Visualization of Quantum Mechanics

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Introduction to QM

- Existence of Atoms & Molecules
- Brownian Motion
- Particle Tunneling
- Particle-in-a-Box
- Harmonic Oscillator
- Molecular Orbitals
- Advanced Topics
STM Apparatus

Low temperature (10 K) ultrahigh vacuum STM
Scanning Tunneling Microscope

Metal Tip

Solid Surface

Metal Tip

Electrons

Solid Surface
Tunneling Spectroscopy

![Diagram of tunneling spectroscopy](image)

- **Metal** and **Vacuum**
- **Tip** and **Sample**
- **Energy Level** $E_f$
- **Energy Gap** $eV$
- **Current** $I$
- **Voltage** $V$
Tunneling Microscopy: Topography

Constant Current STM

Topography

Z

X, Y
Existence of Atoms and Molecules
Imaging Atoms

**Silicon(111)**  
**Ag(110)**
Visualization of Single Molecules

H on Cu(001)
O2 on Pt(111)
C2H2 on Cu(001)
Fe(CO)2 on Ag(110)
Visualization of Single Molecules

- H on Cu(001)
- O$_2$ on Pt(111)
- C$_2$H$_2$ on Cu(001)
- Fe(CO)$_2$ on Ag(110)
50,000,000x Magnification
Galileo, 1992
3,900,000 Miles
Reines Hall
UC Irvine
Brownian Motion
H Atom
Single Atom Tracking

(a)  

(b)  

(c)  

(d)
Random Walk of Single H Atom

Single Atom Tracking:
H Thermal Diffusion

T = 74 K
time = 69 s
Single Atom Thermal Diffusion

The graph shows the relationship between temperature (K) and hop rate (s\(^{-1}\)) for different types of atoms. The inset bar graph represents the distribution of some parameter N. The main graph has data points for Hydrogen and Deuterium, indicating differences in hop rates at various temperatures. The y-axis shows hop rate in s\(^{-1}\), with values ranging from 0.01 to 10, and the x-axis shows temperature in K, ranging from 65 to 80.
Particle Tunneling

Pre-1900 Physics (Classical Physics)

Impenetrable Barrier

Post-1900 Physics (Quantum Physics)

Tunneling Effect
Over-Barrier vs. Tunneling

Over-Barrier

Tunnel

195 meV

70 meV

2.55 Å

H

Cu
Hydrogen Atom Diffusion

Temperature (K)

Hop Rate (s⁻¹)

D (cm².s⁻¹)

1000/T (K⁻¹)

10⁻⁶

10⁻⁴

10⁻²

10⁰

10⁻⁴

10⁻²

10⁻⁰

10⁻¹⁶

10⁻¹⁸

10⁻²⁰

10⁻²²

H

D

Temperature (K)

Hop Rate (s⁻¹)

D (cm².s⁻¹)

10⁻³

10⁻¹⁹

10⁻¹⁷

10⁻¹⁵

10⁻¹³

10⁻¹¹

H

D

1000/T (K⁻¹)
Vacuum Tunneling

Tunnel Current vs. Tip-Sample Distance

Tip = W; Sample = Pt(111)
Particle-in-a-Box
Single Gold Atoms on NiAl(110)
Gold Chains: 1 to 20 Atoms
20-Atom Au Chain

Assembled

Disassembled

75X75 Å

Low

High
Electron in a 1-D Box

Au\textsubscript{20} chain

\[ m_{\text{eff}} = 0.5m_{\text{free}} \]

\[ E = E_0 + \frac{\hbar^2 k^2}{2m_{\text{eff}}} \]

\[ k = \frac{n\pi}{L} \]

Energy (eV)

(Wave Number)\(^2\) (10\(^{20}\) m\(^{-2}\))

Number of Atoms

Energy (eV)

lowest energy peaks
Pd$_{20}$ Chain
Single CO Adsorption on 11-Atom Au Chain

\[ \text{Au}_5 - \text{AuCO-Au}_5 \]

Topography

\(+36 \text{ mV}\)

\(-36 \text{ mV}\)
CuPc@2Au₆
Structure of CuPc
Assembly of CuPc@2Au₆
Harmonic Oscillator
Inelastic Electron Tunneling Spectroscopy (IETS)

Conventional IETS: $\sim 10^9$ molecules

STM-IETS: 1 molecule
Elastic vs. Inelastic Tunneling

Diagram showing a tip connected to a metal surface through a vacuum. The diagram illustrates the concept of elastic and inelastic tunneling with energy levels and quantum states indicated.
H Atom
Single H Atom

15 x 15 Å²

Cu(001)

Sample Bias (mV)

$d^2I/dV^2$ (nA/V²)

H

D

51
70
Chemical Identification:
Single Acetylene Molecules on Cu(100)
Inside Single Acetylene
Molecular Orbitals
Seeing LUMO of Mg-Porphine

“Seeing is Believing”
Advanced Topics:
Nano-photonics → “Ångströ-photonics”
Resolution of Optical Spectroscopy

Aperture-based SNOM

- Light
- Tapered fiber
- Adsorbate
- $d < \lambda/2$
- Resolution $\sim 30$ nm

Apertureless SNOM

- Light
- Metallic tip
- Adsorbate
- $D \ll R$
- Resolution $\sim 10$ nm
Localized Electron Transfer
Photo-induced Resonant Tunneling
Coupling Photons to the Tunneling process

=> Angstrom Resolution!
Atomic Scale Non-linear Optics

807 nm ML
$V_c = 0.3 \, \text{V}$

$\propto P^2$

633 nm CW
$V_c = 0.2 \, \text{V}$

$\propto P$
Nonlinear Photon Coupling with Pulsed Laser

![Graph showing charging probability vs sample bias Vc (V) with markers indicating different conditions: Without laser, 807 nm ML. 0.034 mW, and 800 nm CW, 0.146 mW.]

- Charging probability
- Sample bias Vc (V)

Markers:
- Black square: Without laser
- Red circle: 807 nm ML. 0.034 mW
- Pink triangle: 800 nm CW, 0.146 mW
Spatial Resolution of Two-Photon Induced Electron Transfer

![Graph with data points and curves, showing charging probability and apparent height as a function of lateral distance.](image)
Acknowledgement

Barry Stipe
Mohamad Rezaei
Lincoln Lauhon
Hyojune Lee
Mitch Wallis
Niklas Nilius
Xiaohui Qiu

George Nazin
Shiwei Wu
Mats Persson

NSF    DOE
Time Trajectory of Charging Events
Time Trajectory of Charging Events
Time Trajectory of Charging Events
Analysis of the Time Trajectory

\[ \tau = 1.37 \pm 0.02 \]

\[ \tau = 2.93 \pm 0.12 \]

\[ \tau = 5.86 \pm 0.29 \]

\[ \tau = a P^{-2} \]
Quantum Tunneling of Electrons

$T \sim e^{-d \Phi^{1/2}}$

$E_f$ Metal $\rightarrow$ Vacuum $\rightarrow$ Metal $E_f$

$d$
STM Tip

Tungsten Wire

Etched Tungsten Wire

Etched Tungsten Wire

Human Hair
Time trajectory of charging events (pulsed, 96μW)
Time trajectory of charging events (pulsed, 69μW)
Time trajectory of charging events (pulsed, 46μW)
Analysis of the time trajectory (pulsed)

$P = 96 \mu W$

$P = 69 \mu W$

$P = 46 \mu W$

Slope = 2.10 +/- 0.05
Analysis of the time trajectory (CW)

- $P = 263 \, \mu W$
- $P = 173 \, \mu W$
- $P = 131 \, \mu W$
- $P = 76 \, \mu W$
Time trajectory of charging events (CW, bottom left, 131 μW)
Analysis of the time trajectory (CW)

- $P = 263 \, \mu W$
- $P = 173 \, \mu W$
- $P = 131 \, \mu W$
- $P = 76 \, \mu W$
Analysis of the time trajectory (CW)

Slope (red) = 1.05
Slope (blue) = 1.27 +/- 0.05
Analysis of the time trajectory (CW)

Slope = 1.05
Analysis of the time trajectory (CW and pulsed)
Tip-Induced Plasmon Modes

Plasmon “size” : $\sqrt{dR}$
Laser illumination of STM junction
Function of laser power controller (LPC)
Function of laser power controller (LPC)
Junction Temperature increase upon laser illumination

- **Left graph**
  - Slope = 0.50 K/mW
  - \( \lambda = 633 \text{ nm, CW} \)
  - Ag tip

- **Right graph**
  - Slope = 0.69 K/mW
  - \( \lambda = 800 \text{ nm, ML} \)
  - Ag tip