Quantum Tunneling

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Abstract

This worksheet will introduce the theory and applications of **quantum tunneling**. Herein, we will calculate the probability of quantum tunneling as a function of particle energy, particle mass, and barrier energy. Among the many applications of quantum tunneling, we will focus on the **scanning tunneling microscope** method used for atomic-level characterization of nanosurfaces, as well as **resonant tunneling diodes** used in nanoelectronics. Application uses the Maple Quantum Chemistry Toolbox.

I. Introduction

Classical mechanics predicts that particles which do not have sufficient energy to overcome a potential barrier will not be able to pass to the other side of the barrier (Figure 1A) and will instead be reflected, with zero probability of transmission. The quantum mechanical phenomenon of **tunneling** describes the phenomenon in which particles with lower energy ($E < U(x)$) can still penetrate through a barrier, which would otherwise be classically forbidden (Figure 1B). As a consequence of wave-particle duality, the wave nature of matter at the quantum level means that there is a finite, non-zero probability of the particle to transverse through the barrier.

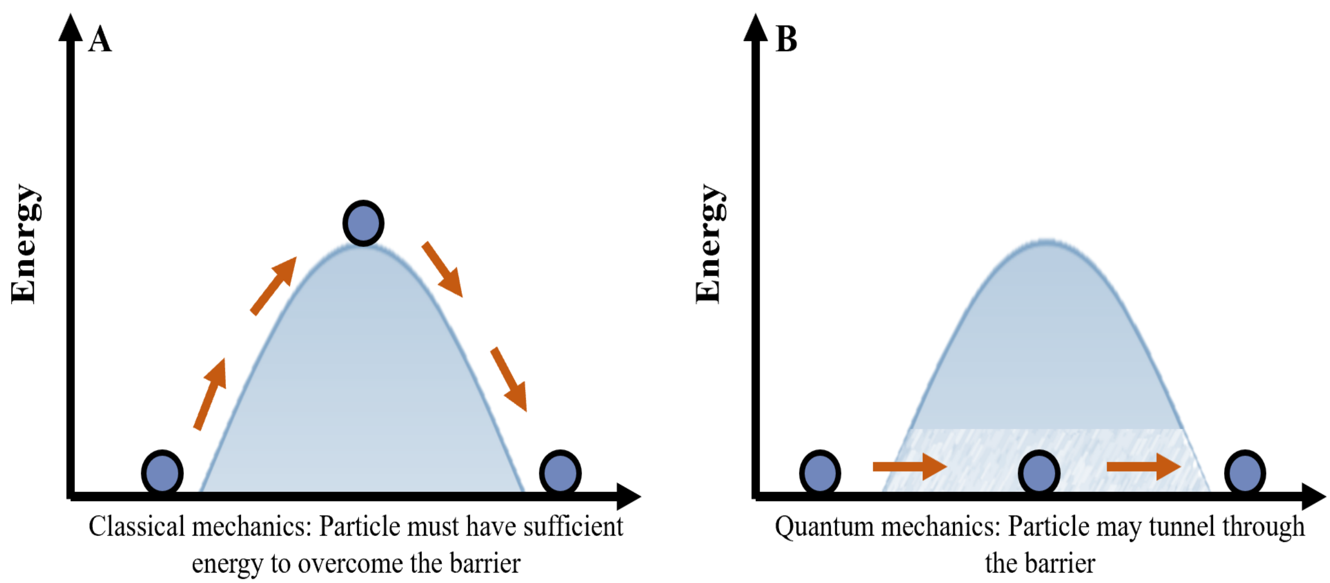

Figure 1: Classical versus quantum motion of particles encountering a barrier

II. Theory

Time-Independent Schr dinger Equation

A uniform, time-independent beam of particles traveling along the x-axis that encounters a potential barrier may be described by the following Schrdinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x) \qquad \text{(Equation 1)}$$

where *E* is the energy of the particle, *m* is the mass of the particle, *U(x)* is the potential energy of the barrier,   is Planck's constant, and ψ is the wavefunction of the particle. In one-dimensional space, the barrier spans from 0 to *L* and is described by the following potential energy function

$$U(x) = \begin{cases} 0, \text{ when } x < 0 \\ U_0, \text{ when } 0 \le x \le L \\ 0, \text{ when } x > L \end{cases} \qquad \text{(Equation 2)}$$

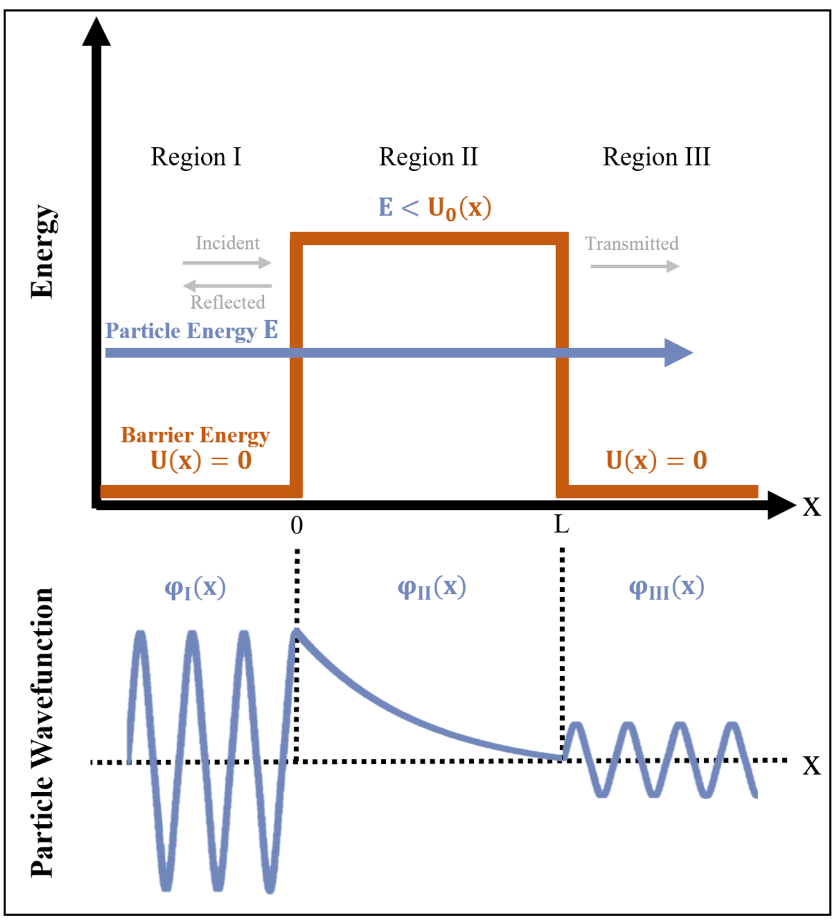

Figure 2: Energy and wavefunction of particles encountering a potential barrier, with three regions described in one-dimensional space

Thus, the barrier creates three unique regions that correspond to three different behaviors of the particles, as illustrated in Figure 2. In Regions I and III, the barrier potential $U(x) = 0$, the energy of the particle is greater than the energy of the barrier ($E > U$), and the particle is able to move freely. The solution to the Schr dinger equation for these two regions take the same form, described in Equations 3 and 4

$$\psi_I(x) = A \cdot e^{i \cdot k \cdot x} + B \cdot e^{-i \cdot k \cdot x} \qquad \text{(Equation 3)}$$

$$\psi_{III}(x) = F \cdot e^{i \cdot k \cdot x} + G \cdot e^{-i \cdot k \cdot x} \qquad \text{(Equation 4)}$$

$$k = \sqrt{2\,mE \,/\, \hbar^2} \qquad \text{(Equation 5)}$$

where the amplitudes (A, B, F, and G) may be different depending on the region. The solutions to Equations 3 and 4 are given as sine waves: the incident wave (+*ikx* term) is traveling toward positive x, and the reflected wave (-*ikx* term) is traveling toward negative x. Because the transmitted particle traveling in the positive x direction in Region III will not encounter another barrier, the amplitude G must be zero in Equation 4.

In Region II, the barrier potential $U_0(x) > 0$ and we consider the case where the energy of the particle is less than that of the barrier ($E < U_0(x)$). Within the confines of the barrier, the particle is not able to travel freely. The solution to the Schr dinger equation takes the form of a real exponential

$$\psi_{II}(x) = C \cdot e^{q \cdot x} + D \cdot e^{-q \cdot x} \qquad \text{(Equation 6)}$$

$$q = \sqrt{2\,m\left(U_0 - E\right) \,/\, \hbar^2} \qquad \text{(Equation 7)}$$

Solutions to Equations 3, 4, and 6 can be found by applying boundary conditions. First, conditions are imposed that require the wavefunction and its derivative to be continuous at the boundary between Regions I to II and Regions II to III

At the boundary where $x = 0$:

$$\psi_I = \psi_{II} \qquad \text{(Equation 8B)}$$

$$A \cdot e^{i \cdot k \cdot x} + B \cdot e^{-i \cdot k \cdot x} = C \cdot e^{q \cdot x} + D \cdot e^{-q \cdot x} \qquad \text{(Equation 8B)}$$

$$\frac{\partial}{\partial x}\left(\psi_I\right) = \frac{\partial}{\partial x}\left(\psi_{II}\right) \qquad \text{(Equation 9A)}$$

$$i \cdot k \cdot A - i \cdot k \cdot B = q \cdot C - q \cdot D \qquad \text{(Equation 9B)}$$

At the boundary where $x = L$:

$$\psi_{II} = \psi_{III} \qquad \text{(Equation 10A)}$$

$$C \cdot e^{q \cdot x} + D \cdot e^{-q \cdot x} = F \cdot e^{i \cdot k \cdot x} \qquad \text{(Equation 10B)}$$

$$\frac{\partial}{\partial x}\left(\psi_{II}\right) = \frac{\partial}{\partial x}\left(\psi_{III}\right) \qquad \text{(Equation 11A)}$$

$$q \cdot C \cdot e^{q \cdot L} + q \cdot \mathrm{D} \cdot e^{-q \cdot L} = i \cdot k \cdot F \cdot e^{i \cdot k \cdot L} \qquad \text{(Equation 11B)}$$

By requiring ψ values to be equal to one another at the boundaries where $x = 0$ and $x = L$, continuity of the wavefunction at the boundaries is ensured. Furthermore, the continuity of the wavefunction at the barrier where $x = 0$ must be independent of the energy of the particle, such that it can describe the possibility for the particle to be reflected by the barrier or transmitted through the barrier.

Collectively, Equations 1 through 11 describe the wavefunction associated with a particle as continuous and sinusoidal on either side of the barrier, and as an exponential decay within the barrier. As a result of the exponential decay experienced by the particle within the barrier, the wave amplitude in Region III is smaller than in Region I. For further details on the theory of quantum tunneling, we refer to References [1] through [3].

Probability of Quantum Tunneling

A particle traveling in the $+x$ direction may be transmitted or reflected upon encountering the potential barrier. The transmission coefficient T describes the probability that the particle will tunnel through the barrier. For full details on the derivation of this parameter, we refer to Reference [3]. Briefly, transmission is approximated as the ratio of the transmitted wave intensity ($\psi_{tra}(x) = F \cdot e^{i \cdot k \cdot x}$) to the incident wave intensity ($\psi_{in}(x) = A \cdot e^{i \cdot k \cdot x}$)

$$T = \frac{\left(\left|\psi_{tra}(x)\right|\right)^2}{\left(\left|\psi_{in}(x)\right|\right)^2} = \left[1 + \left(\frac{k^2 + q^2}{2 \cdot k \cdot q}\right)^2 \sinh^2(q \cdot L)\right]^{-1} \qquad \text{(Equation 12)}$$

In the following example, we will evaluate the dependence of the transmission coefficient on barrier width L, particle mass m, and particle energy E. Let us consider three scenarios: one scenario where the energy of the particle is high and the mass of the particle is low (SC1); one scenario where both the energy and the mass of the particle are low (SC2); and one scenario where the energy of the particle is low and the mass of the particle is high (SC3). We will use the **`ScientificConstants`** tool to obtain the mass of an electron and the **`AtomicData`** command with QuantumChemistry [4] to obtain the mass of a proton.

```
> with(ScientificConstants);
[AddConstant, AddElement, AddProperty, Constant, Element, GetConstant, GetConstants,
    GetElement, GetElements, GetError, GetIsotopes, GetProperties, GetProperty, GetUnit,
    GetValue, HasConstant, HasElement, HasProperty, ModifyConstant, ModifyElement]      (3.2.1)
> with(QuantumChemistry);
[AOLabels, ActiveSpaceCI, ActiveSpaceSCF, AtomicData, BondAngles, BondDistances,
    Charges, ChargesPlot, ContractedSchrodinger, CorrelationEnergy, CoupledCluster,
    DensityFunctional, DensityPlot3D, Dipole, DipolePlot, Energy, ExcitationEnergies,
    ExcitationSpectra, ExcitationSpectraPlot, ExcitedStateEnergies, ExcitedStateSpins,
    ExcitonDensityPlot, ExcitonPopulations, ExcitonPopulationsPlot, FullCI,
    GeometryOptimization, HartreeFock, Interactive, Isotopes, MOCoefficients, MODiagram,
    MOEnergies, MOIntegrals, MOOccupations, MOOccupationsPlot, MOSymmetries, MP2,
    MolecularData, MolecularDictionary, MolecularGeometry, NuclearEnergy,
    NuclearGradient, OscillatorStrengths, Parametric2RDM, PlotMolecule, Populations,
    Purify2RDM, RDM1, RDM2, RTM1, ReadXYZ, Restore, Save, SaveXYZ, SearchBasisSets,
    SearchFunctionals, SkeletalStructure, SolventDatabase, Thermodynamics,
    TransitionDipolePlot, TransitionDipoles, TransitionOrbitalPlot, TransitionOrbitals,
    Variational2RDM, VibrationalModeAnimation, VibrationalModes, Video]      (3.2.2)
> with(ColorTools) :
> myblue := ColorTools:-Color([113, 135, 188]) :
> mygray := ColorTools:-Color([195, 213, 229]) :
> myteel := ColorTools:-Color([222, 232, 241]) :
> myred := ColorTools:-Color([197, 90, 17]) :
> m := evalf(Constant('m[e]'));
```

$$m := 9.10938356 \times 10^{-31} \tag{3.2.3}$$

```
> hbar := 6.58 * 10^(-16);
```

$$\hbar := 6.58000000 \times 10^{-16} \tag{3.2.4}$$

```
> E := 5; U0 := 10;
```

$$E := 5$$

$$U0 := 10 \tag{3.2.5}$$

```
> protonA := AtomicData("H");
protonA := table([name = hydrogen, meltingpoint = 13.81000000 K, names = {hydrogen},
    electronegativity = 2.10000000, symbol = H, boilingpoint = 20.28000000 K, ionizationenergy
    = 13.59840000 eV, atomicweight = 1.00794000 amu, atomicnumber = 1])      (3.2.6)
> protonm := protonA[atomicweight];
```

$$protonm := 1.00794000 \text{ amu} \tag{3.2.7}$$

```
> SC3m := convert(protonm, units,'kg');
```

$$SC3m := 1.67372489 \times 10^{-27} \text{ kg} \tag{3.2.8}$$

> $SC3\_m := 1.67372489 \times 10^{-27}$

$$SC3\_m := 1.67372489 \times 10^{-27} \quad \textbf{(3.2.9)}$$

Values for q and k are calculated according to Equations 5 and 7

> $K := \text{sqrt}(2 * m * E) / \text{hbar};$

$$K := 4.58689291 \quad \textbf{(3.2.10)}$$

> $Q := \text{sqrt}(2 * m * (U0 - E)) / \text{hbar};$

$$Q := 4.58689291 \quad \textbf{(3.2.11)}$$

Next, the transmission coefficient T is expressed according to Equation 12 and the **simplify** command is used to evaluate the expression

> $T := 1 / (1 + ((k^\wedge 2 + q^\wedge 2) / (2 * k * q))^\wedge 2 * \sinh(q * L)^\wedge 2);$

$$T := \frac{1}{1 + \frac{(k^2 + q^2)^2 \sinh(q L)^2}{4 k^2 q^2}} \quad \textbf{(3.2.12)}$$

> $SC1\_TT := simplify(subs(\{k = K, q = Q\}, T));$

$$SC1\_TT := \frac{1}{\cosh(4.58689291\, L)^2} \quad \textbf{(3.2.13)}$$

Next, we define the energies and masses of the particles for SC2 and SC3, and we calculate the transmission coefficient for these scenarios

> $SC2\_E := 2; SC2\_U0 := 10; SC2\_K := \text{sqrt}(2 * m * SC2\_E) / \text{hbar}; SC2\_Q := \text{sqrt}(2 * m * (SC2\_U0 - SC2\_E)) / \text{hbar};$

$$SC2\_E := 2$$
$$SC2\_U0 := 10$$
$$SC2\_K := 2.90100580$$
$$SC2\_Q := 5.80201159 \quad \textbf{(3.2.14)}$$

> $SC3\_E := 2; SC3\_U0 := 10; SC3\_K := \text{sqrt}(2 * SC3\_m * SC3\_E) / \text{hbar}; SC3\_Q := \text{sqrt}(2 * SC3\_m * (SC3\_U0 - SC3\_E)) / \text{hbar};$

$$SC3\_E := 2$$
$$SC3\_U0 := 10$$
$$SC3\_K := 124.35010010$$
$$SC3\_Q := 248.70020020 \quad \textbf{(3.2.15)}$$

> $SC2\_T := 1 / (1 + ((k^\wedge 2 + q^\wedge 2) / (2 * k * q))^\wedge 2 * \sinh(q * L)^\wedge 2); SC3\_T := 1 / (1 + ((k^\wedge 2 + q^\wedge 2) / (2 * k * q))^\wedge 2 * \sinh(q * L)^\wedge 2);$

$$SC2\_T := \frac{1}{1 + \frac{(k^2 + q^2)^2 \sinh(q L)^2}{4 k^2 q^2}}$$

(3.2.16)

$$SC3\_T := \frac{1}{1 + \frac{\left(k^2 + q^2\right)^2 \sinh(q\,L)^2}{4\,k^2\,q^2}} \tag{3.2.16}$$

```
> SC2_TT := simplify(subs({k = SC2_K, q = SC2_Q}, SC2_T)); SC3_TT := simplify(subs({k = SC3_K, q = SC3_Q}, SC3_T));
```

$$SC2\_TT := \frac{1}{-0.56250000 + 1.56250000 \cosh(5.80201159\,L)^2}$$

$$SC3\_TT := \frac{16.00000000}{25.00000000 \cosh(248.70020020\,L)^2 - 9.00000000} \tag{3.2.17}$$

Then we plot transmission T as a function of barrier width L

```
> plot([SC1_TT, SC2_TT, SC3_TT], L = 0 ..0.8, labels = ["Barrier Width", "Transmission"], color = [black, myred, myblue], thickness = 5, legend = ["High Energy, Low Mass", "Low Energy, Low Mass", "Low Energy, High Mass"], legendstyle = [location = right]);
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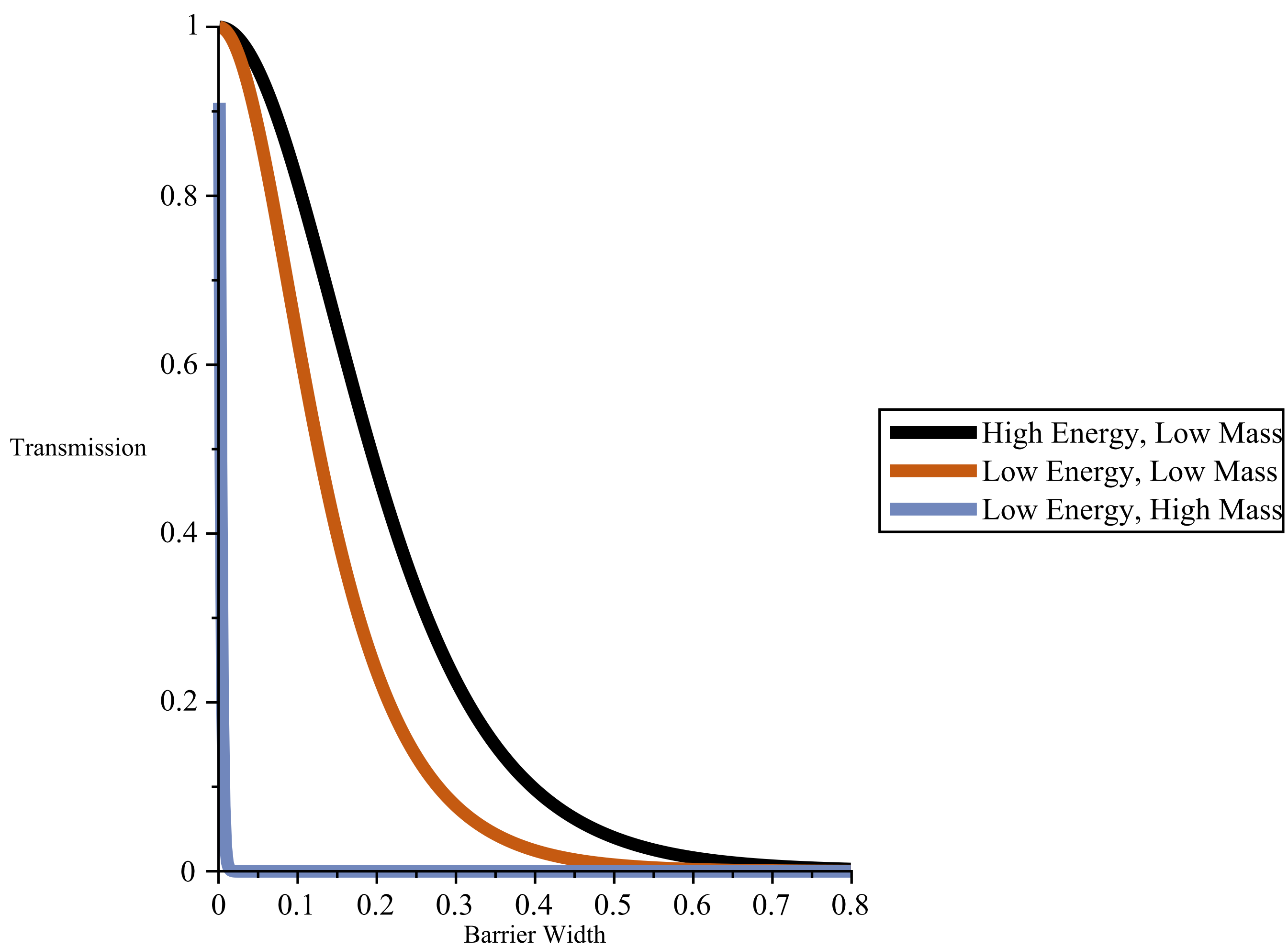

Figure 3: Probability of transmission as a function of barrier width, particle energy, and particle mass

From the overlaid figure, we see that the probability of a particle tunneling through a barrier is dependent on the particle mass, particle energy, and barrier width. It is apparent that particles with the lowest mass and highest energy (black line) have the highest transmission probability. Conversely, particles with the highest mass and lowest energy (blue line) have the lowest transmission probability. Intuitively, this trend agrees with expectation: quantum tunneling is more frequent for microscopic particles and negligible at the macroscopic level. In addition, the probability of tunneling appears to be more dependent on particle mass than on particle energy.

III. Applications

Scanning Tunneling Microscopy

Gerd Binnig and Heinrich Rohrer were awarded the Nobel Prize in Physics in 1986 for their contribution to the development of scanning tunneling microscopy (STM), which measures the topography of conductive surfaces at the atomic level [5]. The STM method involves a sharp conductive tip that is placed within tunneling distance of a conductive surface, as shown in Figure 4. The wave of the STM tip electrons (ψ_T) and the surface electrons (ψ_S) overlap, resulting in a tunneling current of electrons through the gap between the tip and the surface. Measuring the local magnitude of the tunneling current, as a function of tip position, provides information on variations in electron density and renders an atomic image of the sample surface with Angstrom-level precision. The STM method can be applied to characterize nanomaterials such as carbon nanotubes, superlattices, or conductors, and the resulting images can inform upon structure-function relationships.

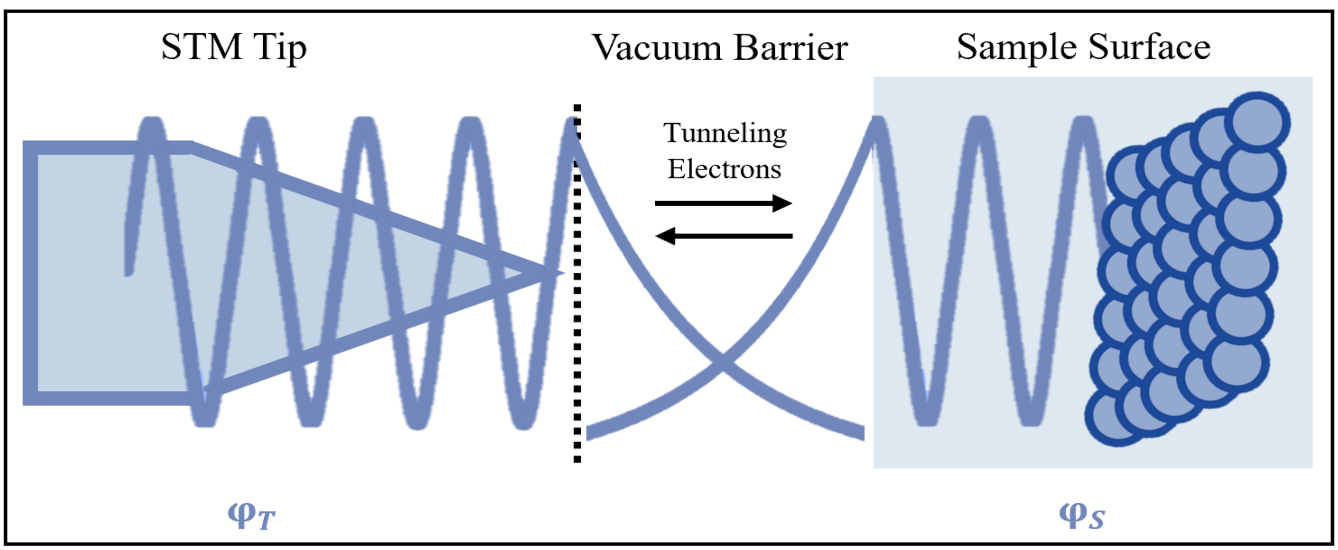

Figure 4: Schematic of scanning tunneling microscope

The high sensitivity of the STM method is due to the exponential decay experienced by tunneling electrons in the vacuum barrier. As demonstrated in Section II and Figure 3 above, the probability for quantum tunneling is strongly dependent on barrier width. Indeed, the tunneling current that is measured as a function of the probe-to-sample distance results in a sub-Angstrom resolution. If the probe-to-sample distance changes by only one Angstrom, the resulting current is changed by one order of magnitude.

Resonant Tunneling Diodes

Another application of quantum tunneling is in the development of nanoscale electronics. As shown in Figure 5, a resonant tunneling diode consists of two barriers that are separated by a quantum well, where energy levels are quantized. In one region, an emitter provides an electron source. Without a bias voltage, electrons encountering Barrier I or Barrier II would have a small, finite probability of tunneling through the barriers (as described in Section II). By applying a bias voltage to the diode system, the energy of the emitted electrons can be matched to a quantized energy in the quantum well; this corresponds to resonance energy. At this resonance energy, the transmission coefficient of the electron wave approaches unity and maximizes tunneling current.

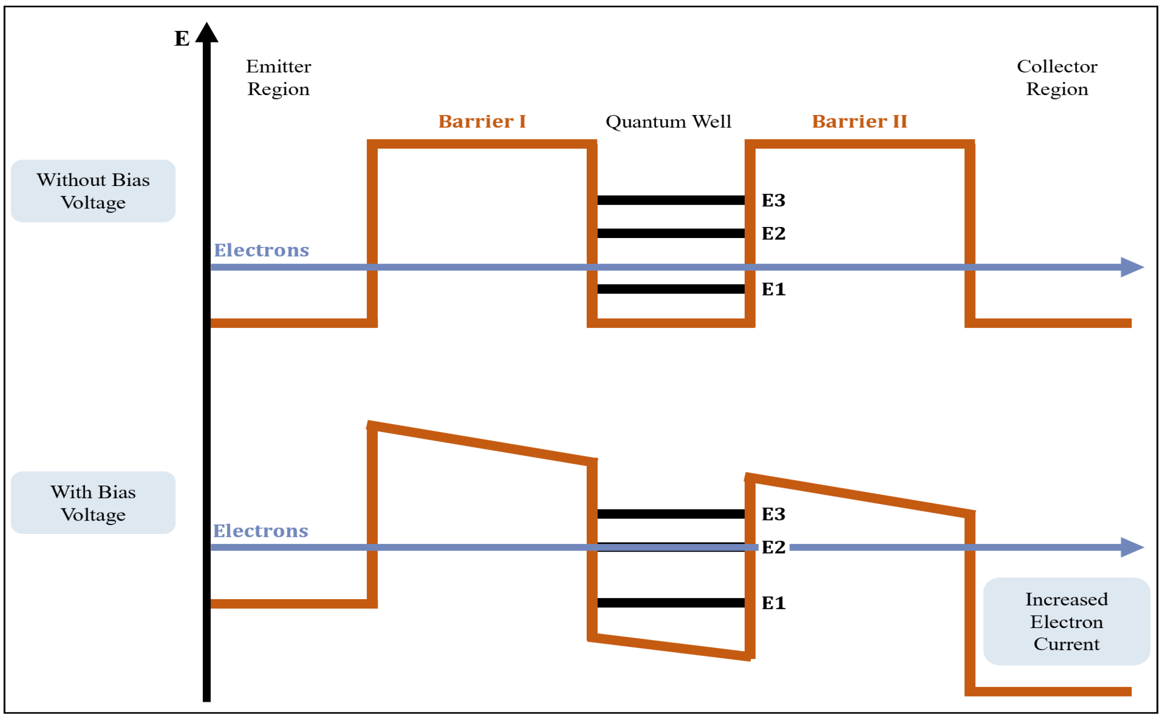

Figure 5: Schematic of resonant tunneling diode

A resonant tunneling diode can be used in place of a conventional transistor. Because resonant tunneling diodes are both nano-size and high-speed, they may be used in the advancement of nanoelectronics such as photodetectors, silicon chips, circuits, and semiconductors [6].

IV. Conclusions

In this Worksheet, we have explored the phenomenon of quantum tunneling. Although classically forbidden, a particle that has lower energy than a potential barrier will have a finite, non-zero probability of tunneling through the barrier at the quantum mechanical level. Calculation of the transmission coefficient in this Worksheet has demonstrated that the probability of quantum tunneling is strongly dependent on particle mass and is also dependent on particle energy and barrier width. The dependence of tunneling current on barrier width has been utilized in the method of scanning tunneling microscopy, which measures the change in tunneling current as a function of probe-to-sample distance. High-resolution atomic images obtained using this method provide information on the structure of nanomaterials. Quantum tunneling is also utilized in resonant tunneling diodes, which provide faster and smaller alternatives to conventional transistors.

Selected References

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