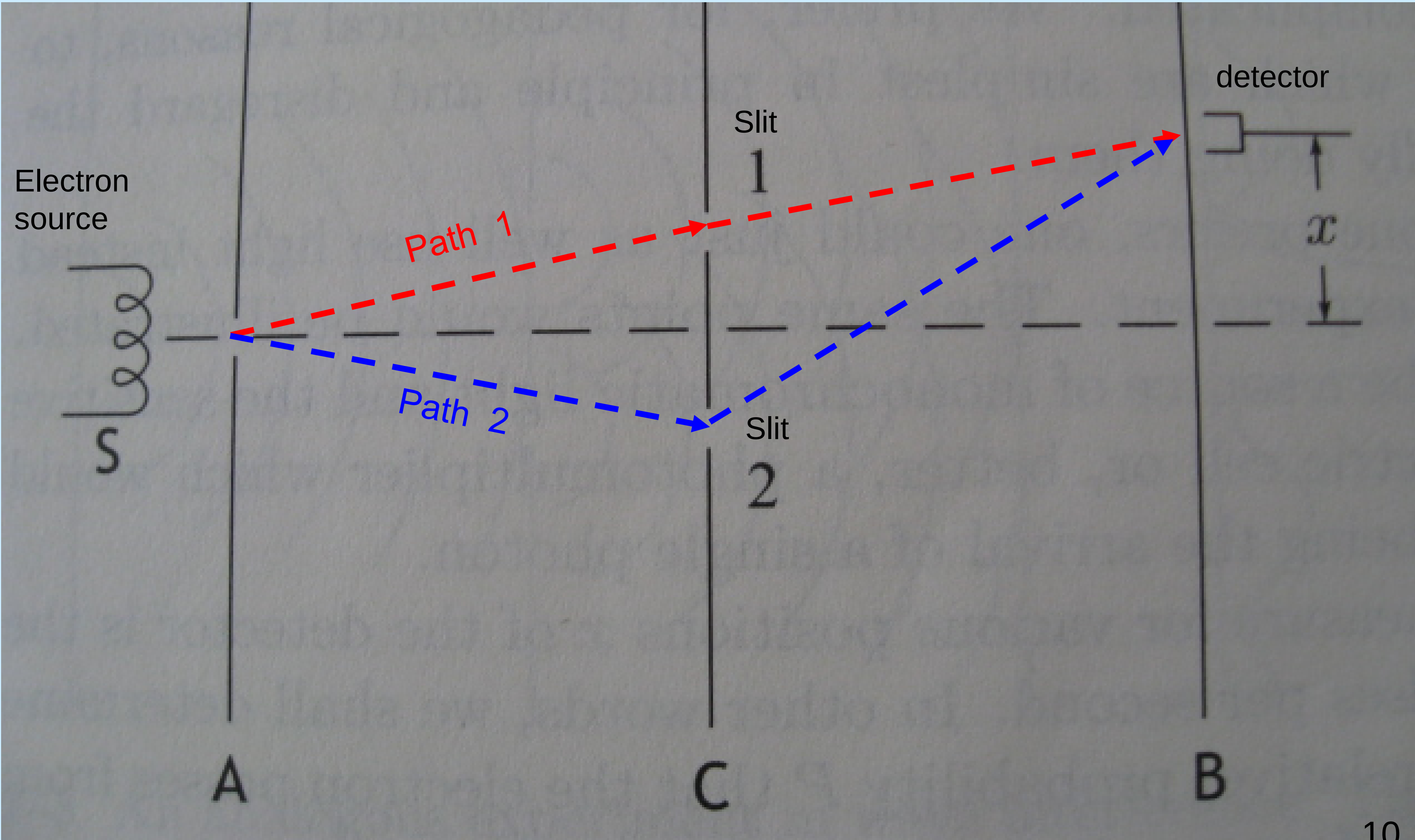

Probability Distributions from Double Slit Experiments

Feynman and Hibbs , “Quantum Mechanics and Path Integrals” pg. 4

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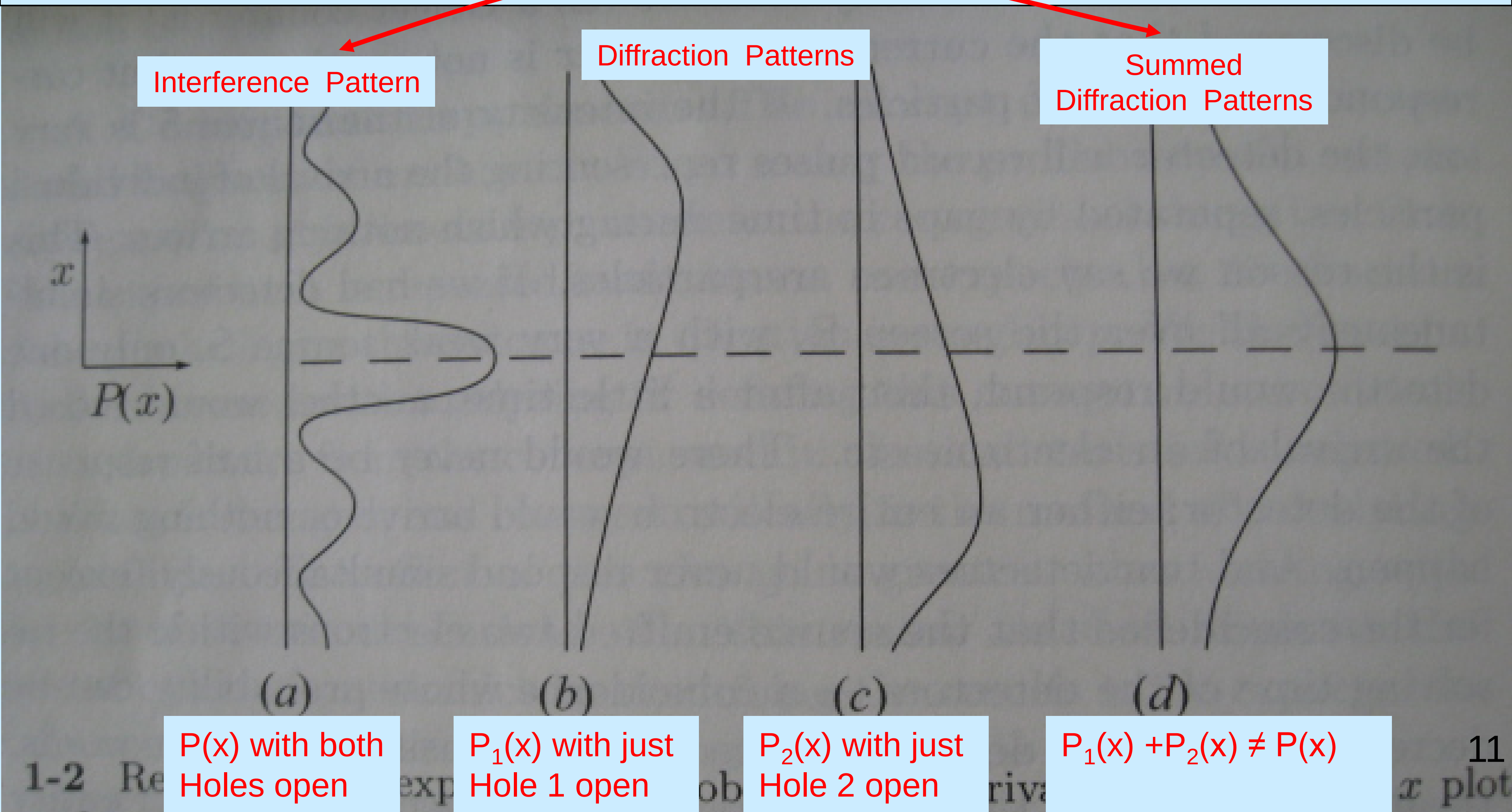

Dirac's Contact Transformation

"The Lagrangian in Quantum Mechanics" : 1932

$$\emptyset_{j[b,a]} \sim e^{\frac{i}{\hbar} S_{j[b,a]}}$$

The amplitude for a single path "j"

Where: S = 'Action' for path 'j' (from 'a' to 'b')
= the time integral of Lagrangian

$$S = \int_{t_a}^{t_b} \mathcal{L}\, \partial t \rightarrow \text{Action}$$

$$\mathcal{L} = \left\{ (\text{K.E.}) - (\text{P.E.}) \right\} \rightarrow$$ Lagrangian: Classical Newtonian Mechanics

Classical Mechanics meets **Wave** Mechanics !

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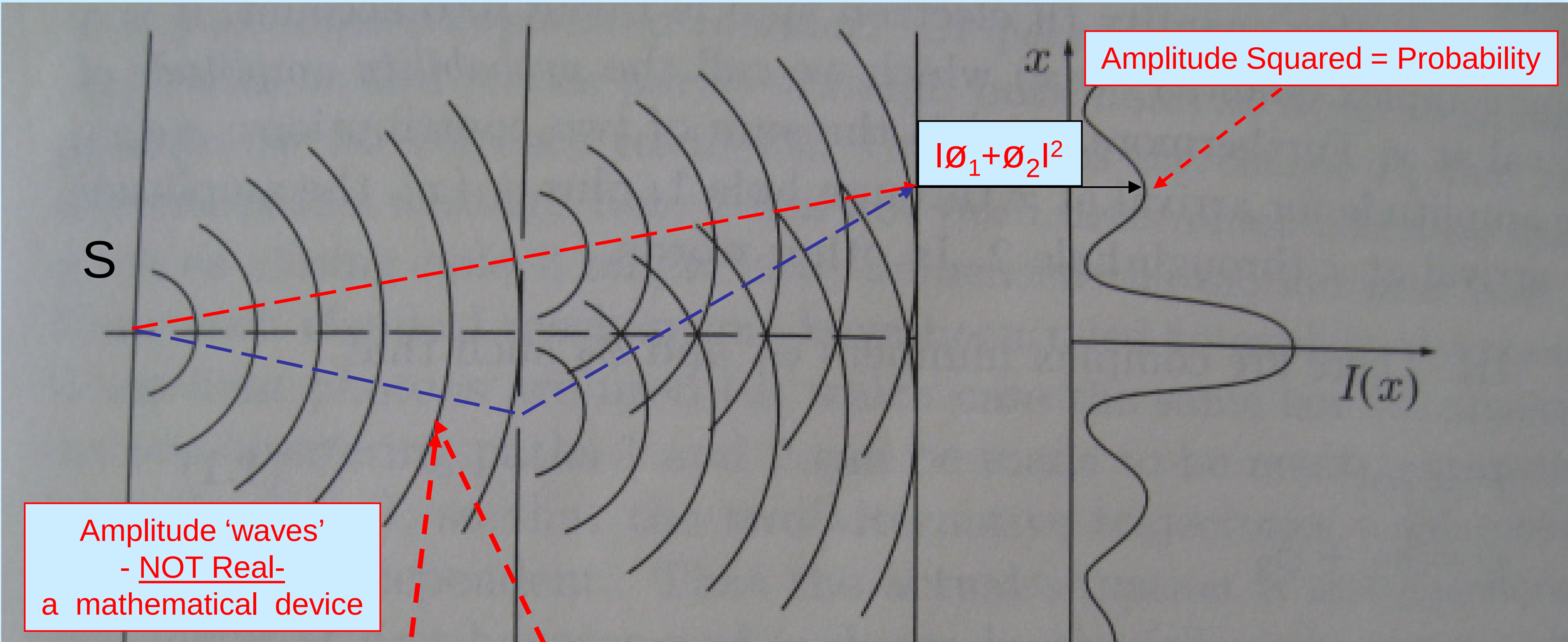
Analogous Experiment in Wave Interference



$$Ø_j[b,a] \sim e^{\frac{i}{\hbar} S_j} = \cos(S_j/\hbar) + i \sin(S_j/\hbar)$$

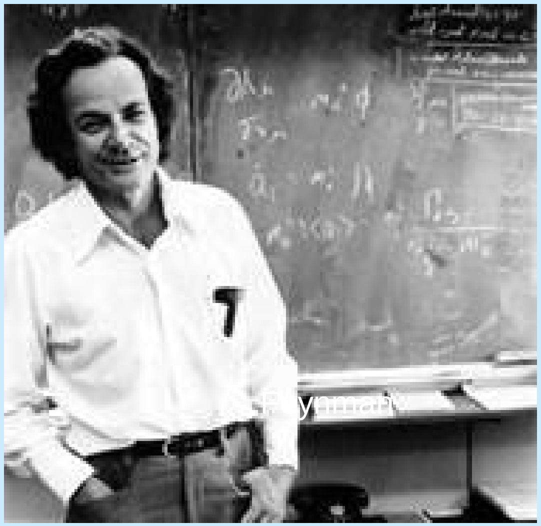
← Euler's Formula

Feynman and Hibbs , "Quantum Mechanics and Path Integrals" pg. 5

"… The easiest way to represent wave amplitudes is by complex numbers..." -Feynman

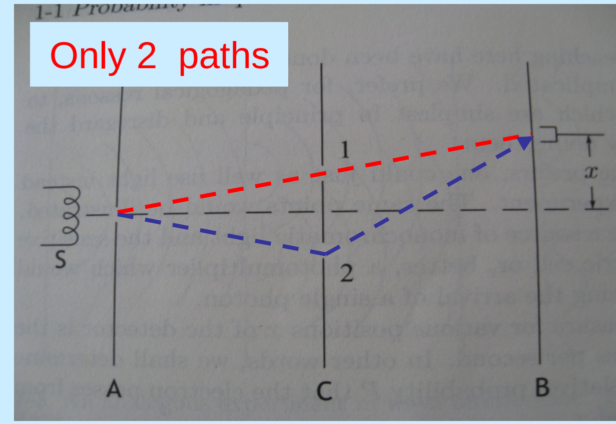
Feynman's Wave Equation

Can Derive Schrodinger Equation from this Concept



Sum over ***all*** possible paths in **time** and **space**

$$\Psi[b(t_b)] = \sum \{e^{\frac{i S}{\hbar}} \Psi[a(t_a)]\}$$



Recall:

$$S = \int_{t_a}^{t_b} \mathcal{L}\, \partial t \rightarrow \text{Action}$$

$$\mathcal{L} = (\text{K.E.}) - (\text{P.E.})$$

Feynman's Wave Equation

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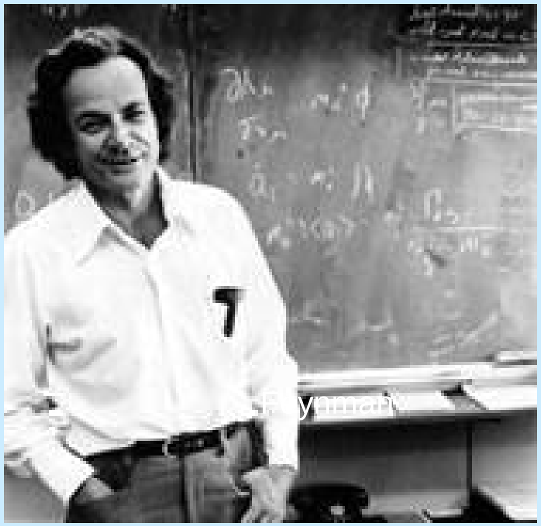
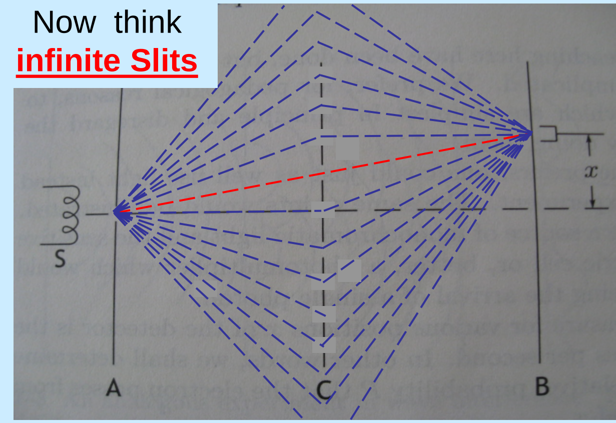


Sum over ***all*** possible paths in **time** and **space**

$$\Psi[b(t_b)] = \sum \{e^{\frac{iS}{\hbar}} \Psi[a(t_a)]\}$$

Now think **infinite Slits**



Recall:

$$S = \int_{t_a}^{t_b} \mathcal{L}\, \partial t \rightarrow \text{Action}$$

$$\mathcal{L} = (\text{K.E.}) - (\text{P.E.})$$

Can be solved

but

Conceptual Approach today

The Principle of Least Action

The Lagrangian = {K.E.} – {P.E.}

$$S = \text{Action} = \int_{t_a}^{t_b} \left(\frac{m}{2} v^2 - V_{(x,y,z)} \right) \partial t$$

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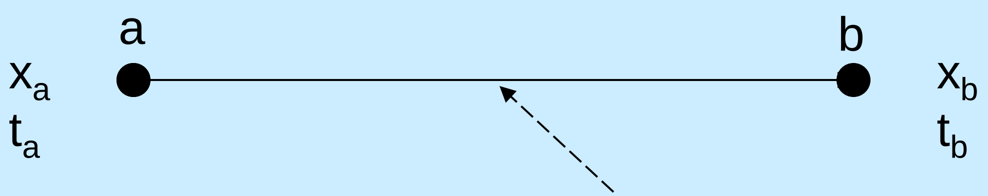
0 for free particle

Action of a Free particle



Classical Path
From ‘a’ to ‘b’
(constant velocity)

The Principle of Least Action

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Action of a Free particle

$$S_{cl} = \frac{m}{2} \left(\frac{\Delta x}{\Delta t} \right)^2 (\Delta t)$$

Classical ‘Action’

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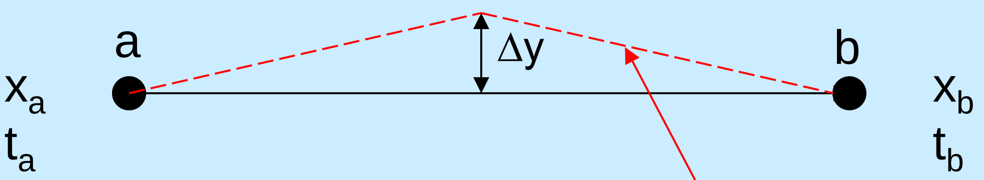

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non-classical **Paths**:
think
Double Slit

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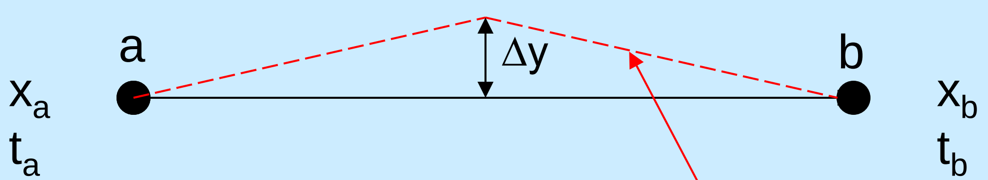

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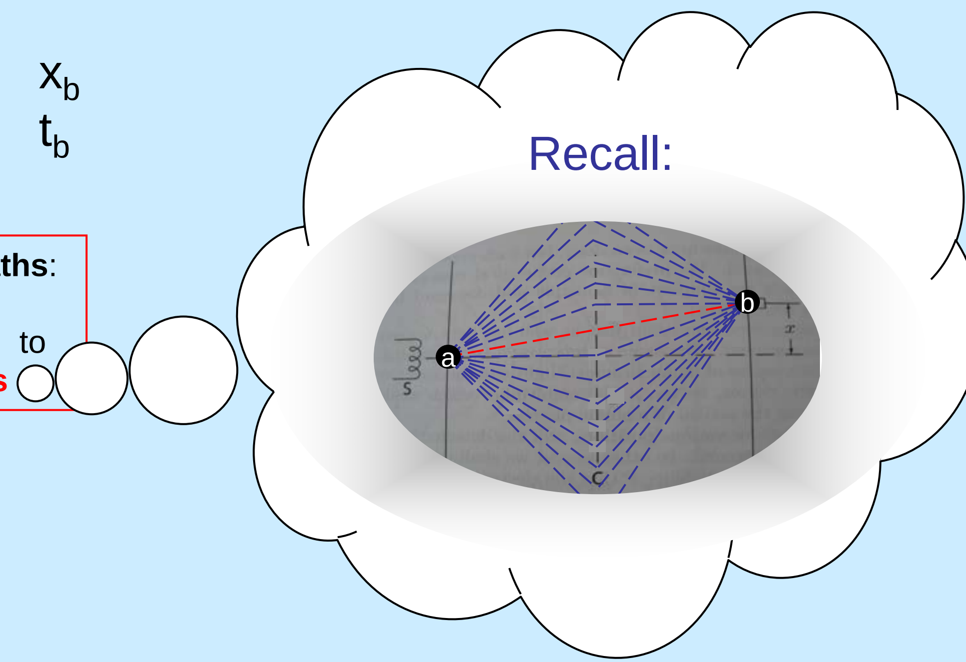
Double Slit to
Infinite Slits



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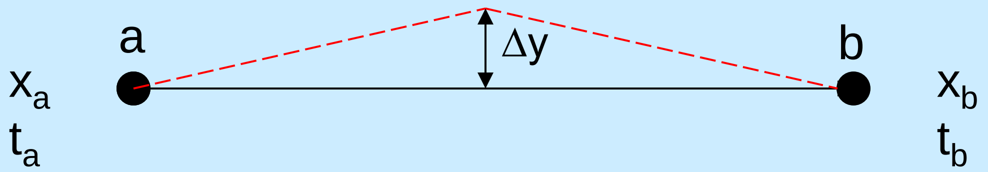

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Classical ‘Action’
$\Delta y = 0$

$$S_{\Delta y} = \frac{m}{2} \left\{ \left(\frac{\Delta x}{\Delta t} \right)^2 + \left(\frac{2\,\Delta y}{\Delta t} \right)^2 \right\} (\Delta t)$$

Action of Alternate Paths
(non-classical Action)

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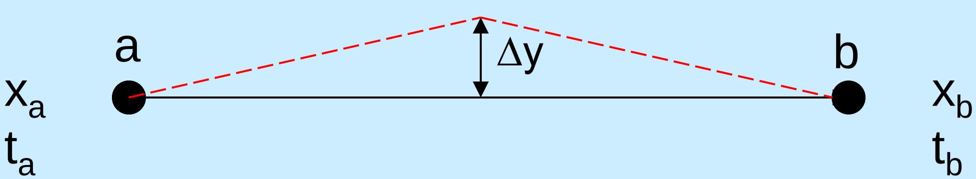

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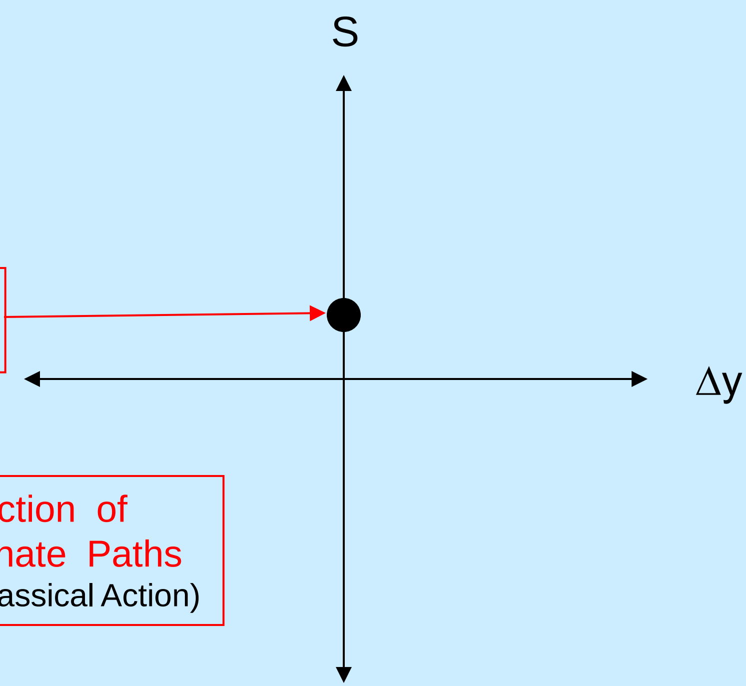

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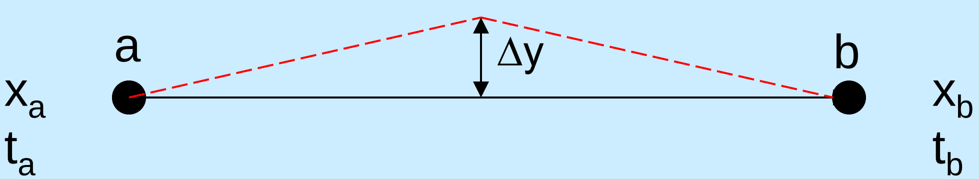

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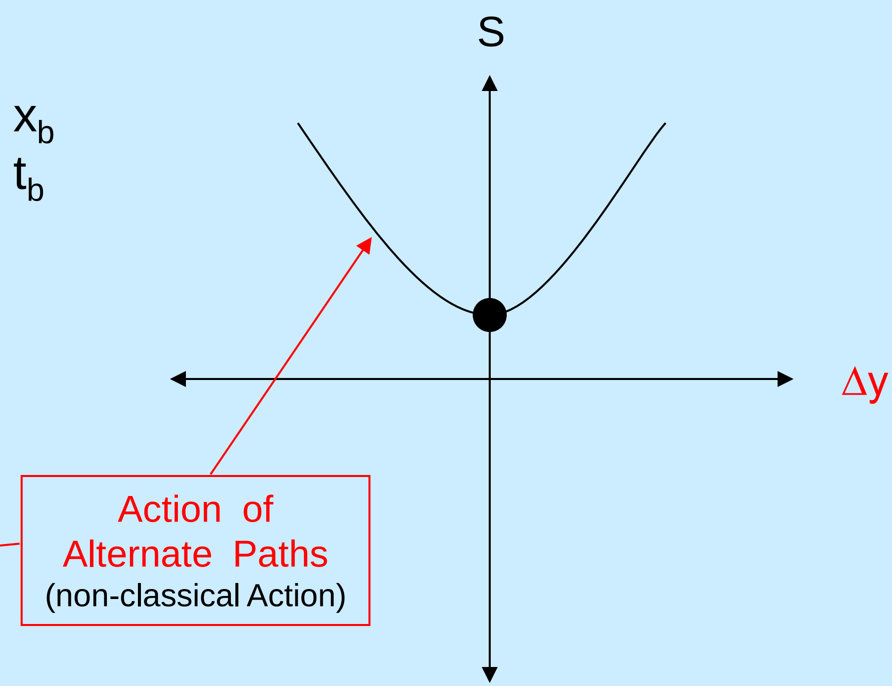

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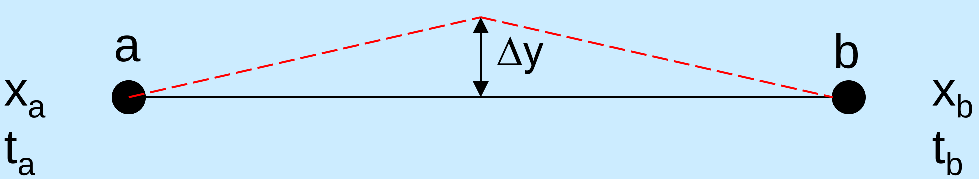

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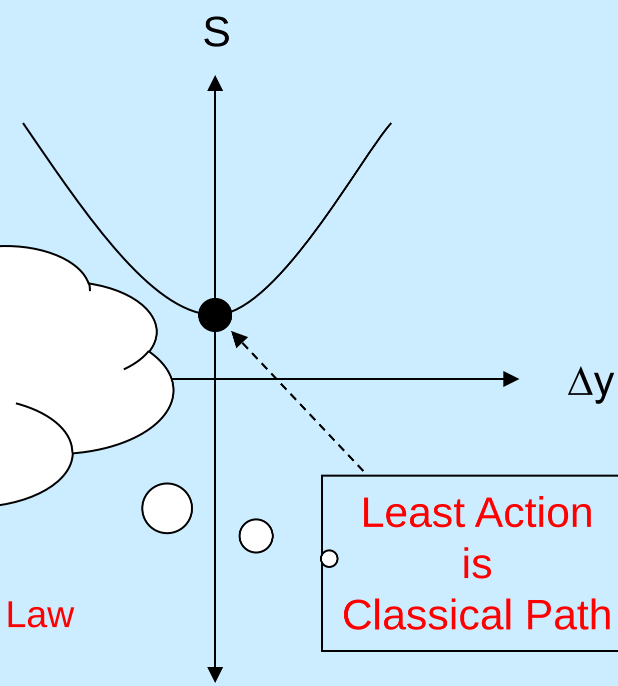
Classical Path ➔ Extremum

$$\left(\text{i.e. } \frac{dS}{dy} = 0 = ma - F\right)$$

Newtons's 2nd Law



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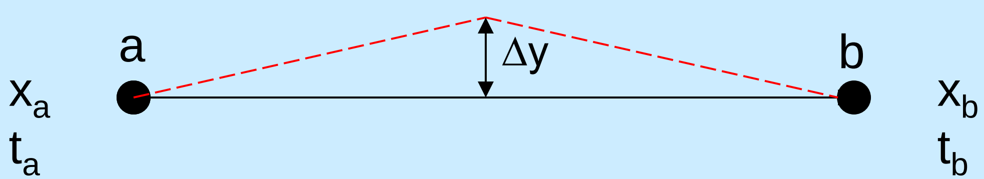
Recall:
D_2^* Classical Motion
An Extremum

Action of a Free particle



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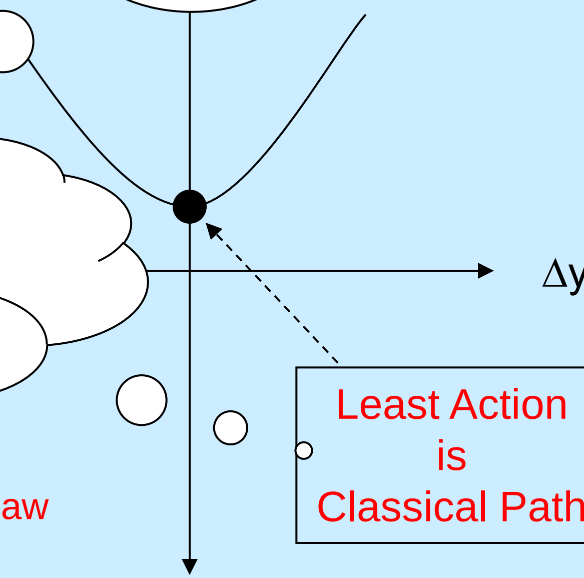
Classical Path ➔ Extremum

(i.e. $\frac{dS}{dy} = 0 = ma - F$)

Newtons's 2nd Law

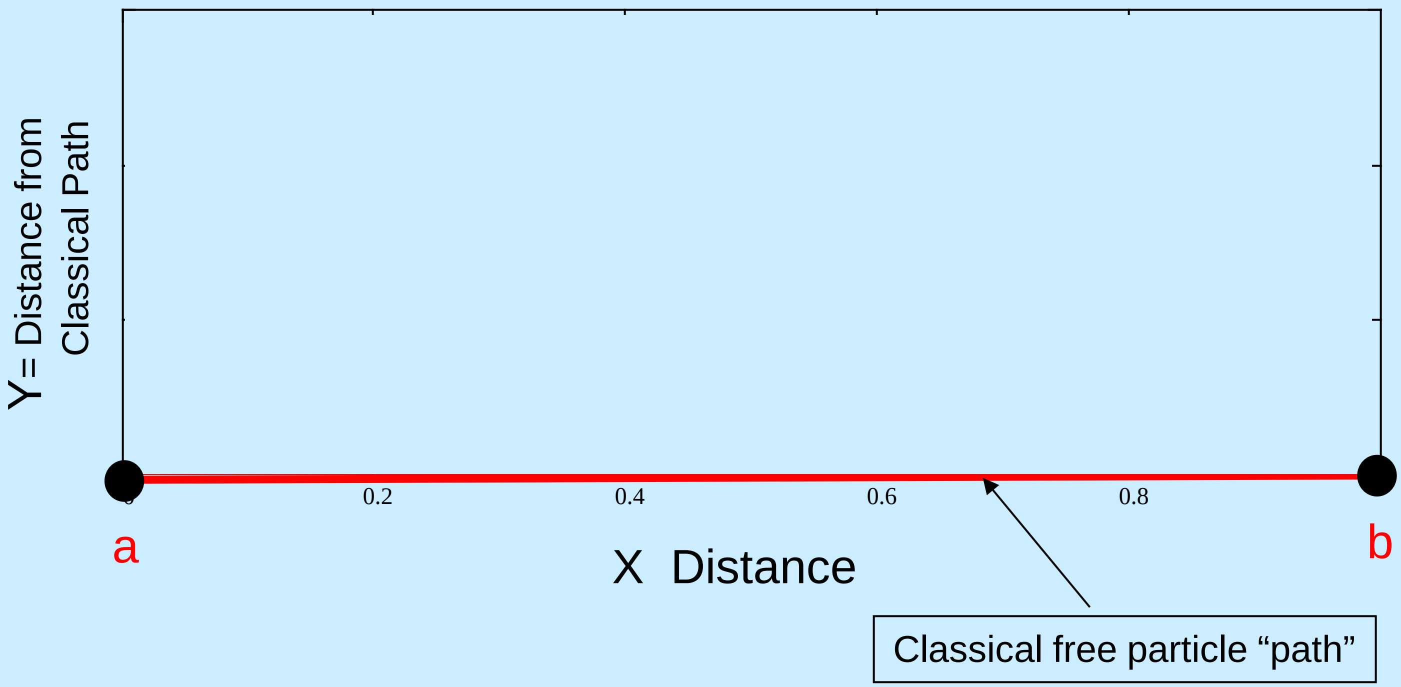


Least Action is Classical Path

Summing Amplitudes of Paths

‘Free Particle’ Examples

$$S = \text{Action} = \int_{t_a}^{t_b} \frac{m}{2}\left(v[x,t]^2 + v[y,t]^2 \right) \partial t$$



Summing Amplitudes of Paths

‘Free Particle’ Examples

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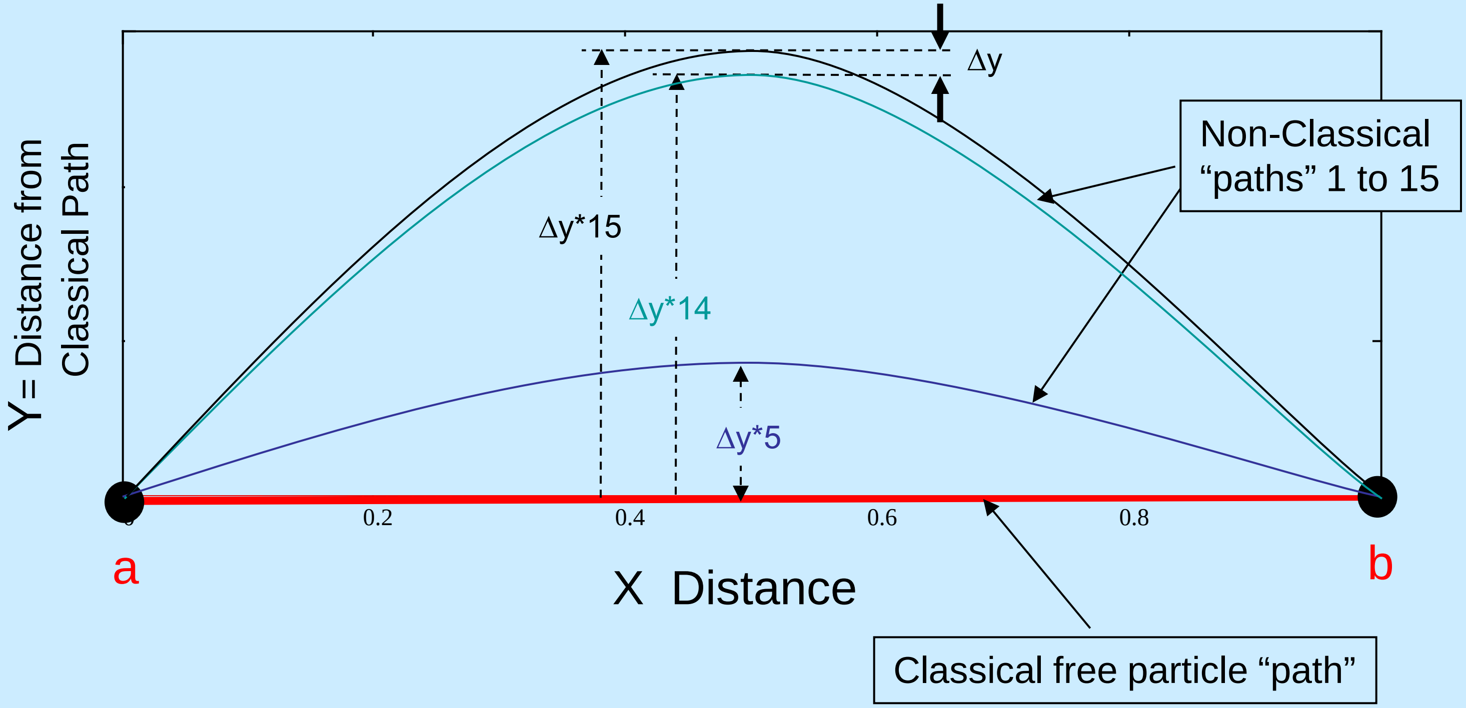
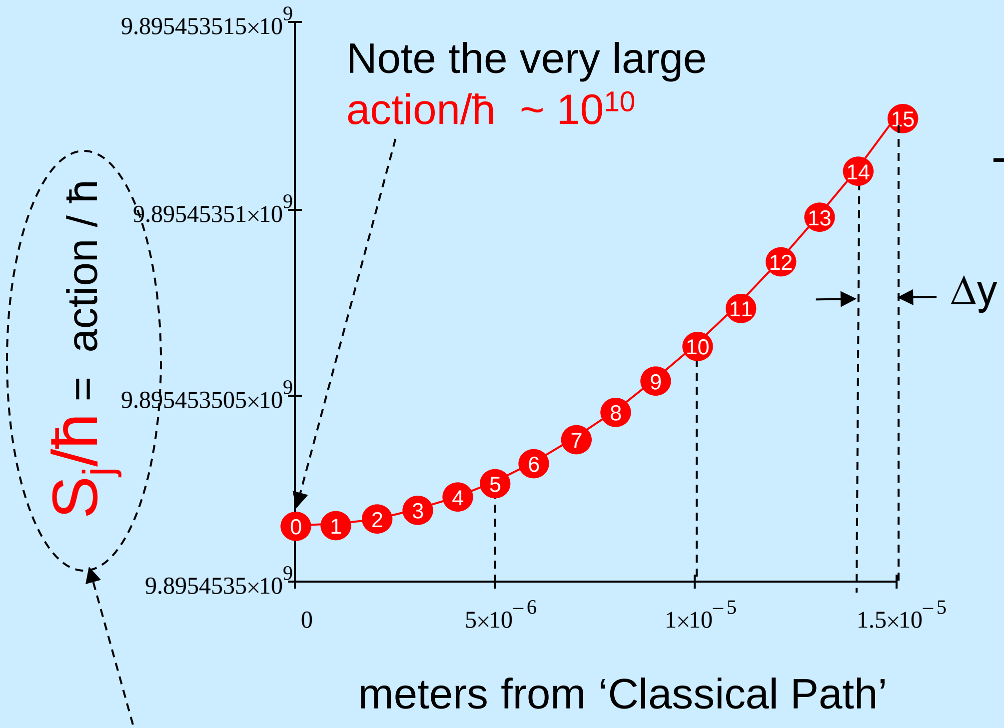


Example #1: Electron with 1 meter path at ~13.6 eV

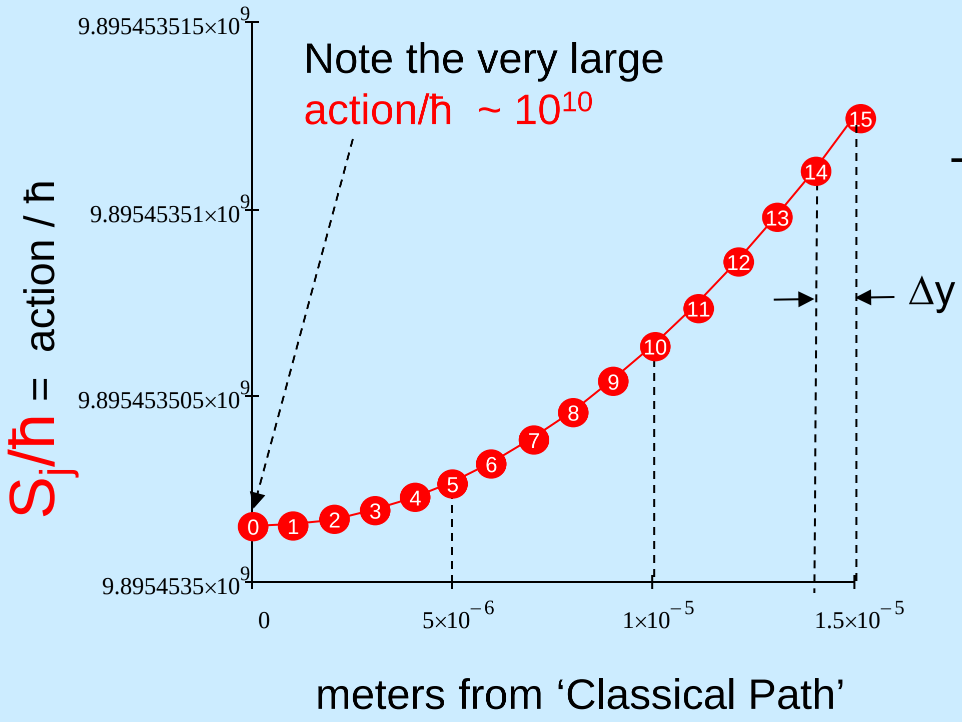


Sum of Paths

$$\text{Total Amplitude} = \sum_{J=0}^{15} e^{iS(j)/\hbar}$$

Action in units of Planks Constant

Example #1: Electron with 1 meter path at ~13.6 eV



Sum of Paths

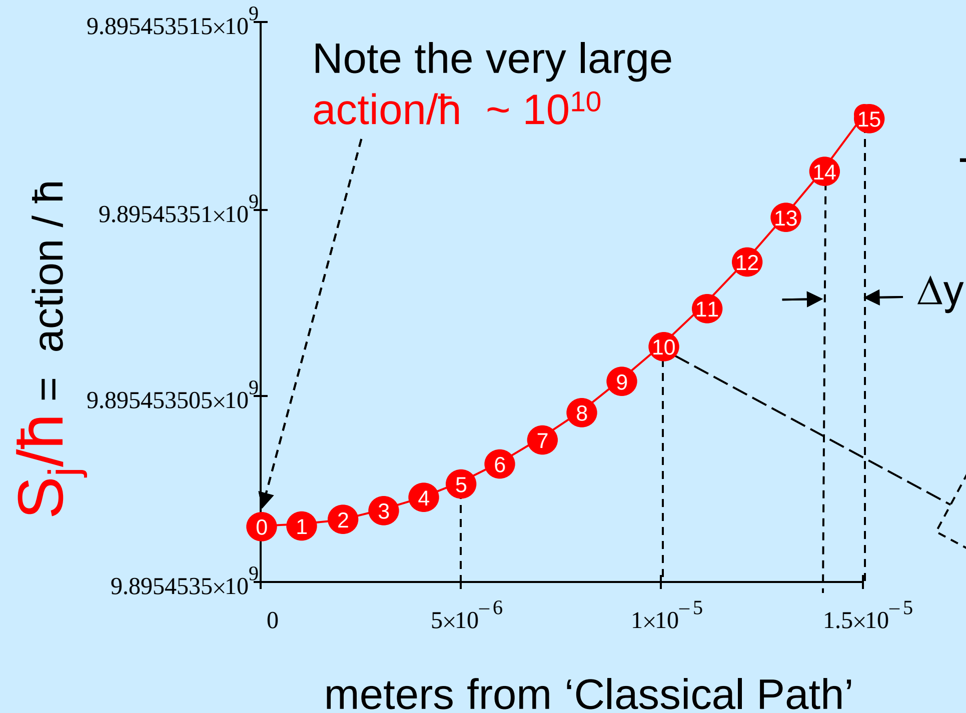
$$\text{Total Amplitude} = \sum_{J=0}^{15} e^{iS(j)/\hbar}$$

$$= \sum_{J=0}^{15} [\cos(S_j/\hbar) + i \sin(S_j/\hbar)]$$

Like adding Vectors
in the Complex Plane

imaginary

Example #1: Electron with 1 meter path at ~13.6 eV



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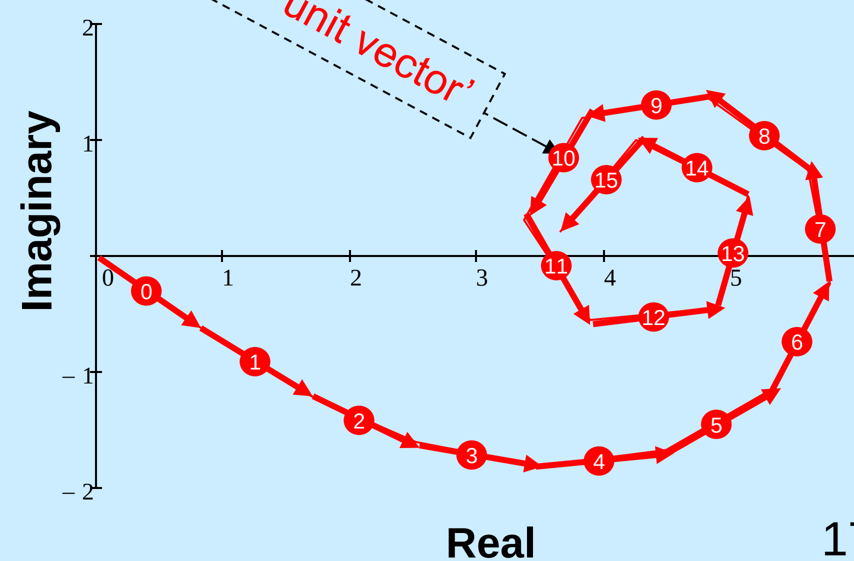
x= Real y= imaginary

Complex Plane

Each dot has a '~unit vector'



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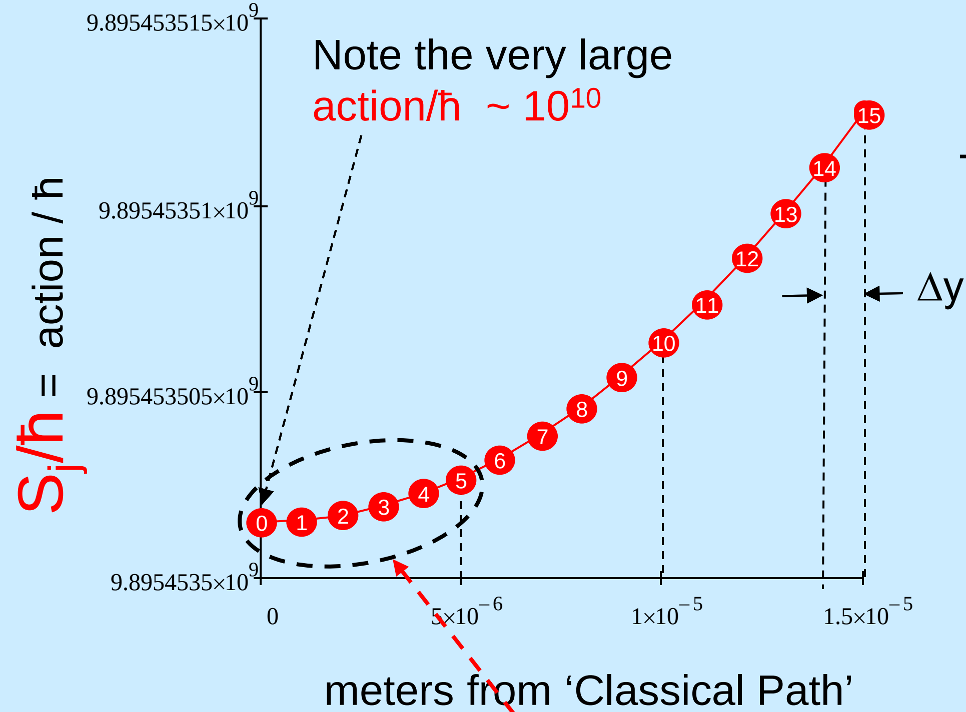

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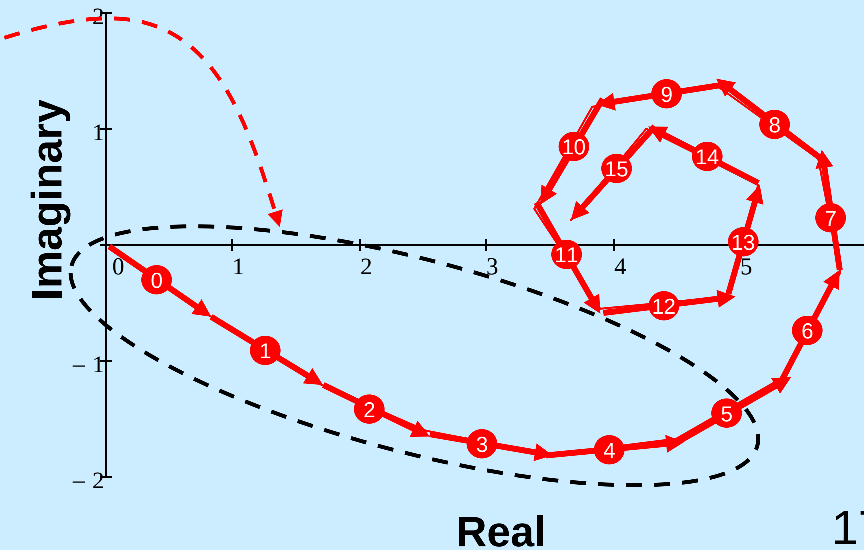
Complex Plane

Paths near ***Extremum***
Contribute to
'Sum of amplitudes'
(i.e. 'Observables')



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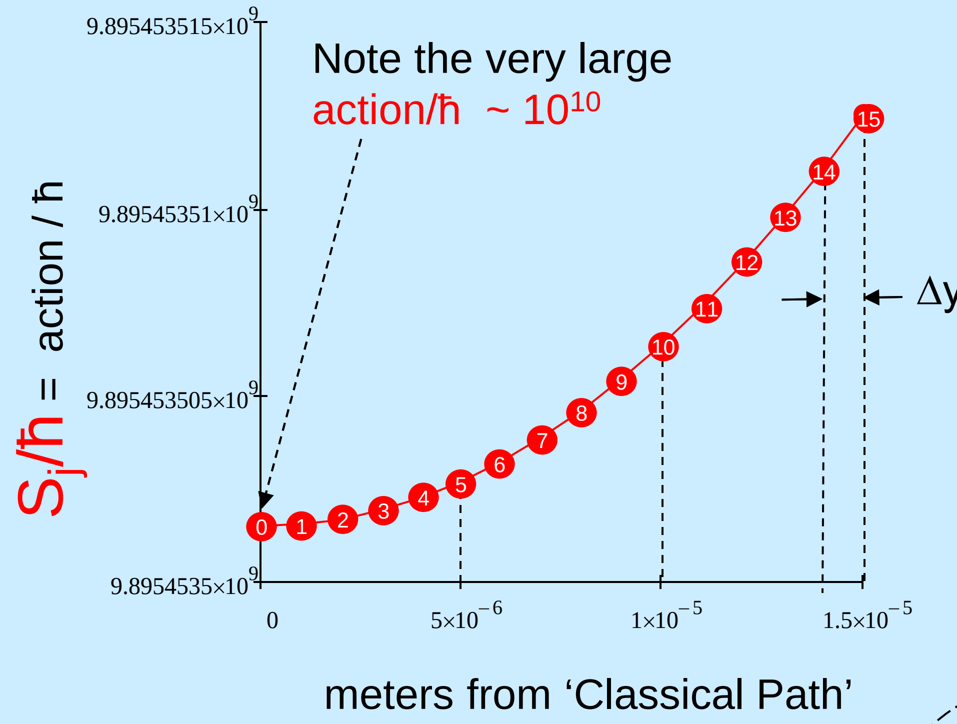

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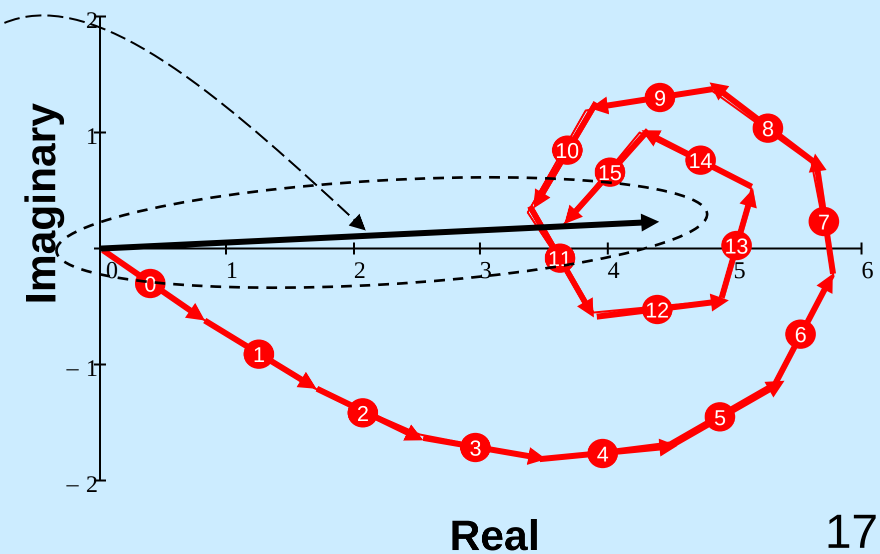

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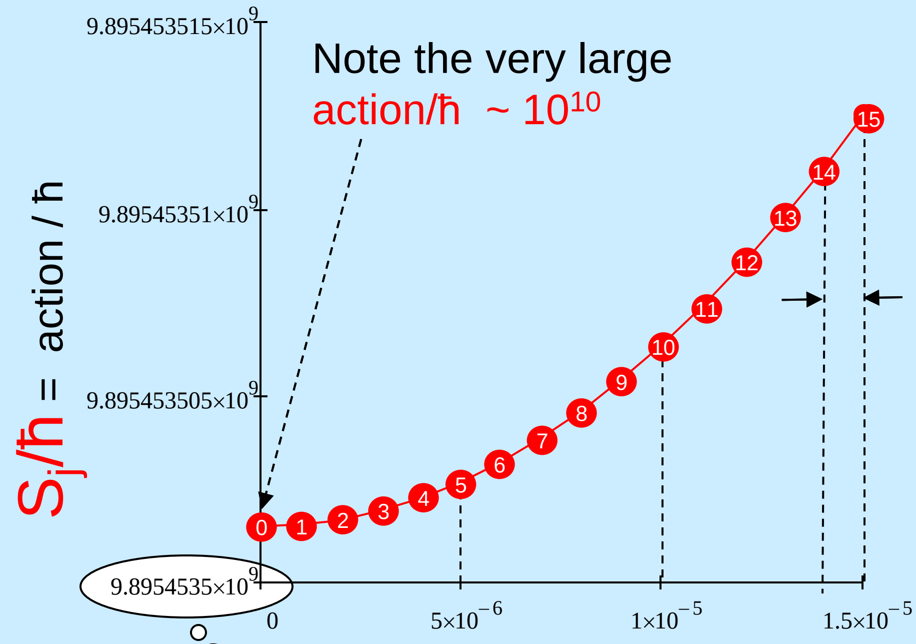

meters from 'Classical Path'

Remember:

Large 'Action' = Small Deviation from Classical Path

Sum of Paths

$$\text{Total Amplitude} = \sum_{J=0}^{15} e^{iS(j)/\hbar}$$

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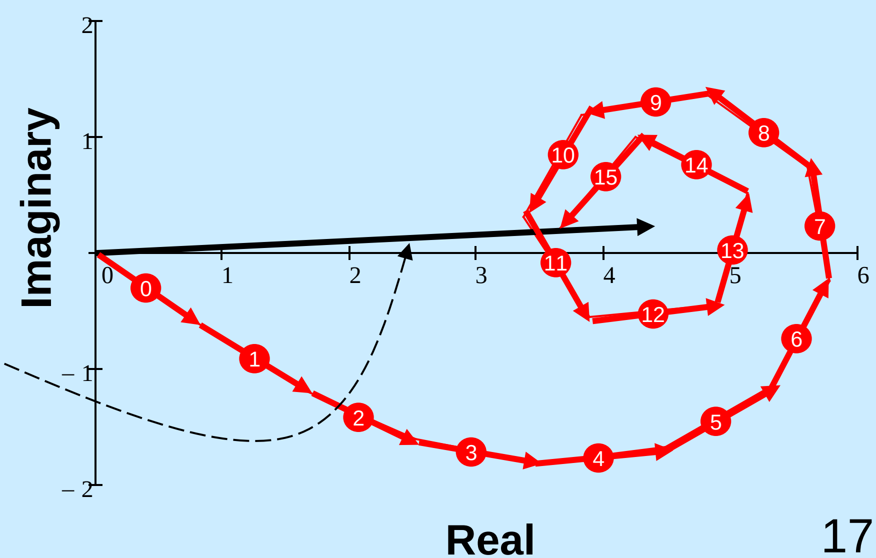
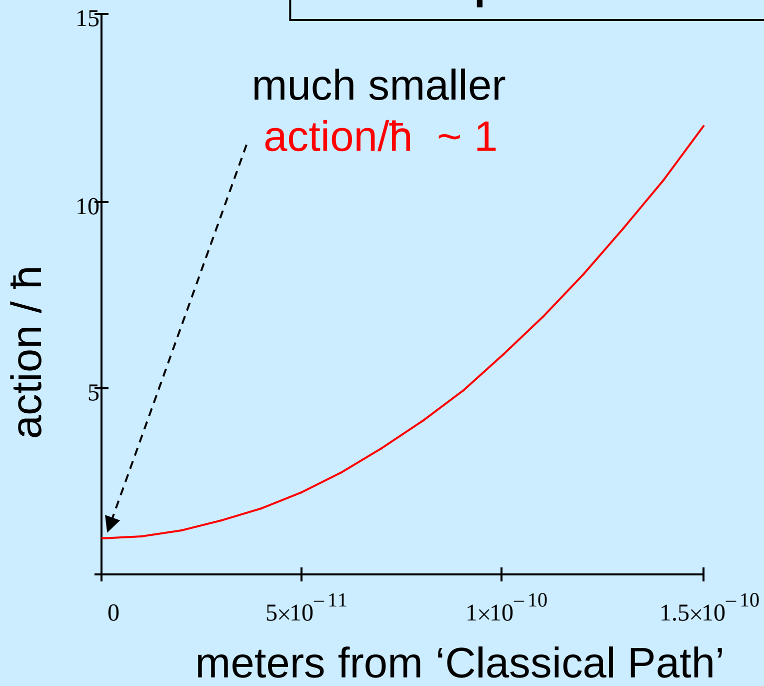
Complex Plane



Resultant deviation from Classical path ~ 4.5 microns

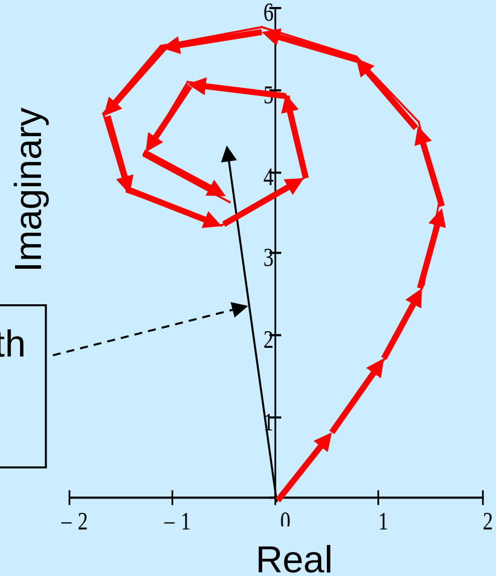
Example #2: Electron with 1 Angstrom Path at ~13.6 eV

Hydrogen Electron K.E.



Sum of Paths

Complex Plane



Deviation from Classical path
~ 0.45 Angstroms
(diameter ~0.9 Angstrom)

Example #2: Electron with 1 Angstrom Path at ~13.6 eV

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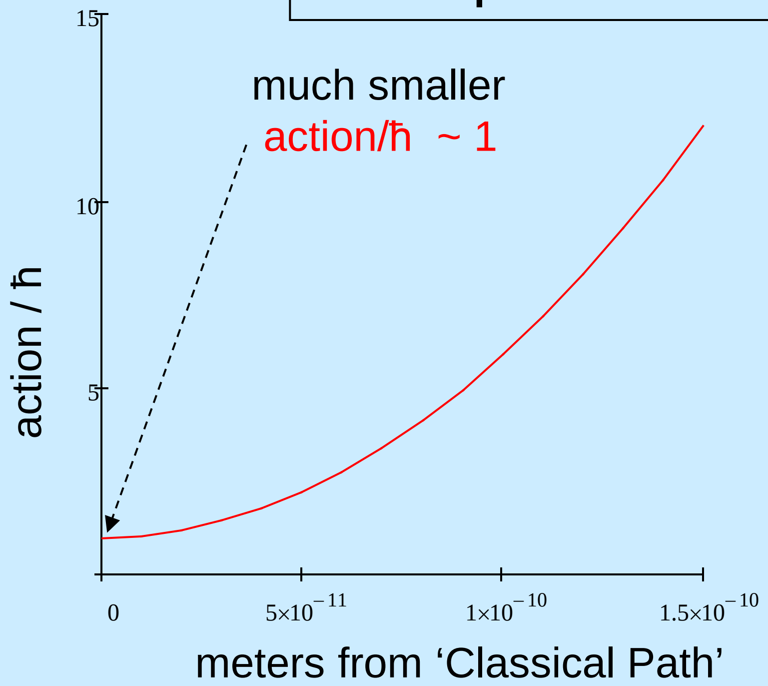

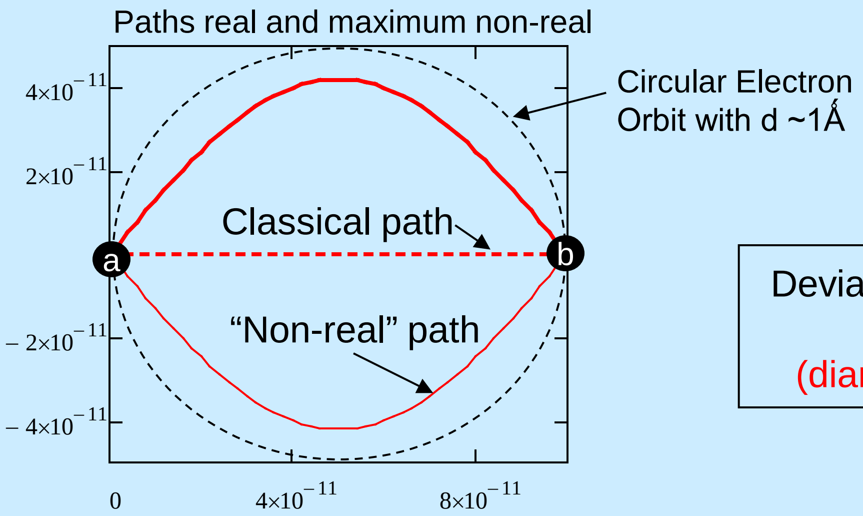

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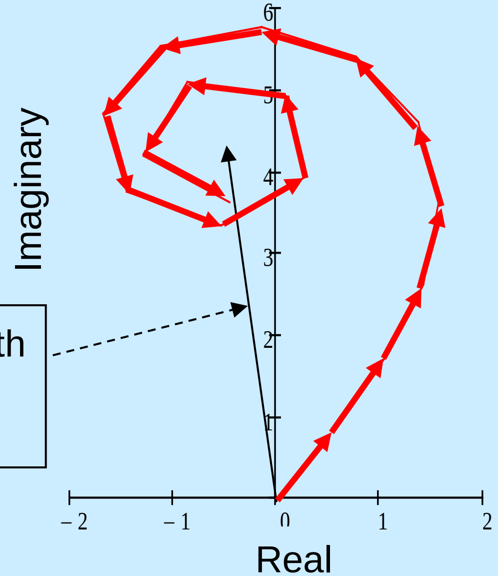
Sum of Paths
Complex Plane



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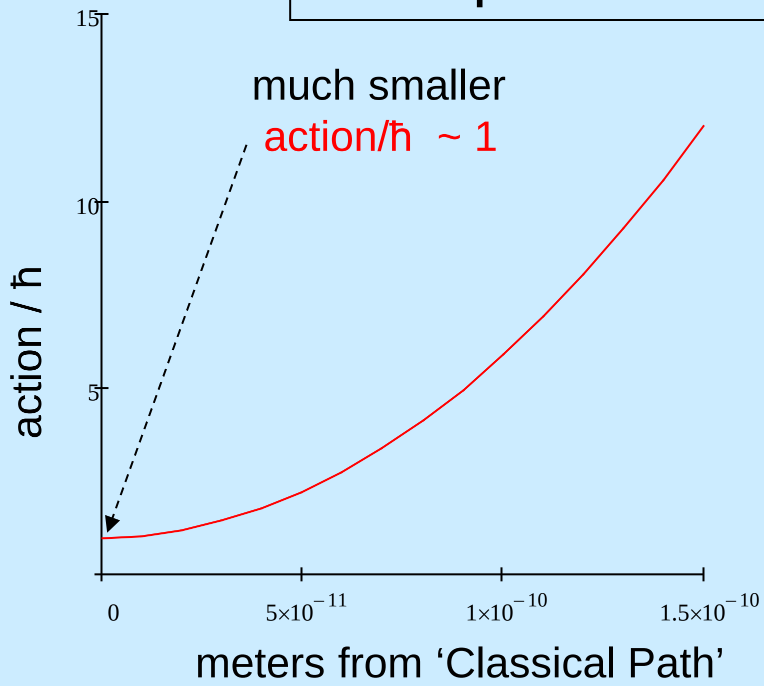
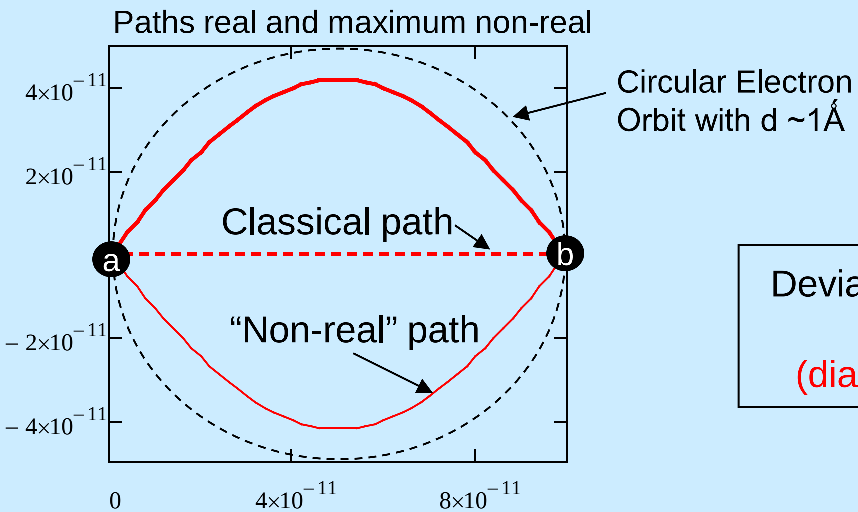


Origin of Atomic Dimensions

-Determined by Plank's Constant-

Sum of Paths

Complex Plane



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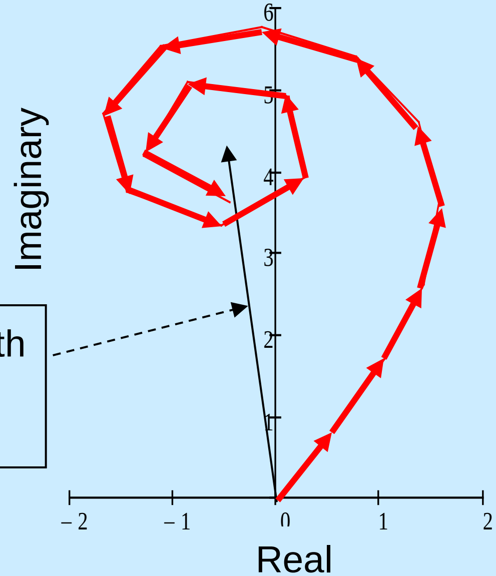

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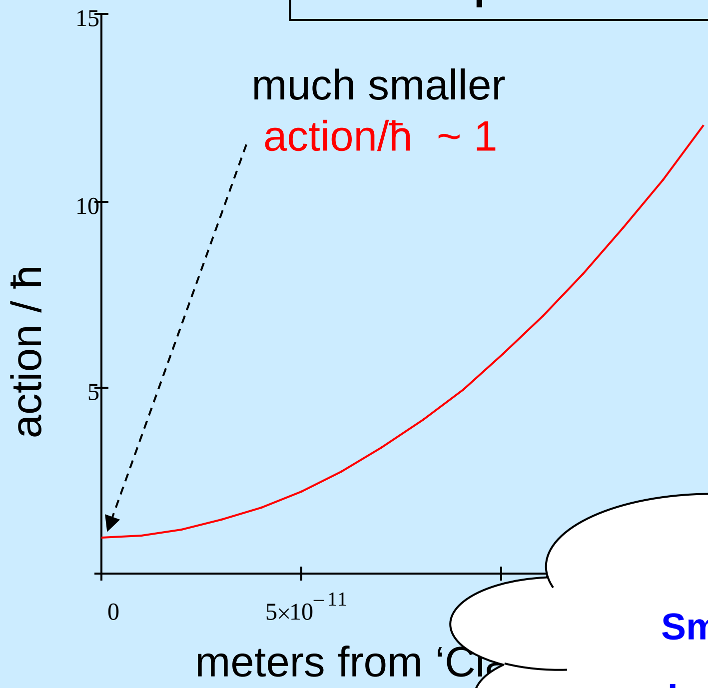


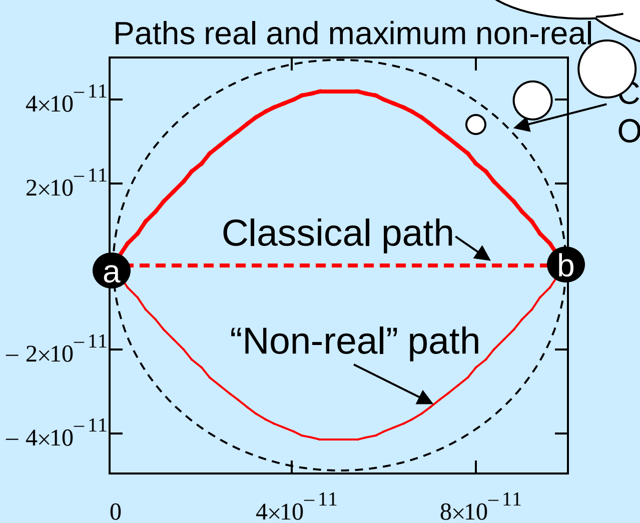
Origin of Atomic Dimensions

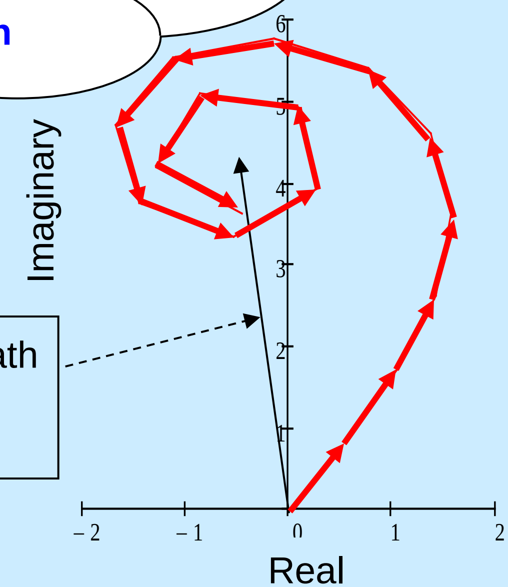
-Determined by Plank's Constant-

Remember:

Small 'Action' ➔ ill-defined Path

Large 'Action' ➔ Classical Path





Deviation from Classical path
~ 0.45 Angstroms
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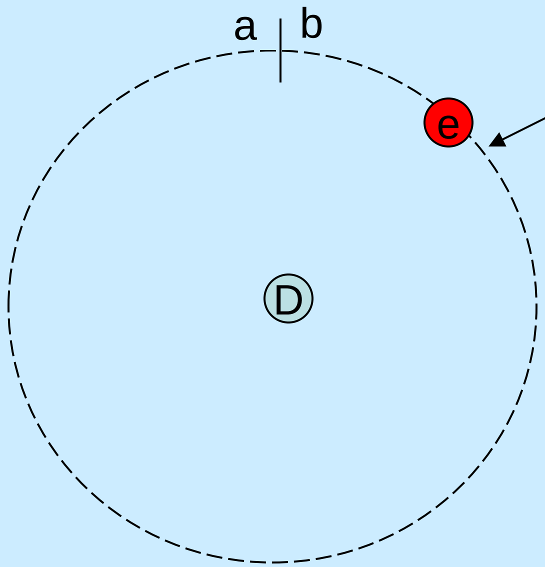
Stationary State Requirement

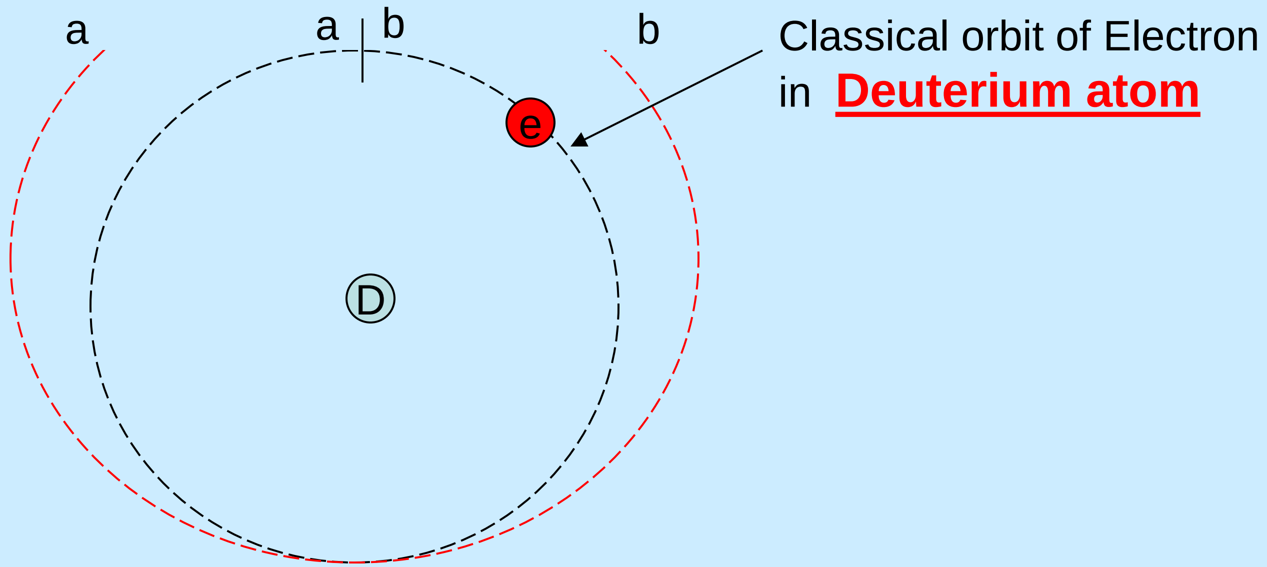
Repeating Amplitude of Path



Classical orbit of Electron in **Deuterium atom**

Stationary State Requirement

Repeating Amplitude of Path



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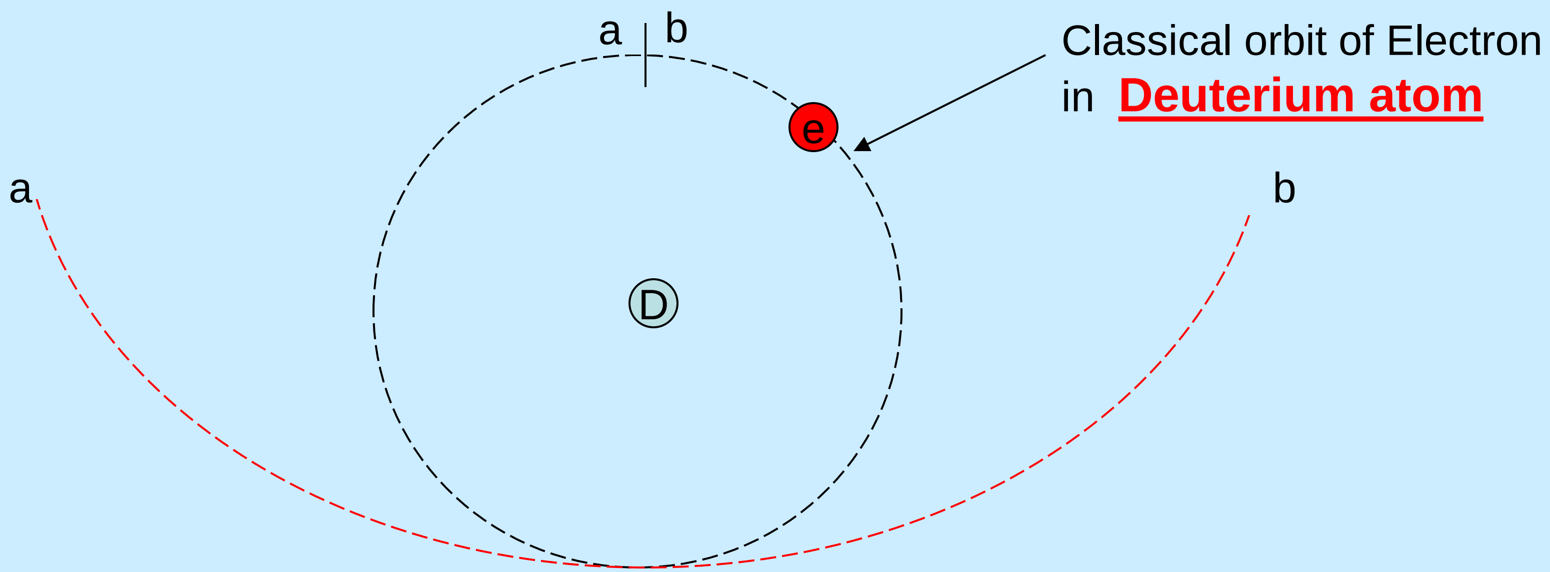

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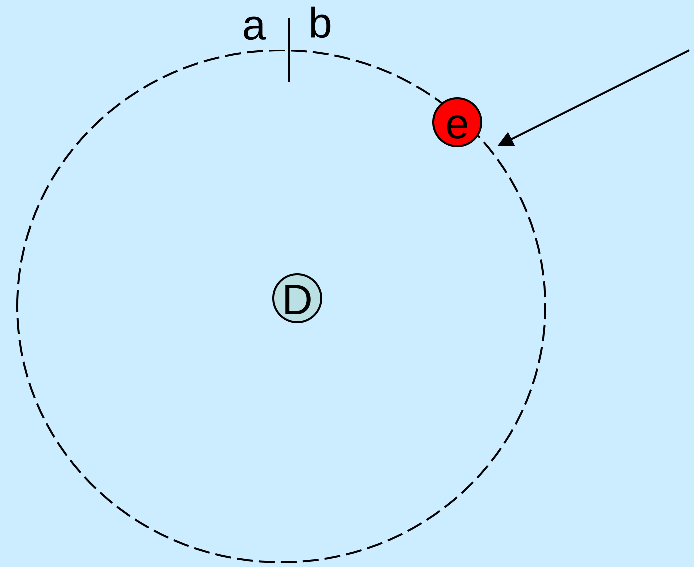

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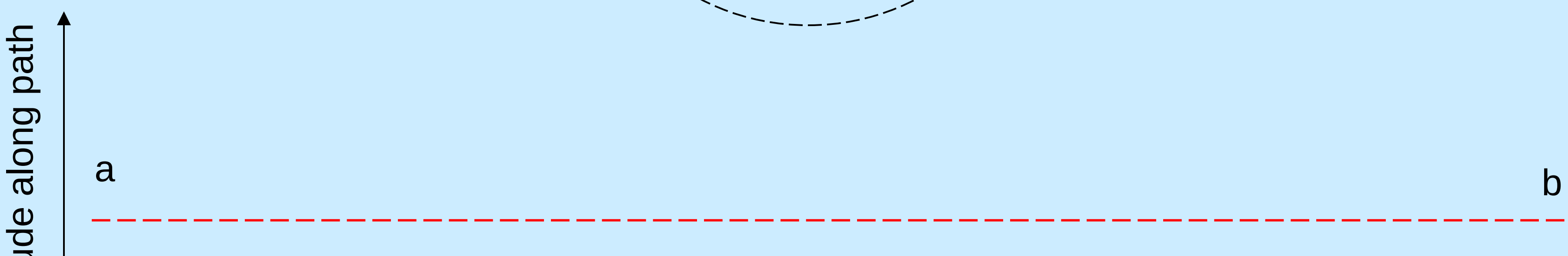
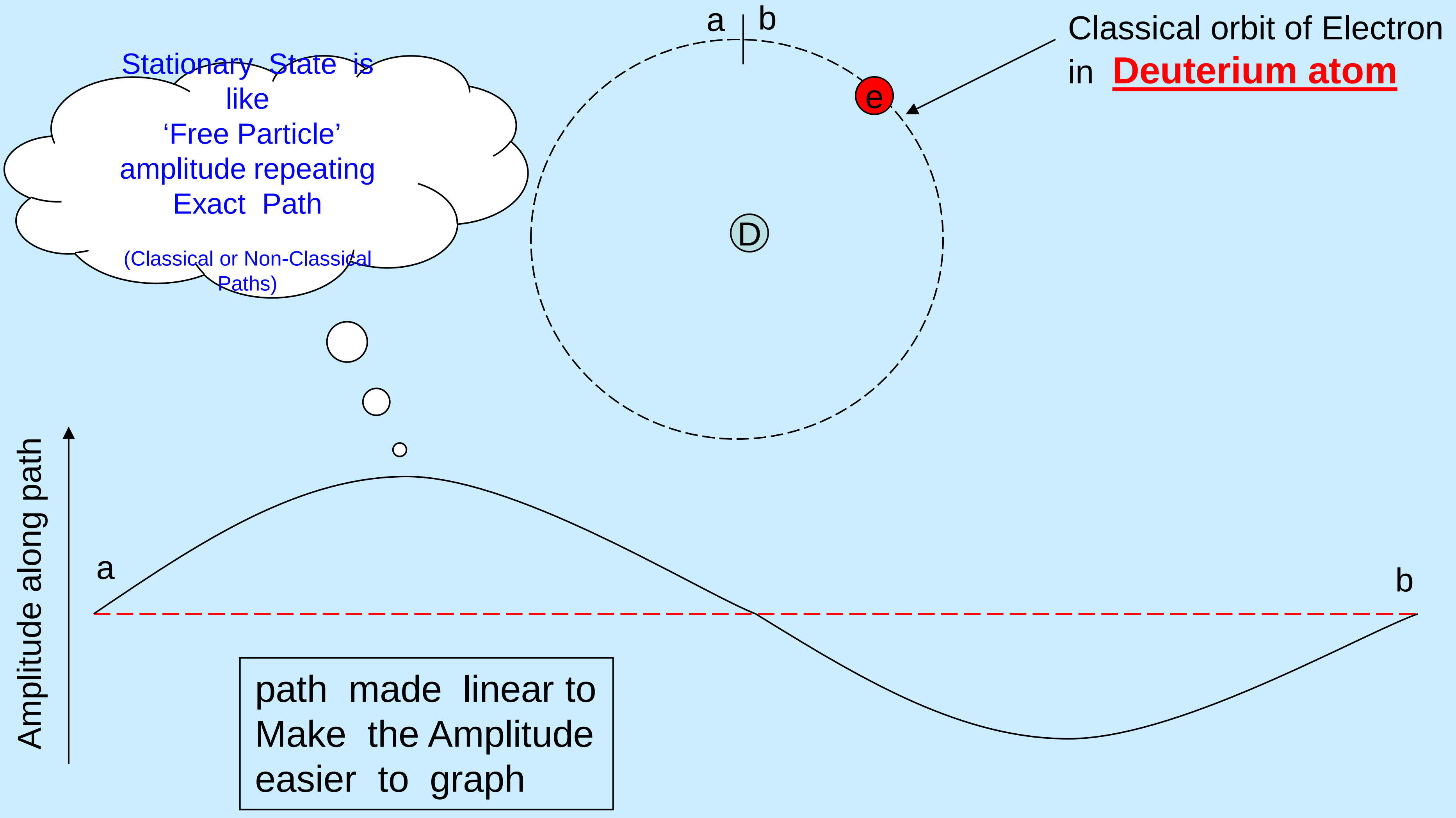


path made linear to
Make the Amplitude
easier to graph

Stationary State Requirement

Repeating Amplitude of Path



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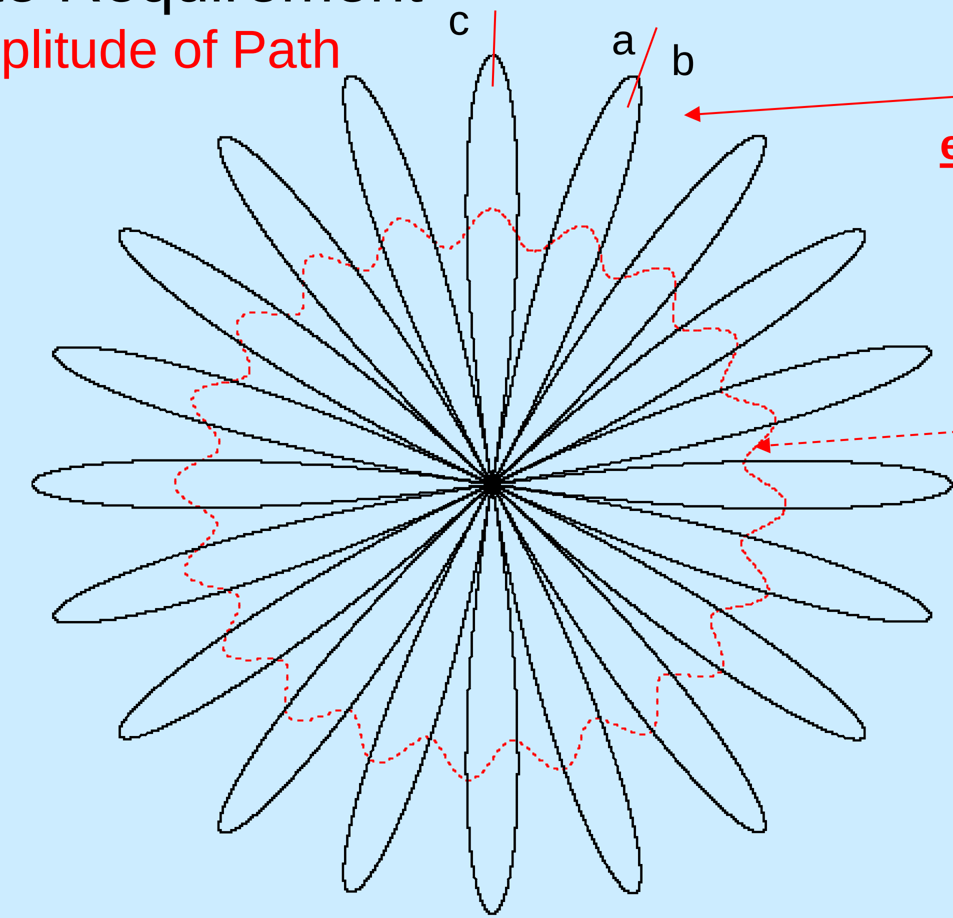


'Dramatized'

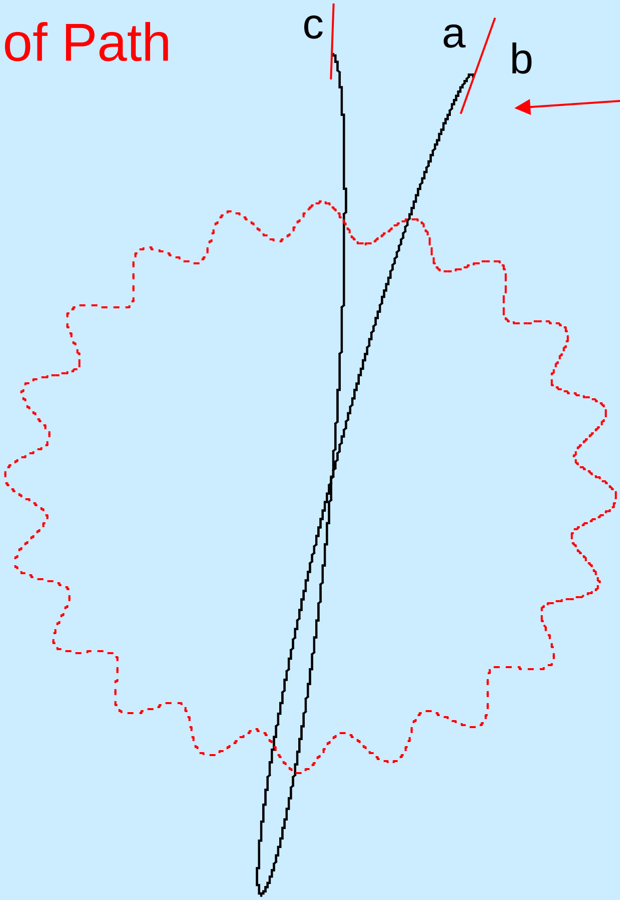
Classical orbit of **electron** in $\mathbf{D_2^*}$ molecule

a ➔ b

Deuterons Classical Orbit

Stationary State Requirement

Repeating Amplitude of Path

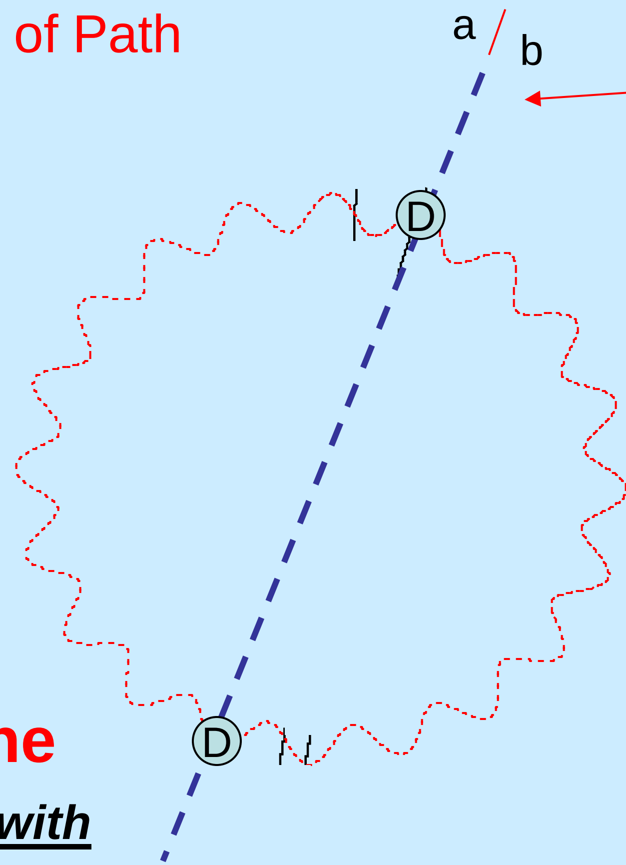


Classical orbit of **electron** in $\mathbf{D_2^*}$ molecule

a ➔ c

Stationary State Requirement

Repeating Amplitude of Path



Classical orbit of **electron** in $\mathbf{D_2^*}$ molecule
With Born-Oppenheimer
a ➔ b

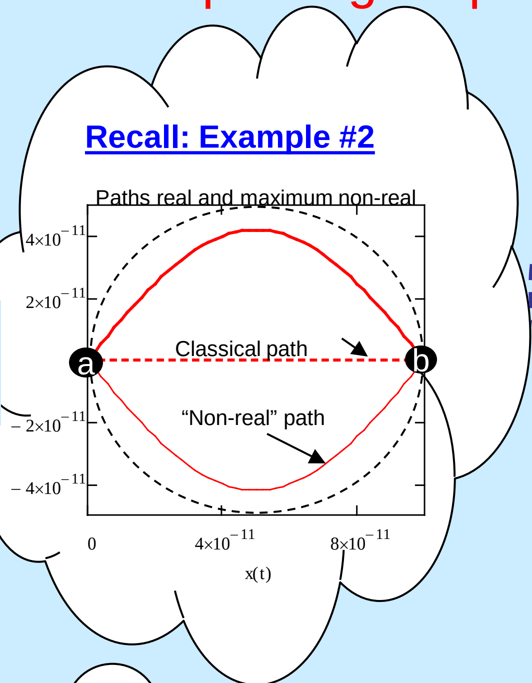
If we invoke the

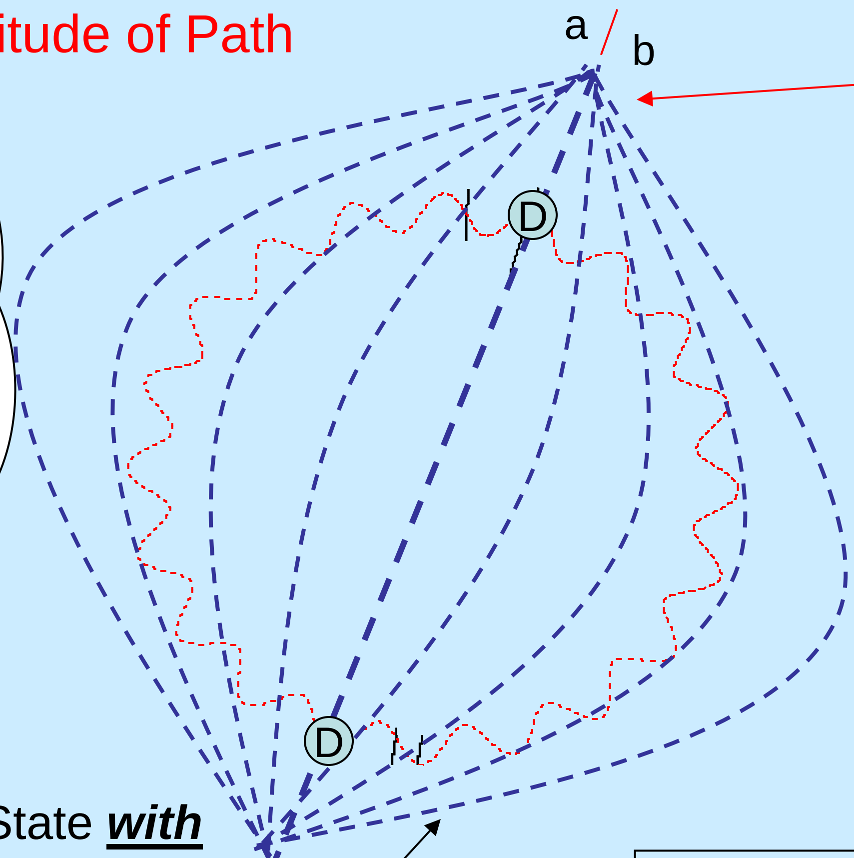
Linear Momentum State ***with***

Born-Oppenheimer

Stationary State Requirement

Repeating Amplitude of Path





Classical orbit of **electron** in $\mathbf{D_2^*}$ molecule
With Born-Oppenheimer
a ➔ b

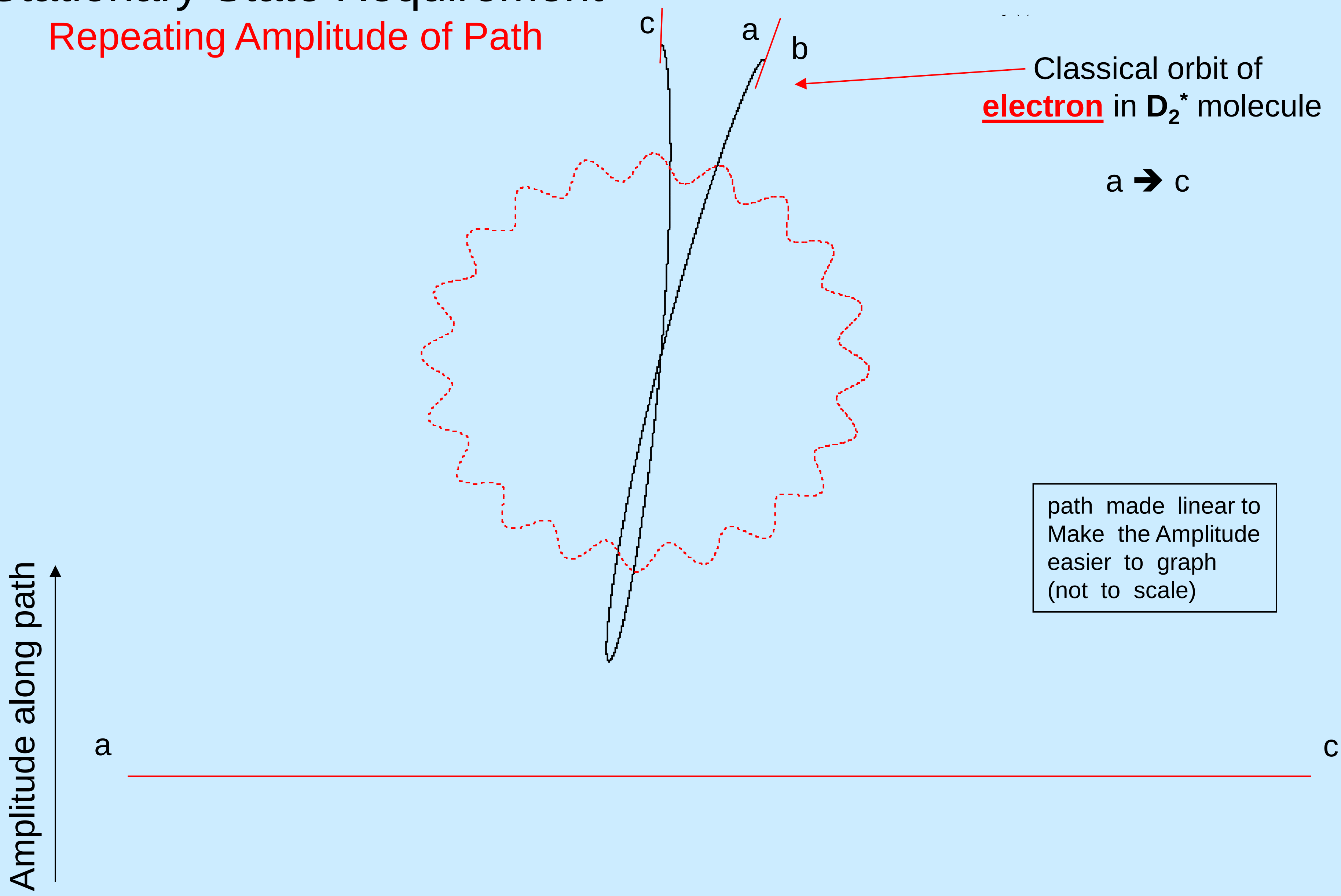
Linear Momentum State ***with***
Born-Oppenheimer

Get other paths with similar probability

Results in **Standard Schrodinger Solution**, (i.e. 'Normal' D_2)

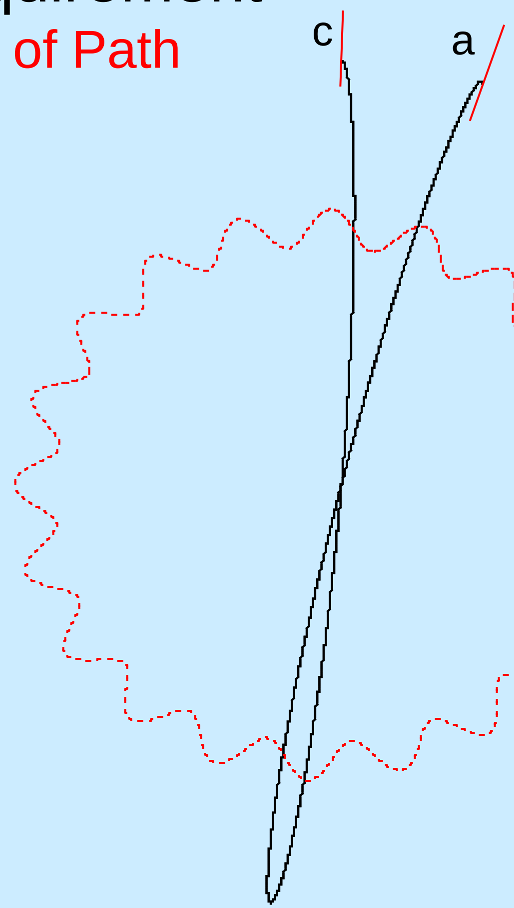
Stationary State Requirement

Repeating Amplitude of Path



Stationary State Requirement

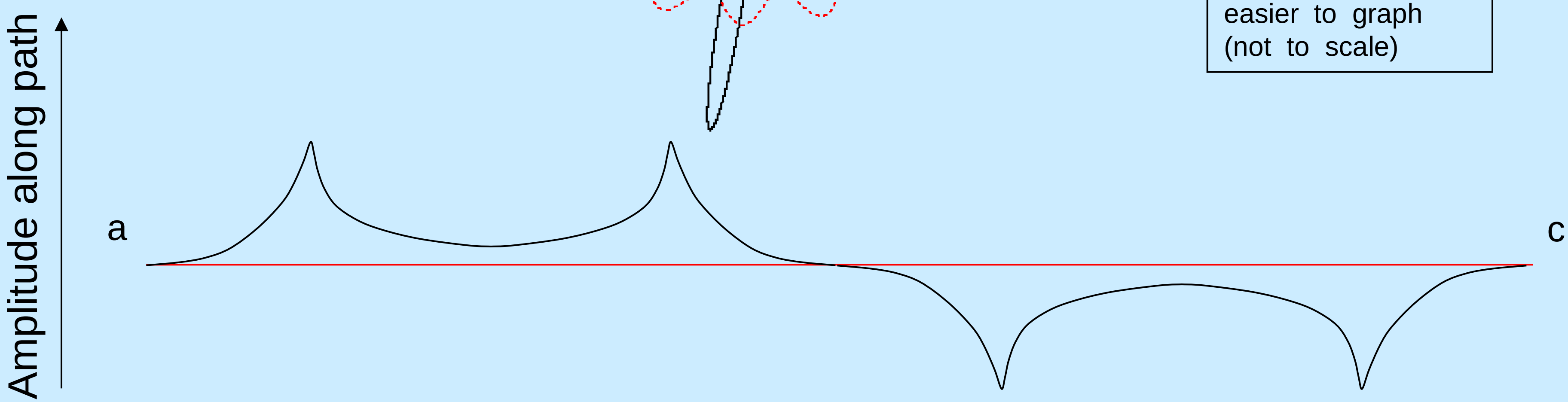
Repeating Amplitude of Path



Classical orbit of **electron** in D_2^* molecule

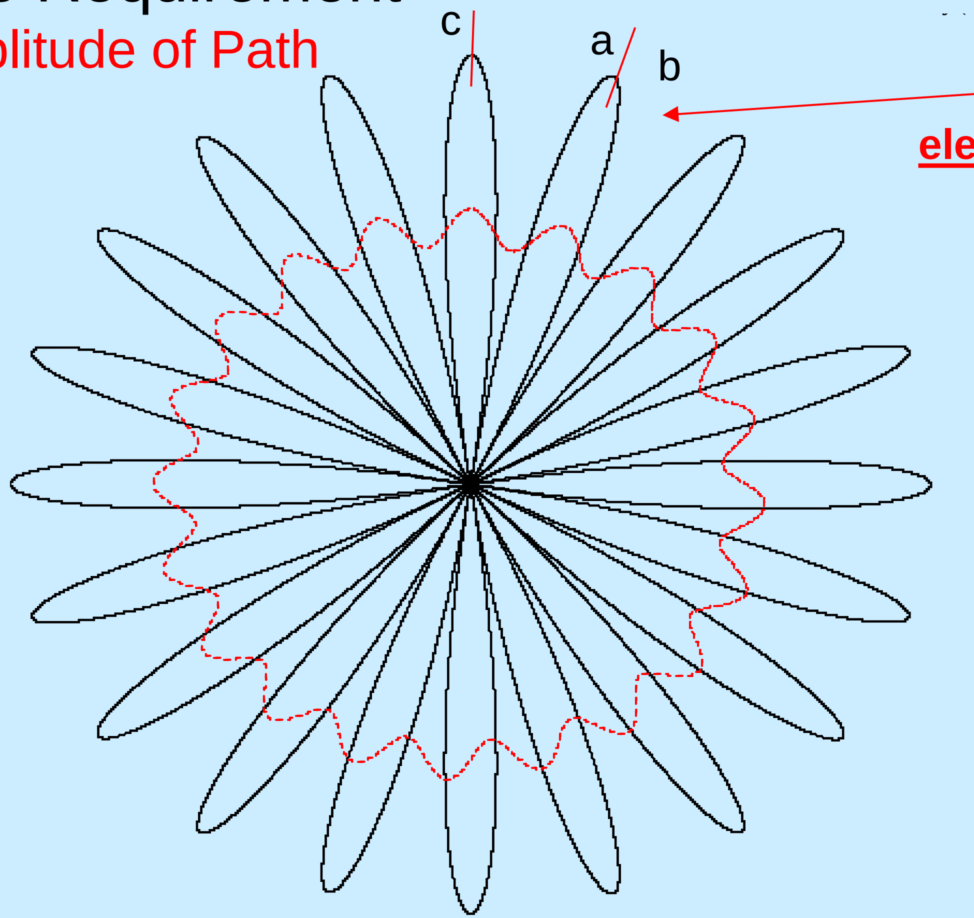
a ➔ c

path made linear to
Make the Amplitude
easier to graph
(not to scale)



Stationary State Requirement

Repeating Amplitude of Path



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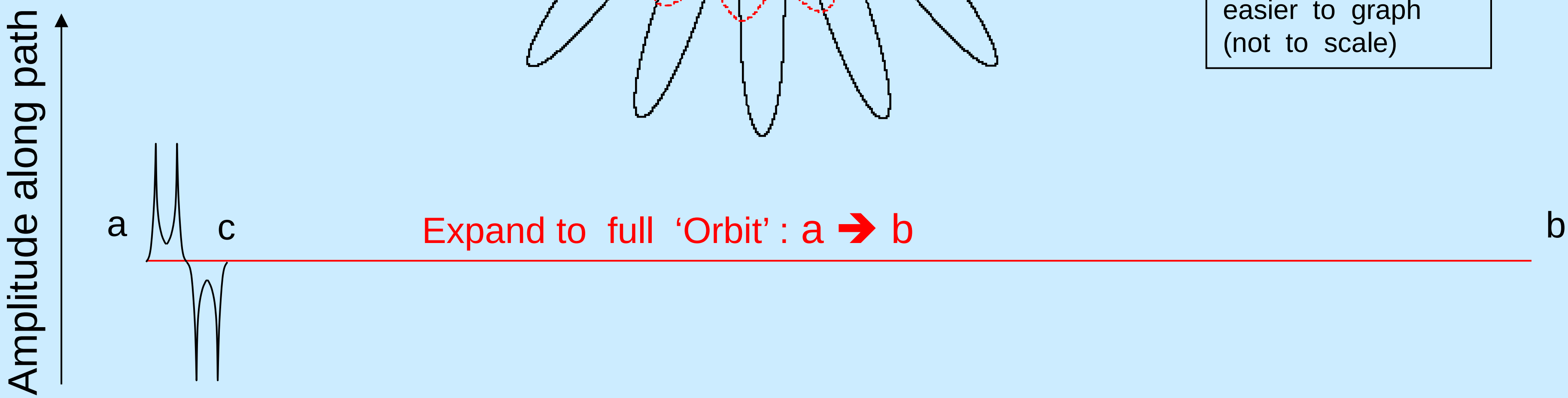
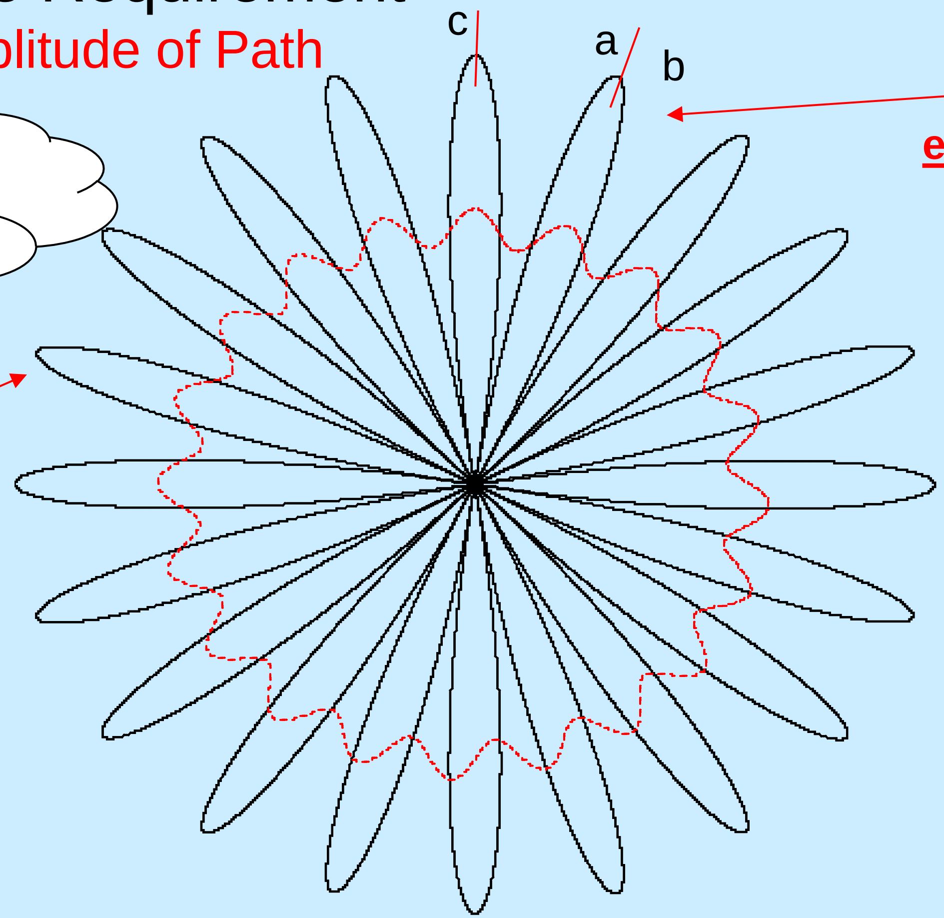


Stationary State Requirement

Repeating Amplitude of Path

Recall that large action
→ Classical like Path



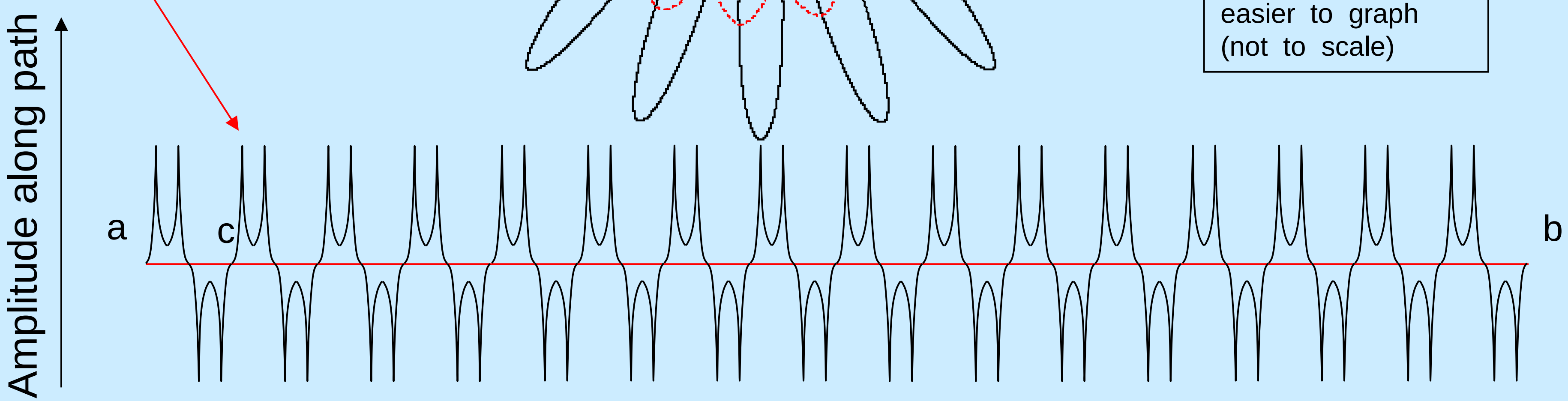
Classical orbit of **electron** in D_2^* molecule

a → b

Very Long Path Gives Very Large Action

Crosses axis ~400 times

path made linear to Make the Amplitude easier to graph (not to scale)



Conceptual Conclusion

{ n~ 400 is like a very large quantum no.= very large Action }

+

{ Action is also Very Sensitive to Large Potential through Nuclei }

→ Classical Like Electron Behavior

- The Born-Oppenheimer Approximation *obscures* this straight forward Quantum Solution
- The Schrodinger Equation Can Not Easily Describe this Correlation
- The Correlation is Accessible through Feynman's Wave Equation over an Orbital Period
- The Q.M. Correlation is defined by an Extremum of the Lagrangian Action of a Classically defined orbit
- Yes ! - The Linear Momentum State ***can*** be derived from Basic 'Accepted' Q.M. Principles

Conceptual Conclusion

n~ 400 is like a very large quantum no.= very large Action

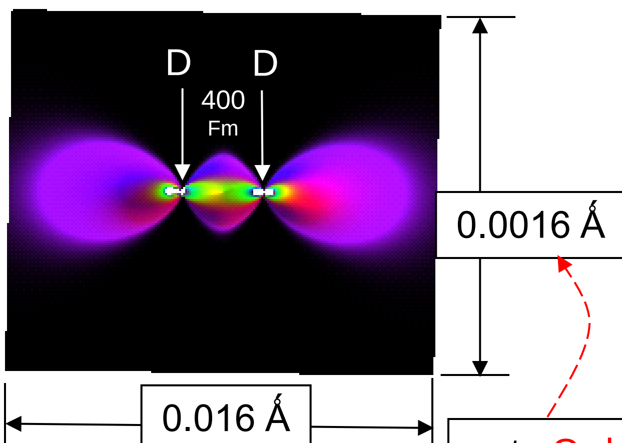
+

Action is also Very Sensitive to Large Potential through Nuclei

→ Classical Like Electron Behavior

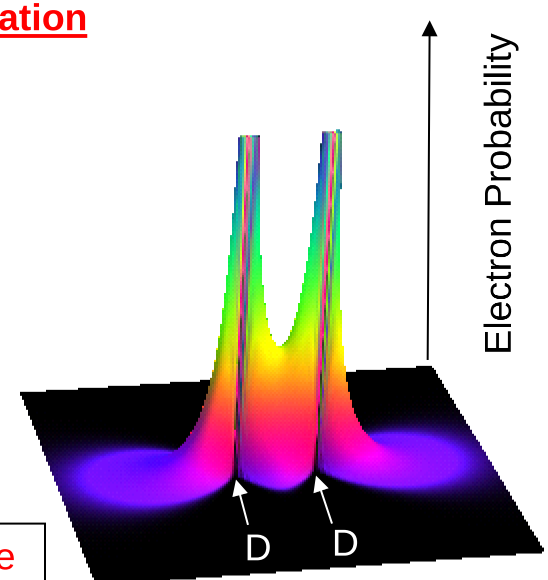
"Linear Momentum State"

Electron Probability Relative to D's
from **Feynman's Wave Equation**



note Order of Magnitude difference in the 2 scales

Top view



Side view

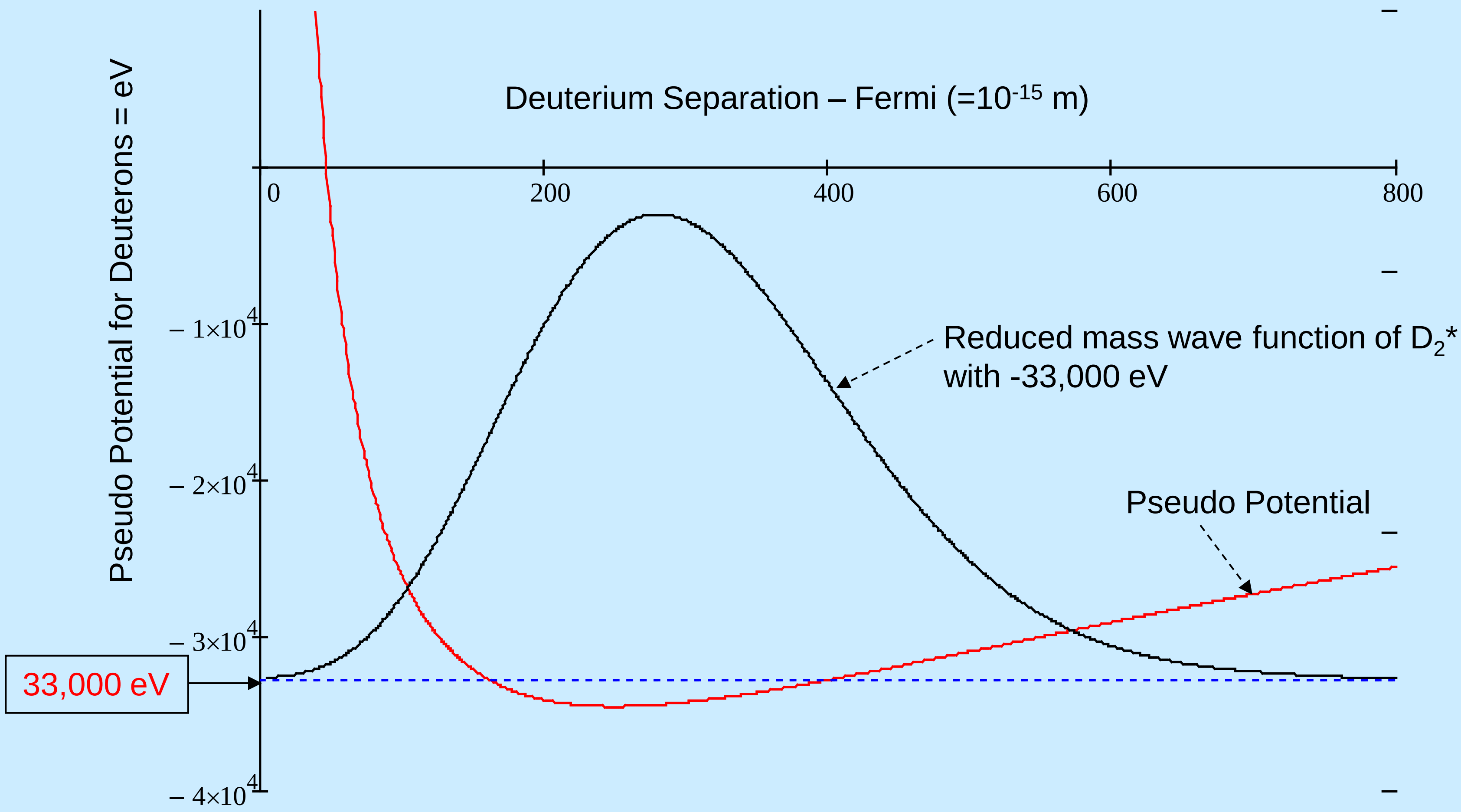
[axially symmetric]


Questions?
Evolution Valley – California Sierras
The 4th Miracle

END of PRESENTATION SLIDES

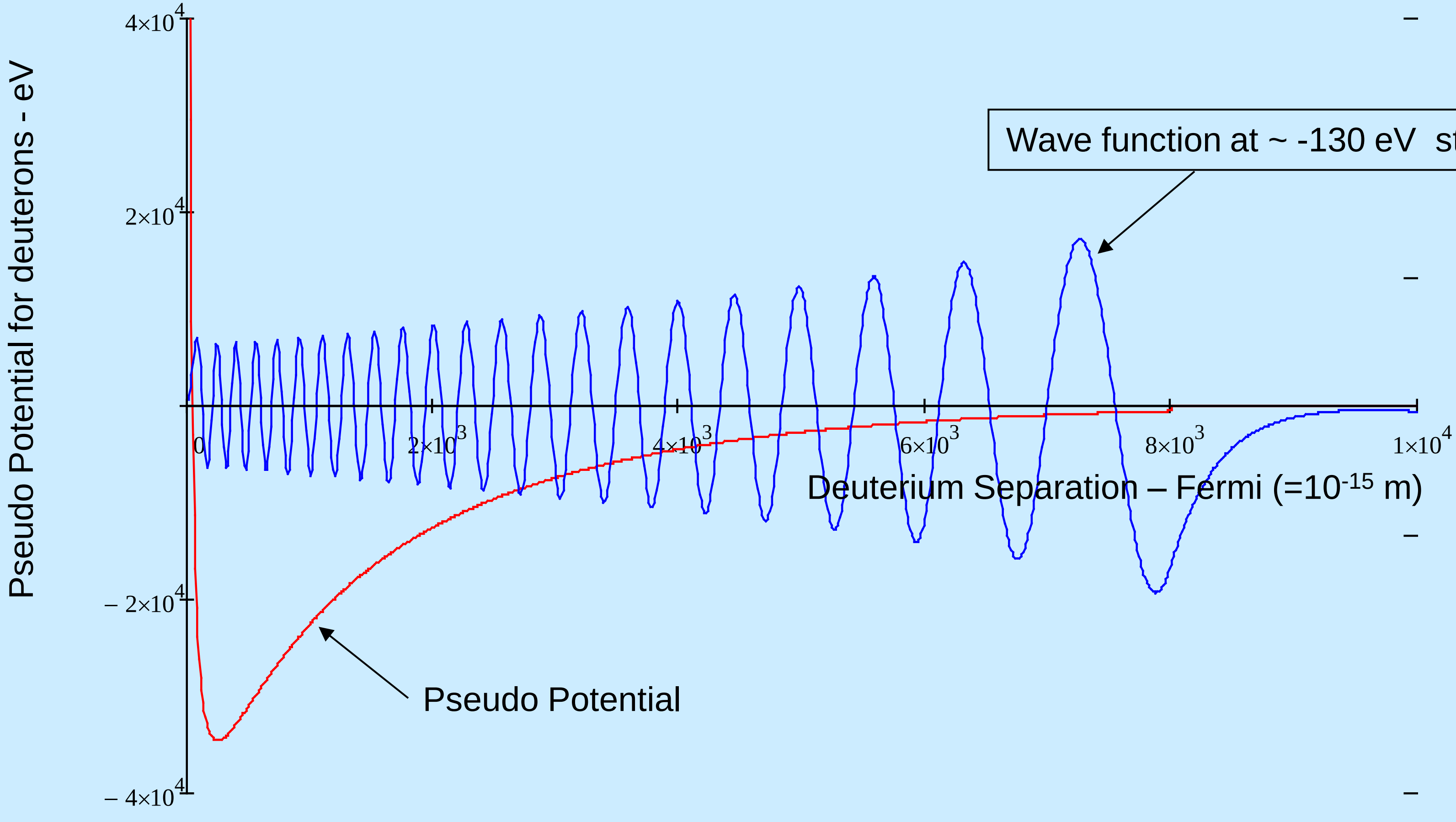
Pseudo Potential and Resulting Ground State Wave Function for D_2*

Calculated numerically with the Schrodinger equation

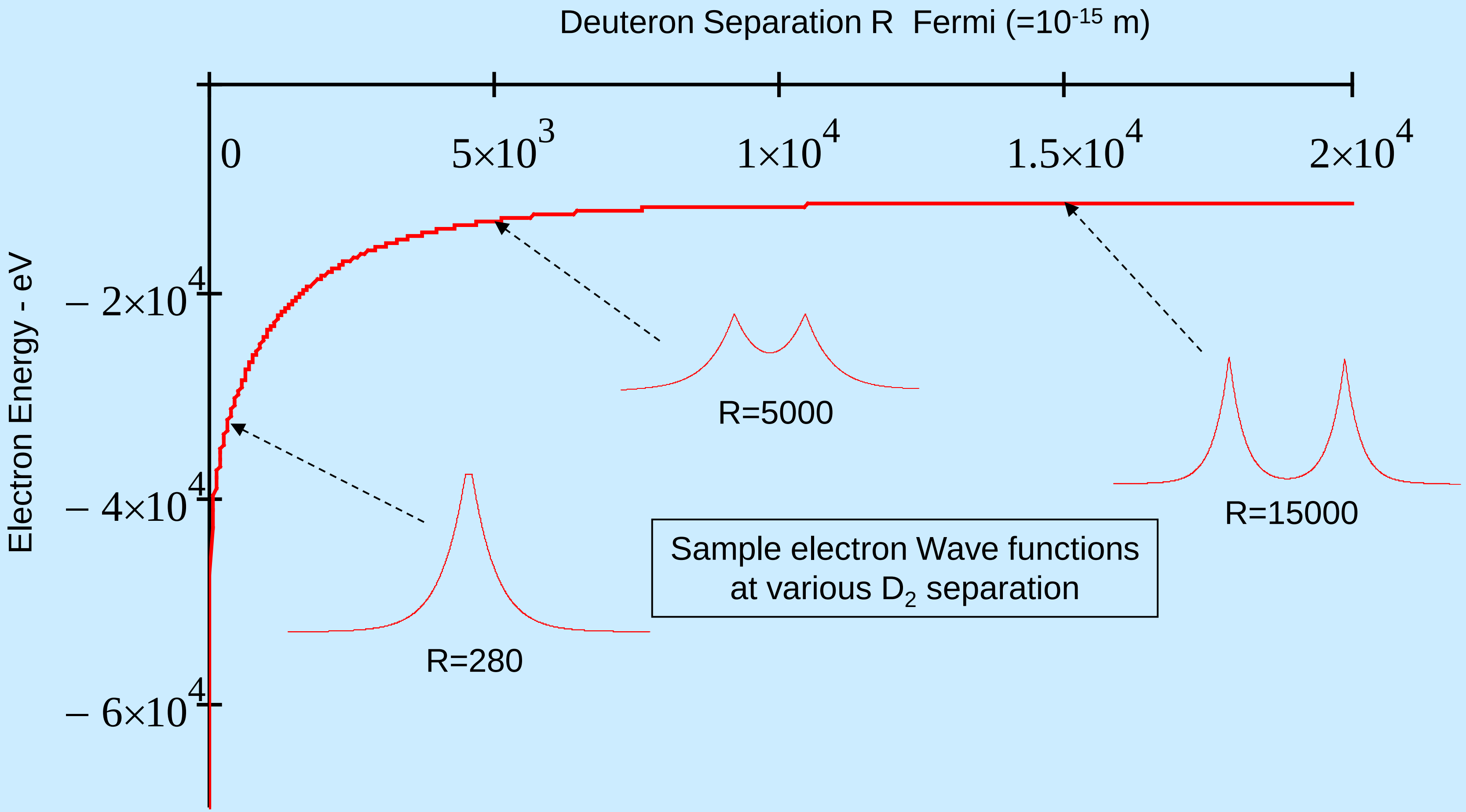


Pseudo Potential and Resulting Excited State Wave Function for D_2^*

Calculated numerically with the Schrodinger equation



Electron Energy as a Function of Deuterium Separation



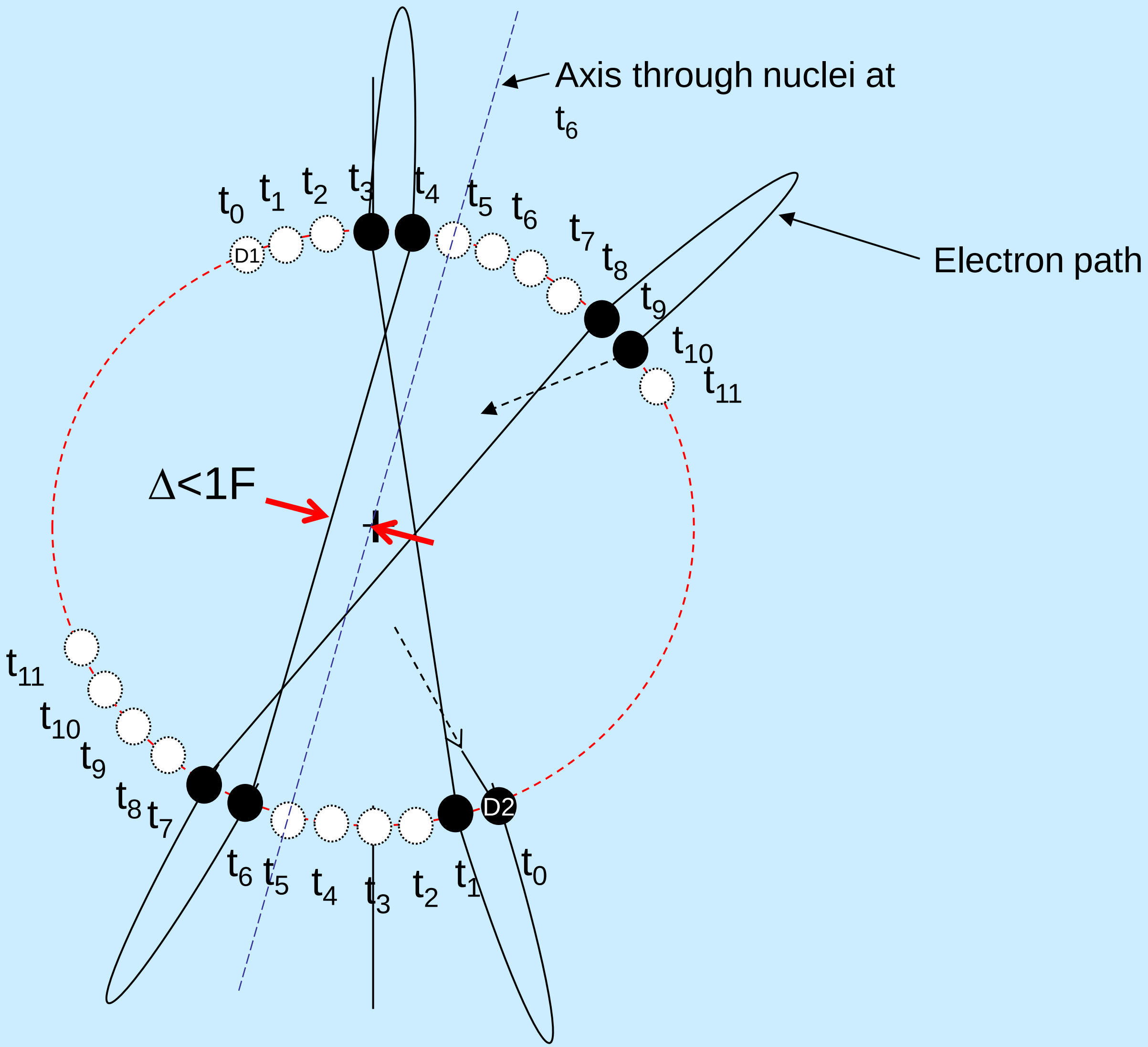
Approximations

Used in Calculation

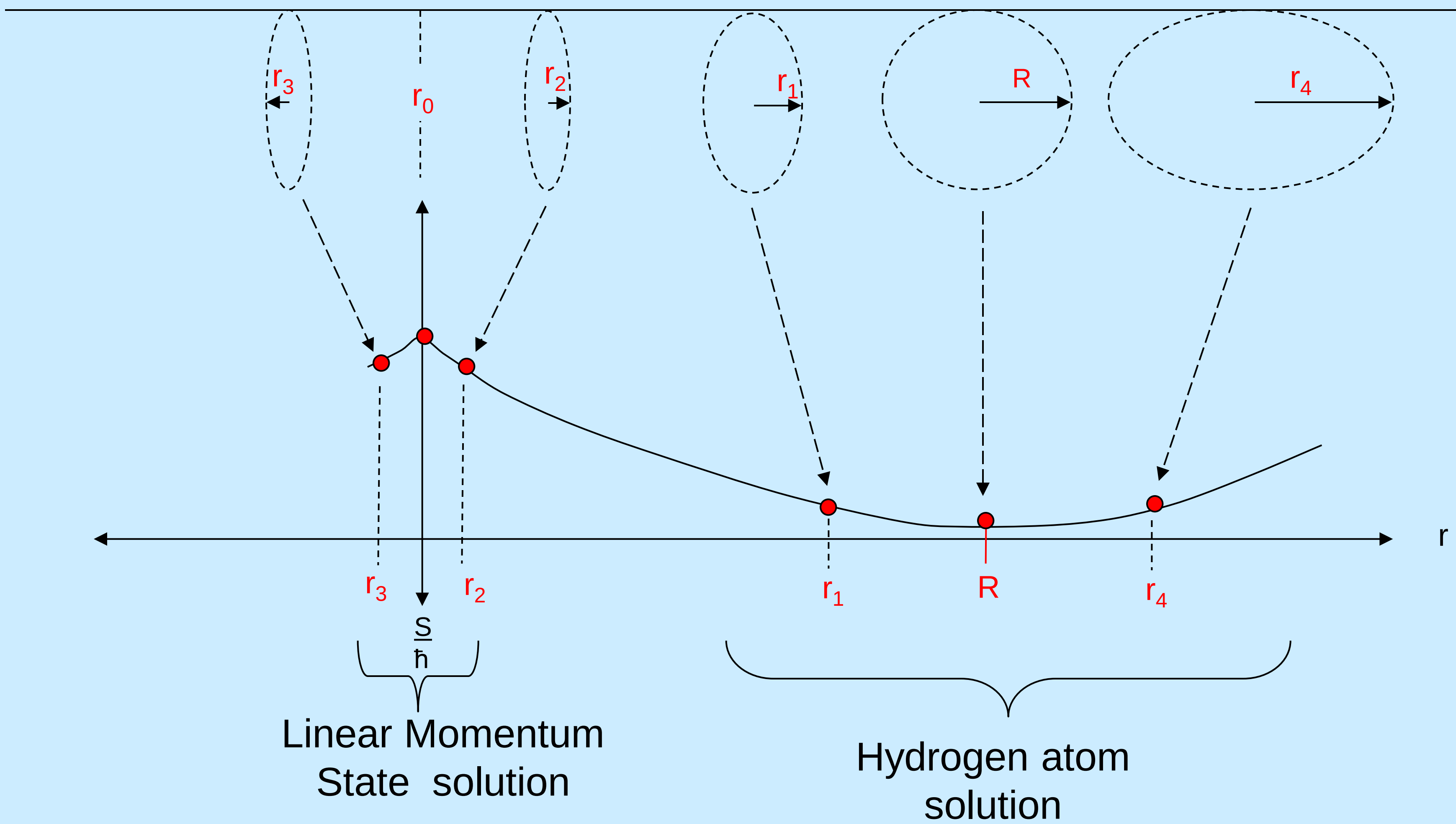
1. Nuclear Charge distribution and Relativistic affect.
   Less accurate electron energy calculation.
   No affect on over all theory, with moderate affect on numbers.

2. Classical path assumed to go through center of mass.
   Very small error in electron Action. Not much affect on results.

Δ= maximum deviation of electron path from the center of potential between the two deuterons

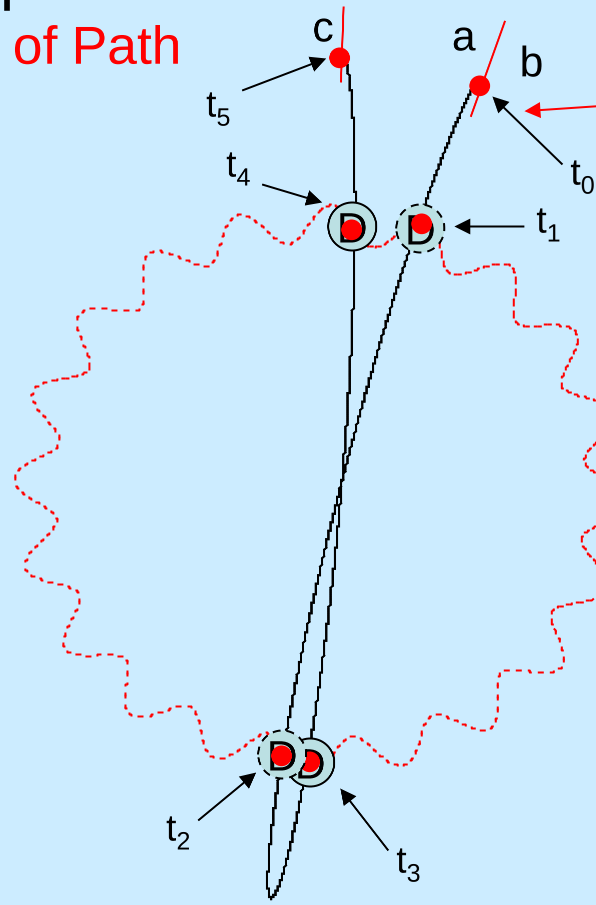


Origin of **'Maximum'** Action for Linear Momentum State from Circular Orbit 'Least Action'



Stationary State Requirement

Repeating Amplitude of Path



Classical orbit of **electron** in D_2^* molecule

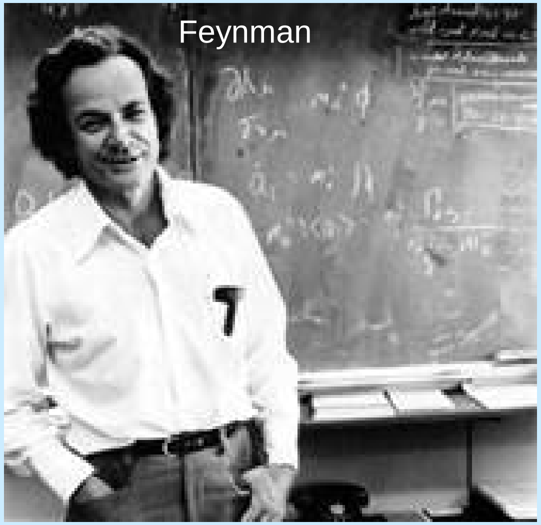
a ➔ c

Need to Solve Feynman's Wave Equation

Can Derive Schrodinger Equation from this Equation

$$\Psi(x_k,t)=\lim_{\varepsilon\to 0}\cdots\int_{x_{k-3}}^{x_{k-2}}\int_{x_{k-2}}^{x_{k-1}}\int_{x_{k-1}}^{x_k}\exp\left[\frac{i}{\hbar}\sum_{i=-\infty}^{k-1}S(x_{i+1},x_i)\right]\frac{dx_{k-1}}{A}\frac{dx_{k-2}}{A}\cdots$$

$$where: S(x_{i+1},x_i)=\varepsilon L\left(\frac{x_{i+1}-x_i}{\varepsilon},x_i\right)$$



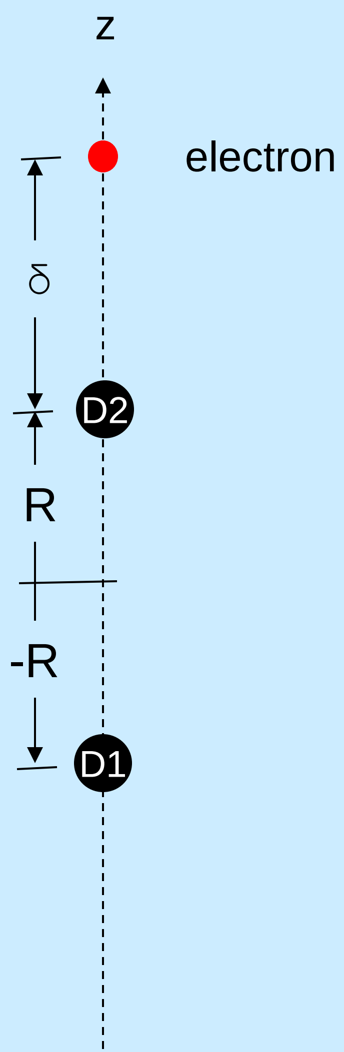
$$L = the\quad Lagrangian$$

= Classical Newtonian Mechanics

This is doable, but we will take an intuitive approach today

Classical Newtonian Simulation

of 3 Particle Bond



$$F_3 = m_3 * a_3 = \frac{d\{V_{1,3} + V_{2,3}\}}{dz}$$

$$F_2 = m_2 * a_2 = \frac{d\{V_{1,2} + V_{2,3}\}}{dz}$$

$$F_1 = m_1 * a_1 = \frac{d\{V_{1,2} + V_{1,3}\}}{dz}$$

Initial conditions

$v_1 = v_2 = v_3 = 0$

$x_1 = -R$
$x_2 = R$
$x_3 = R + \delta$

Note: The proton distribution in the nucleus is used to calculated the charge distribution in the nucleus