ME597/PHYS57000

Fall Semester 2010

Lecture 01

Quantum Tunneling

The STM – basic idea

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Suggested Reading:

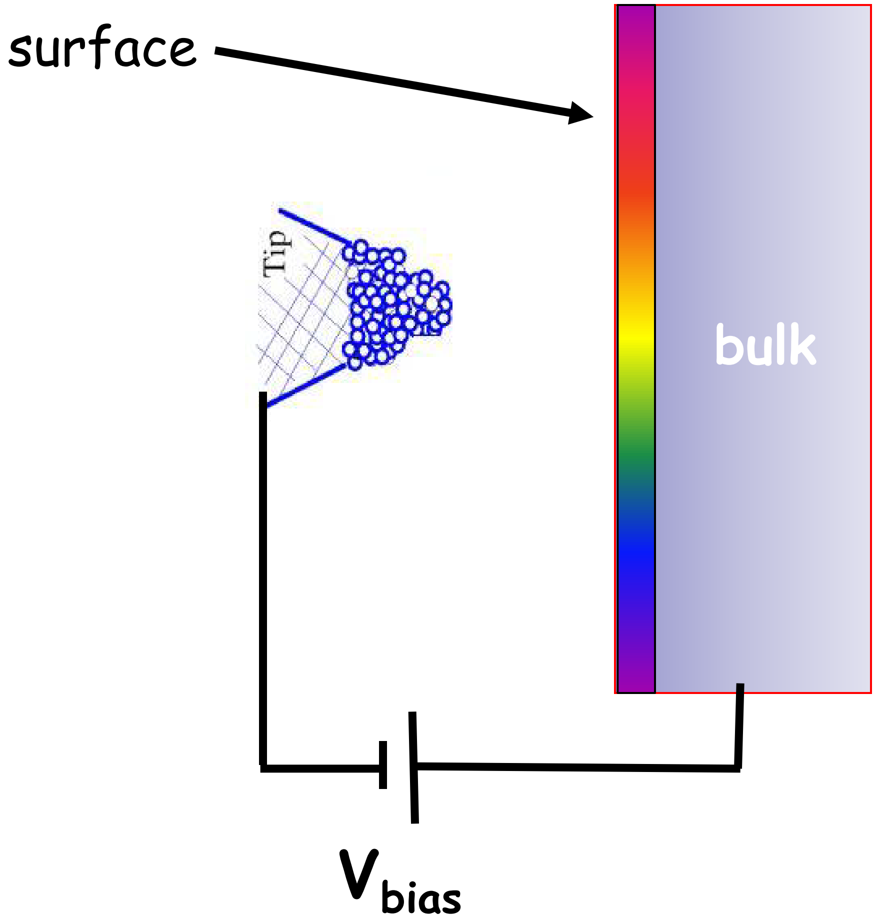
• G. Binnig, H. Rohrer, Ch. Gerber, E. Weibel, “Tunneling through a controllable vacuum gap”, Appl. Phys. Lett. **40**, 178 (1982).

• G. Binnig, H. Rohrer, Ch. Gerber, E. Weibel, Surface studies by scanning tunneling microscopy” Phys. Rev. Lett. **49**, 57 (1982).

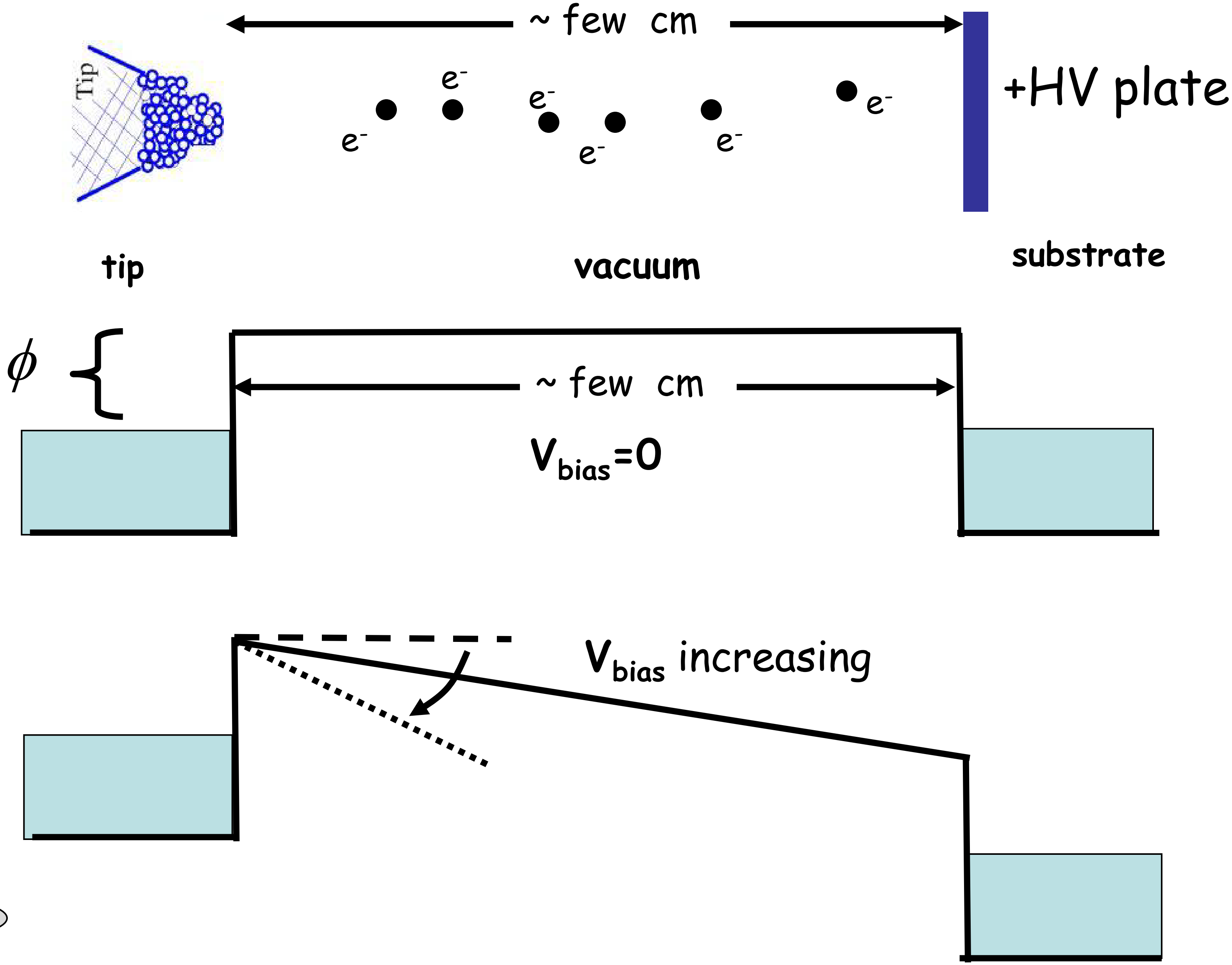
• P.K. Hansma and J. Tersoff, “Scanning tunneling microscopy”, J. Appl. Phys. **61**, R1 (1987).

Critical Realization (*circa* 1980)

Require a proximal probe (a sharp tip) to locally interrogate the surface of a bulk material



The Classical Picture



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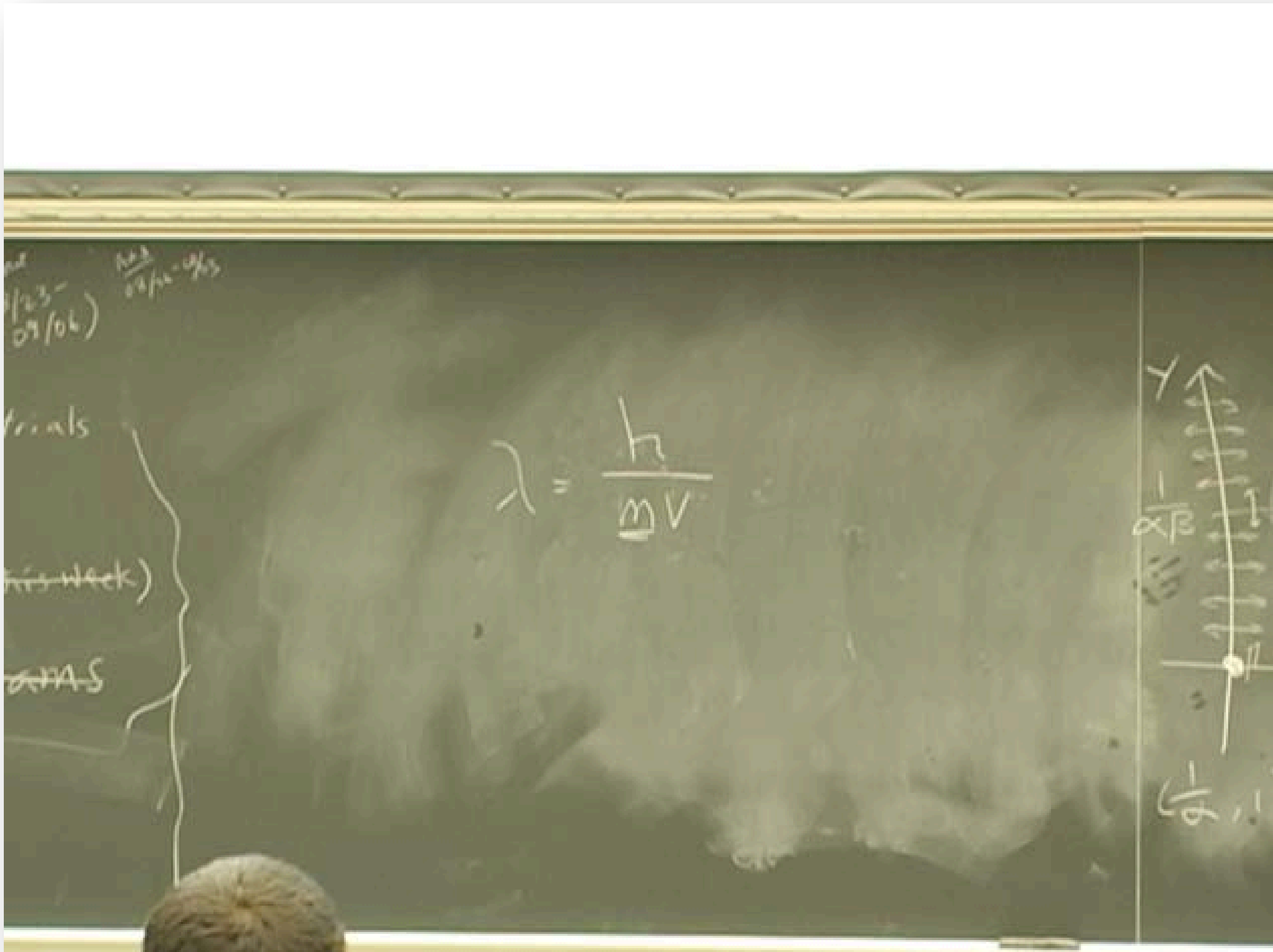
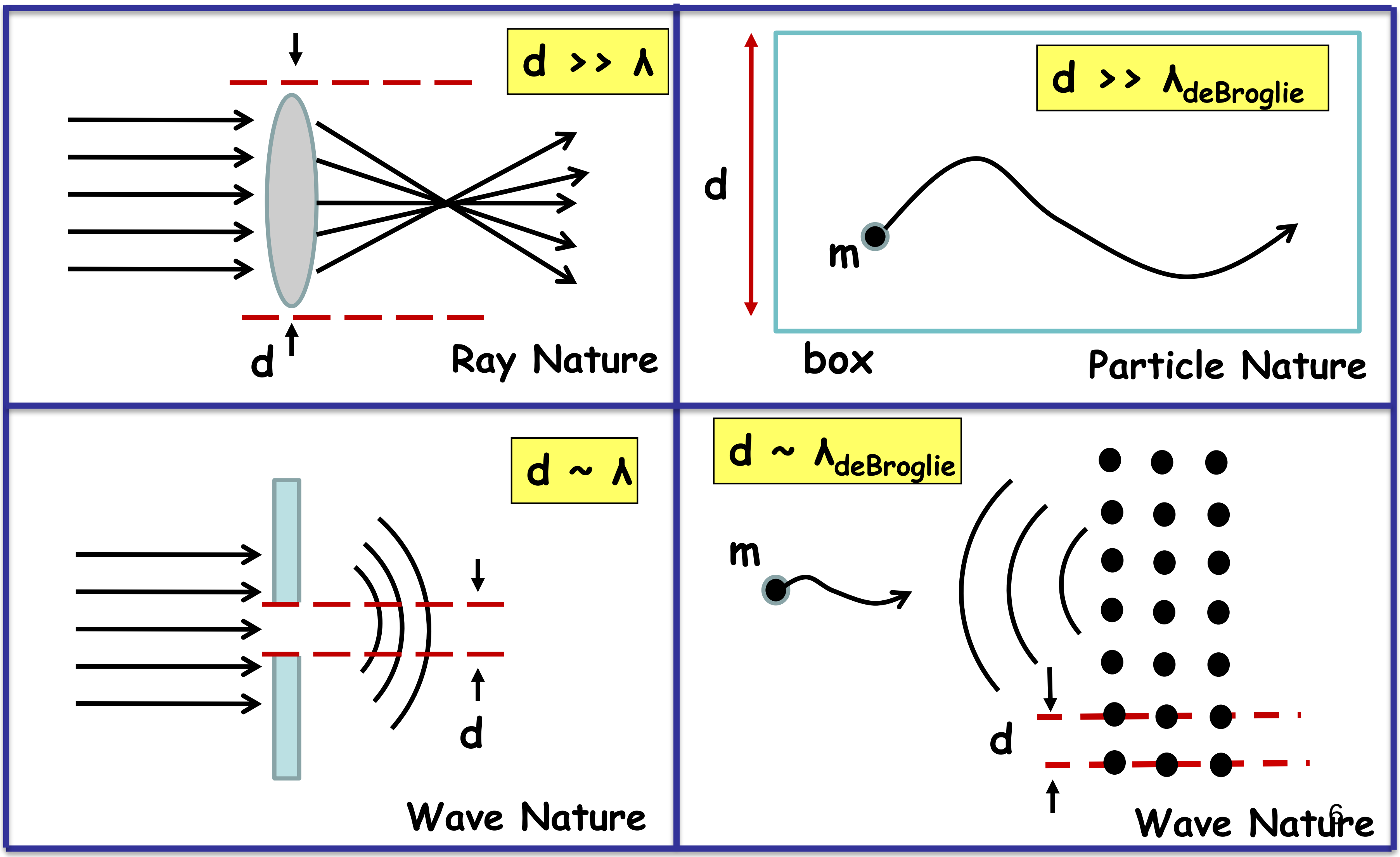
A Fundamental Breakthrough



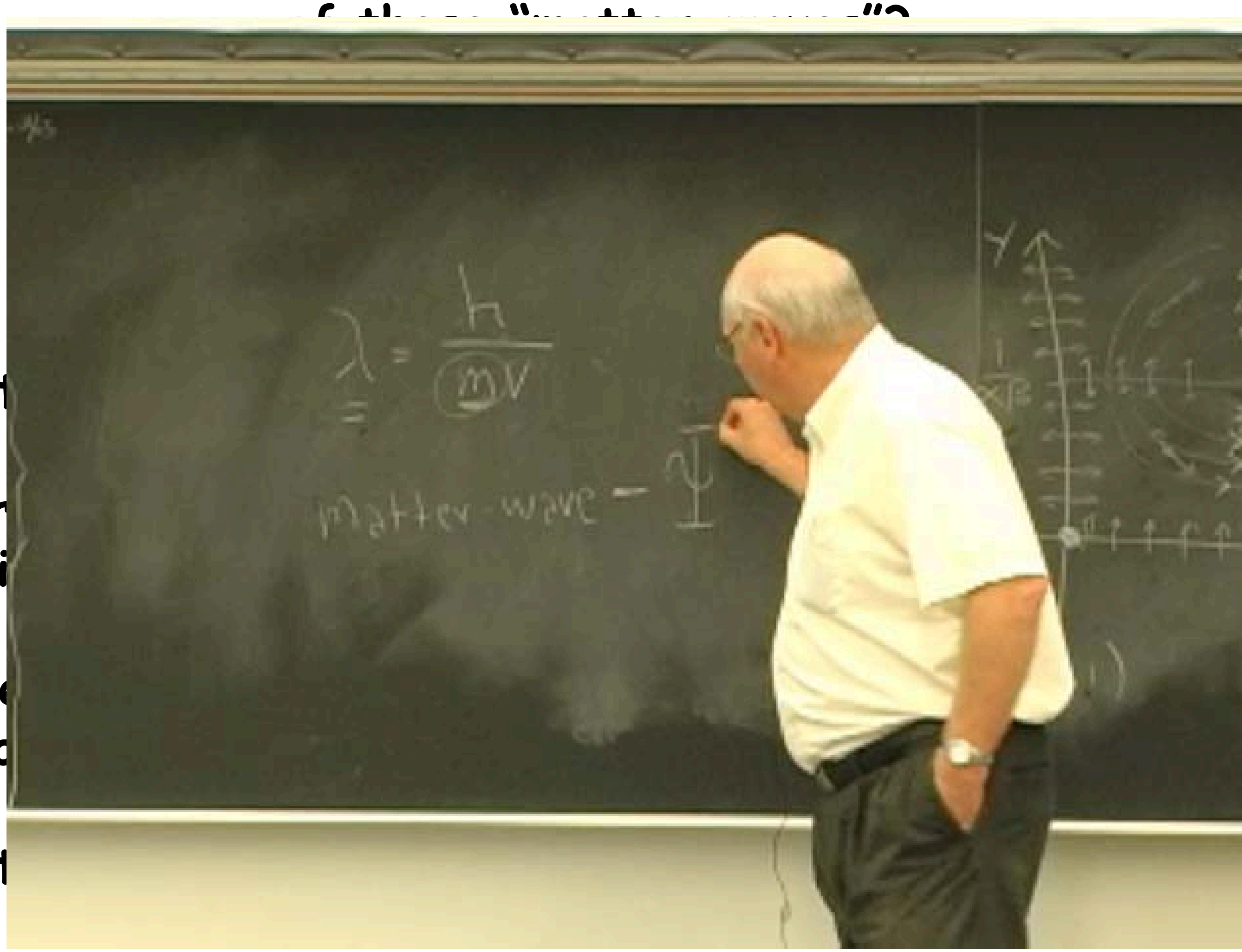
Dual Character

LIGHT

PARTICLE



If particles behave like waves, what is the equation that describes the motion



• Can’t … ved

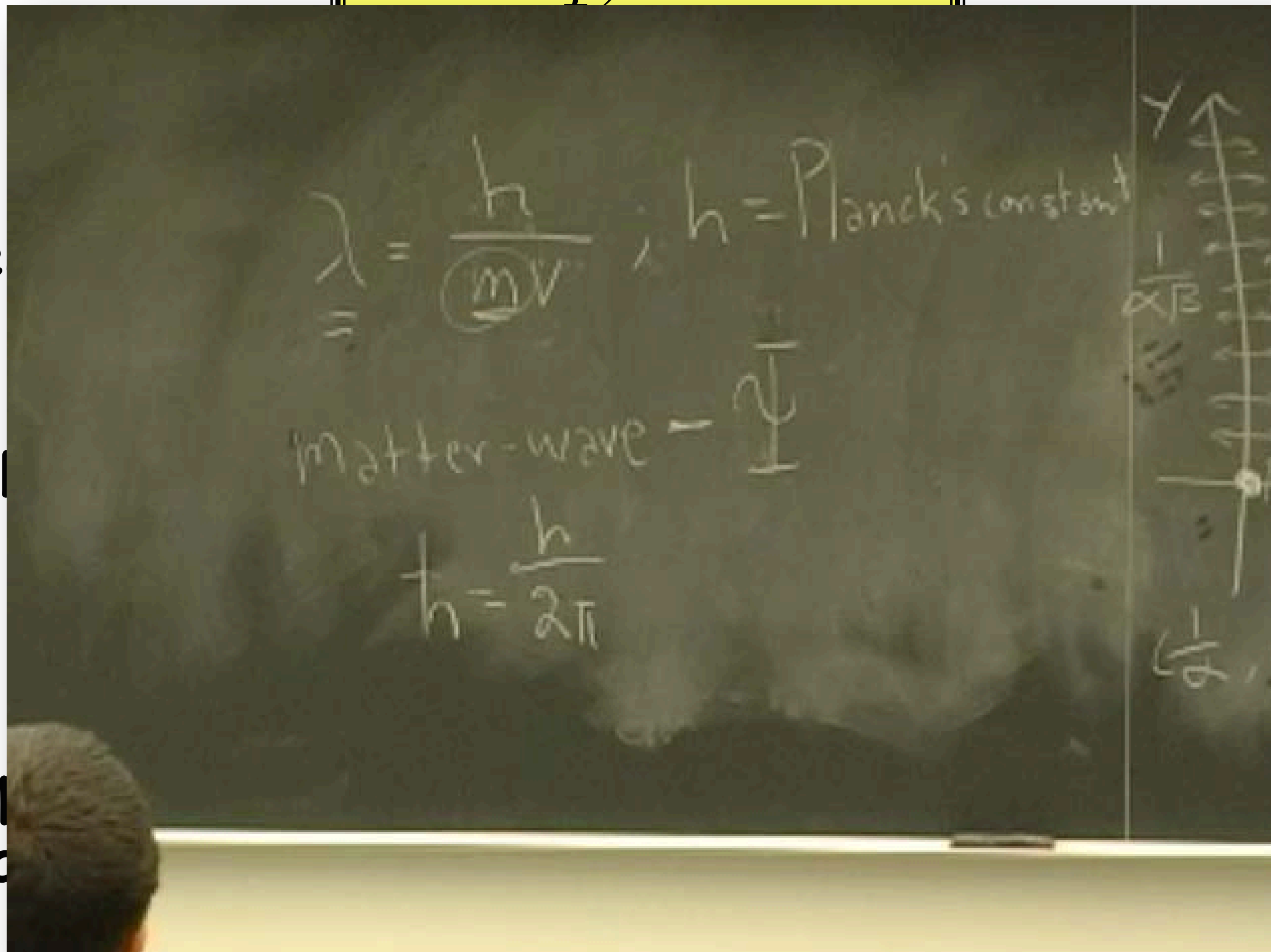
• Schr …
experi …

• Solv … omic
and co …

• Must …

• Describes the wave field of a particle; the so-called matter wave

Define a Hamiltonian *Operator*, H



The

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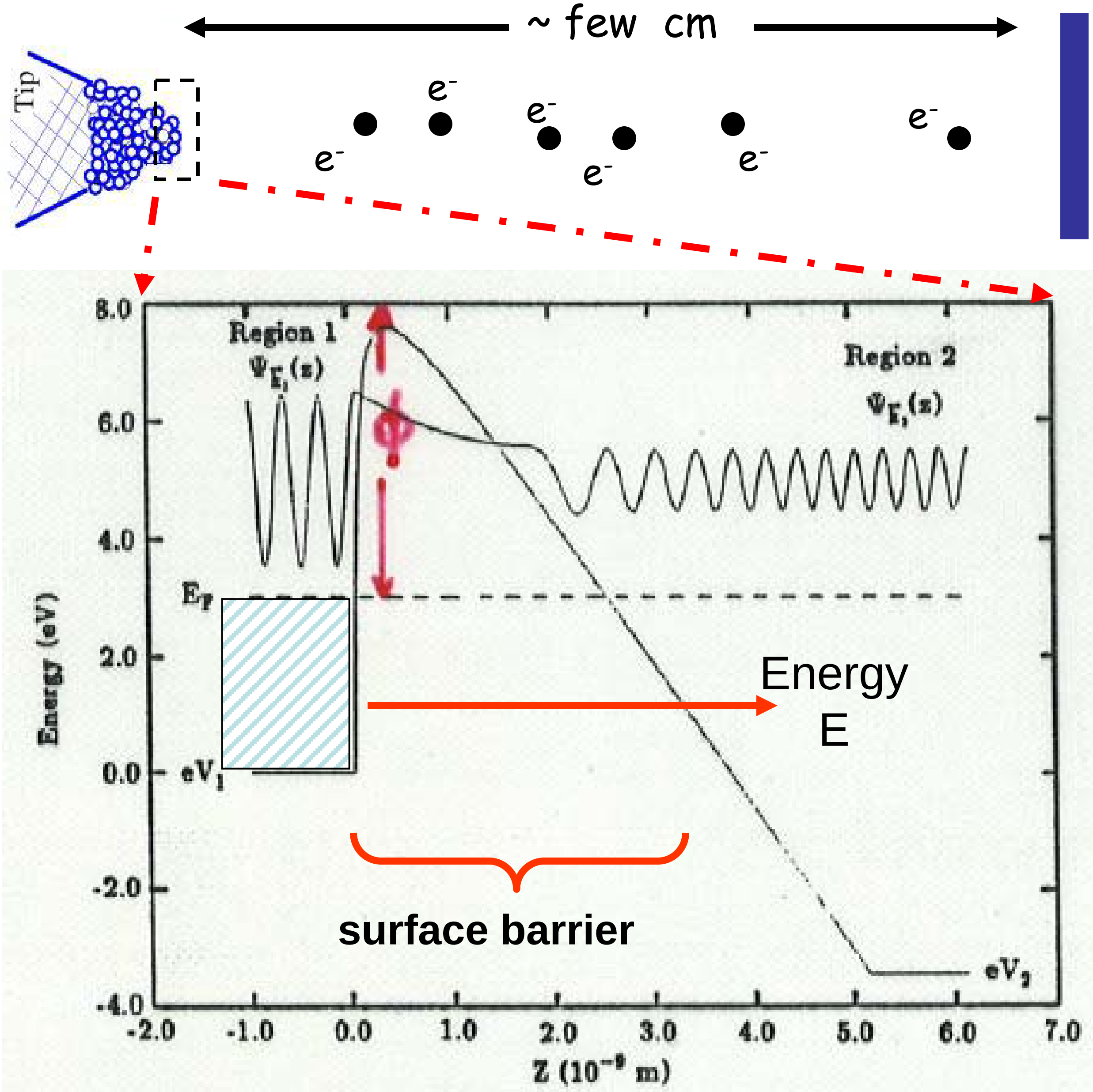
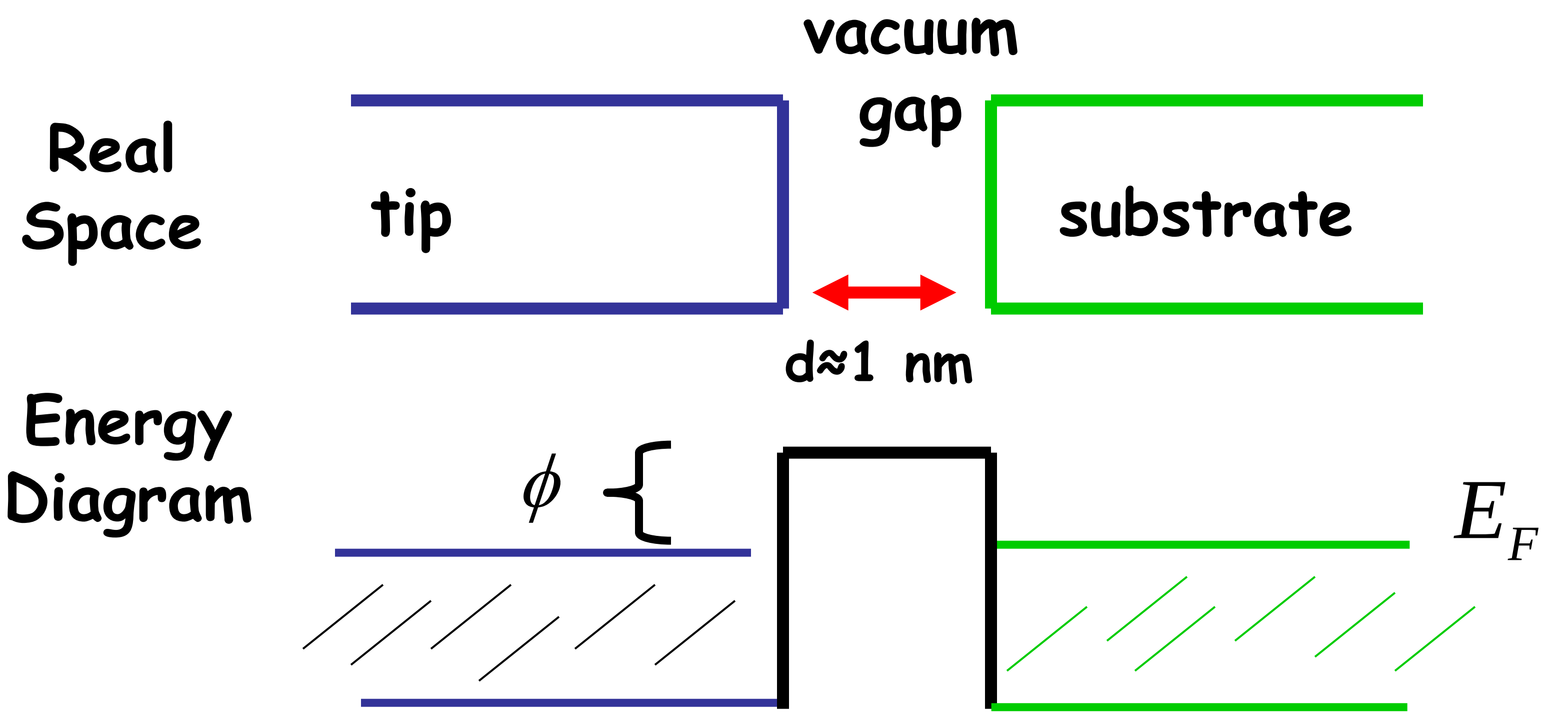
$$\langle X \rangle = \int_{-\infty}^{+\infty} \Psi^*(\vec{r})\, X\, \Psi(\vec{r})\, d^3\vec{r}$$

Physics of Field Emission (~1925)

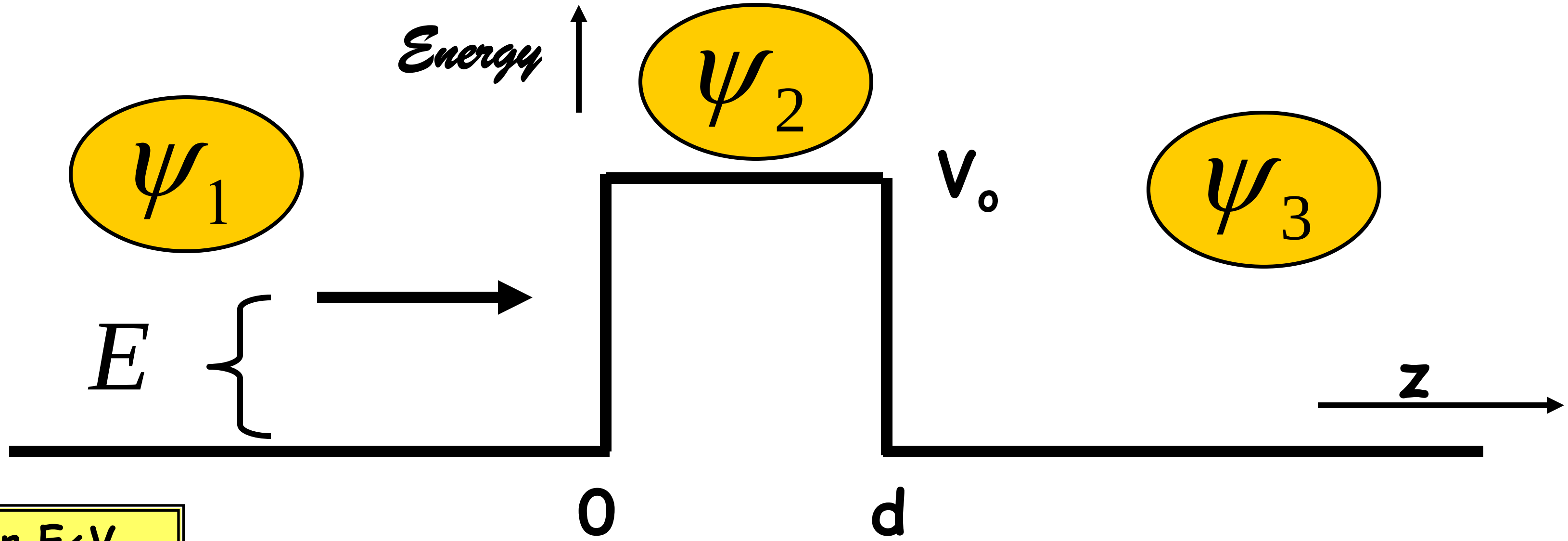


The energy of electron does not change!

What happens if the distance between the two metals is reduced?



The electron wavefunctions for a square barrier can be analytically solved



Valid for $E<V_o$

everywhere $$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dz^2}+U(z)\psi=E\psi$$

$$\psi_1=e^{ikz}+Ae^{-ikz} \qquad \psi_2=Be^{-\alpha z}+Ce^{\alpha z} \qquad \psi_3=De^{ikz}$$

$$U(z)=0 \qquad U(z)=V_o \qquad U(z)=0$$

$$k^2=\frac{2mE}{\hbar^2} \qquad \boxed{\alpha^2=\frac{2m\left(V_o-E\right)}{\hbar^2}} \qquad k^2=\frac{2mE}{\hbar^2}$$

Calculating the Transmission Probability

The classical expression for current density produced by a charge q with velocity v is given by

j=qv

Now, if a single electron is described by a wavefunction Ψ(z,t), then the equivalent QM expression for the current is

j=-|e|<v>

where $\langle v \rangle = \frac{d}{dt}\int_{-\infty}^{\infty} \psi^{*}(z,t)\, z\, \psi(z,t)\, dz$

Evaluating this expression using the time-dependent Schroedinger equation, we can define a probability current density given by

$$j = \frac{-i\hbar}{2m}\left[\psi^{*}\frac{d\psi}{dz} - \psi\frac{d\psi^{*}}{dz}\right]$$

Transmitted current:

$$j_{trans} = \frac{-i\hbar}{2m}\left[\psi_3^* \frac{d\psi_3}{dz} - \psi_3 \frac{d\psi_3^*}{dz}\right] = \frac{\hbar k}{m}\left|D\right|^2$$

Incident current:

$$j_{inc} = \frac{-i\hbar}{2m}\left[\psi_1^* \frac{d\psi_1}{dz} - \psi_1 \frac{d\psi_1^*}{dz}\right] = \frac{\hbar k}{m}$$

Transmission Probability:

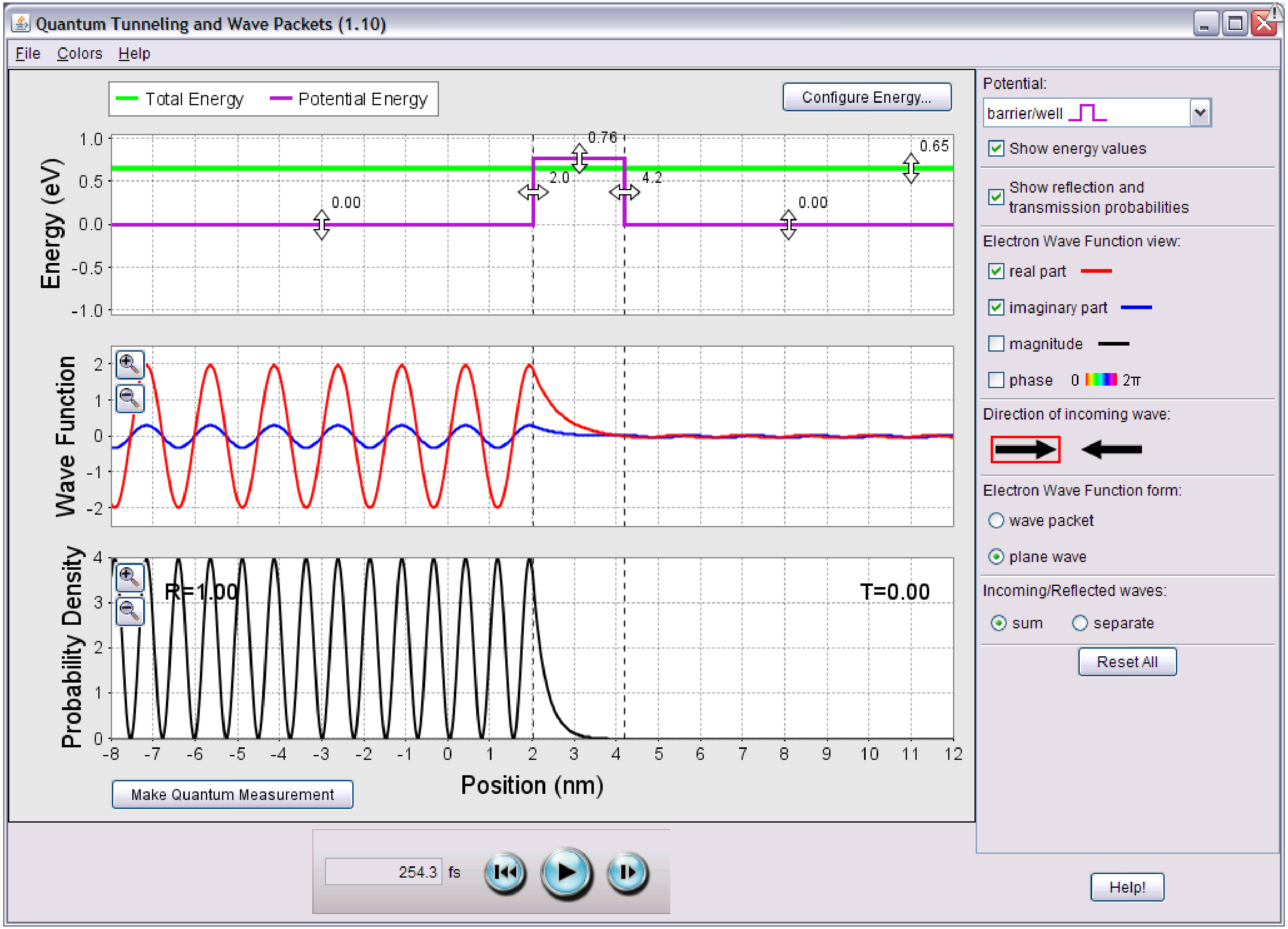
$$T \equiv \frac{j_{trans}}{j_{inc}} = \left|D\right|^2 = \frac{1}{1 + \frac{\left(k^2+\alpha^2\right)^2}{4k^2\alpha^2}\sinh^2(\alpha d)}$$

Valid for E<V$_o$

$$if\ \alpha d \gg 1\,(wide\ \ barrier, low\, energy)$$

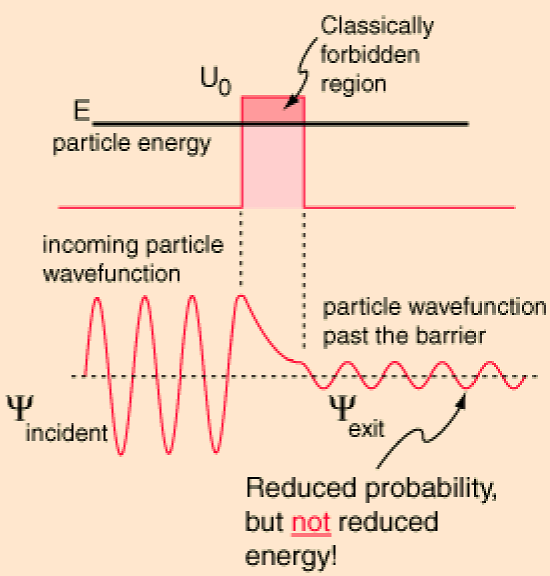
$$T \cong \frac{16k^2\alpha^2}{\left(k^2+\alpha^2\right)^2} e^{-2\alpha d} \qquad \alpha \sim 10-15\, nm^{-1}$$

http://phet.colorado.edu/simulations/sims.php?sim=Quantum_Tunneling_and_Wave_Packets



http://hyperphysics.phy-astr.gsu.edu/Hbase/quantum/barr.html#c1

Barrier Penetration



According to classical physics, a particle of energy E less than the height U_0 of a barrier could not penetrate - the region inside the barrier is classically forbidden. But the wavefunction associated with a free particle must be continuous at the barrier and will show an exponential decay inside the barrier. The wavefunction must also be continuous on the far side of the barrier, so there is a finite probability that the particle will tunnel through the barrier.

As a particle approaches the barrier, it is described by a free particle wavefunction. When it reaches the barrier, it must satisfy the Schrodinger equation in the form

$$\frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x)}{\partial x^2} = (E - U_0)\Psi(x)$$

Useful summary of barrier penetration

In real life, it's always more complicated

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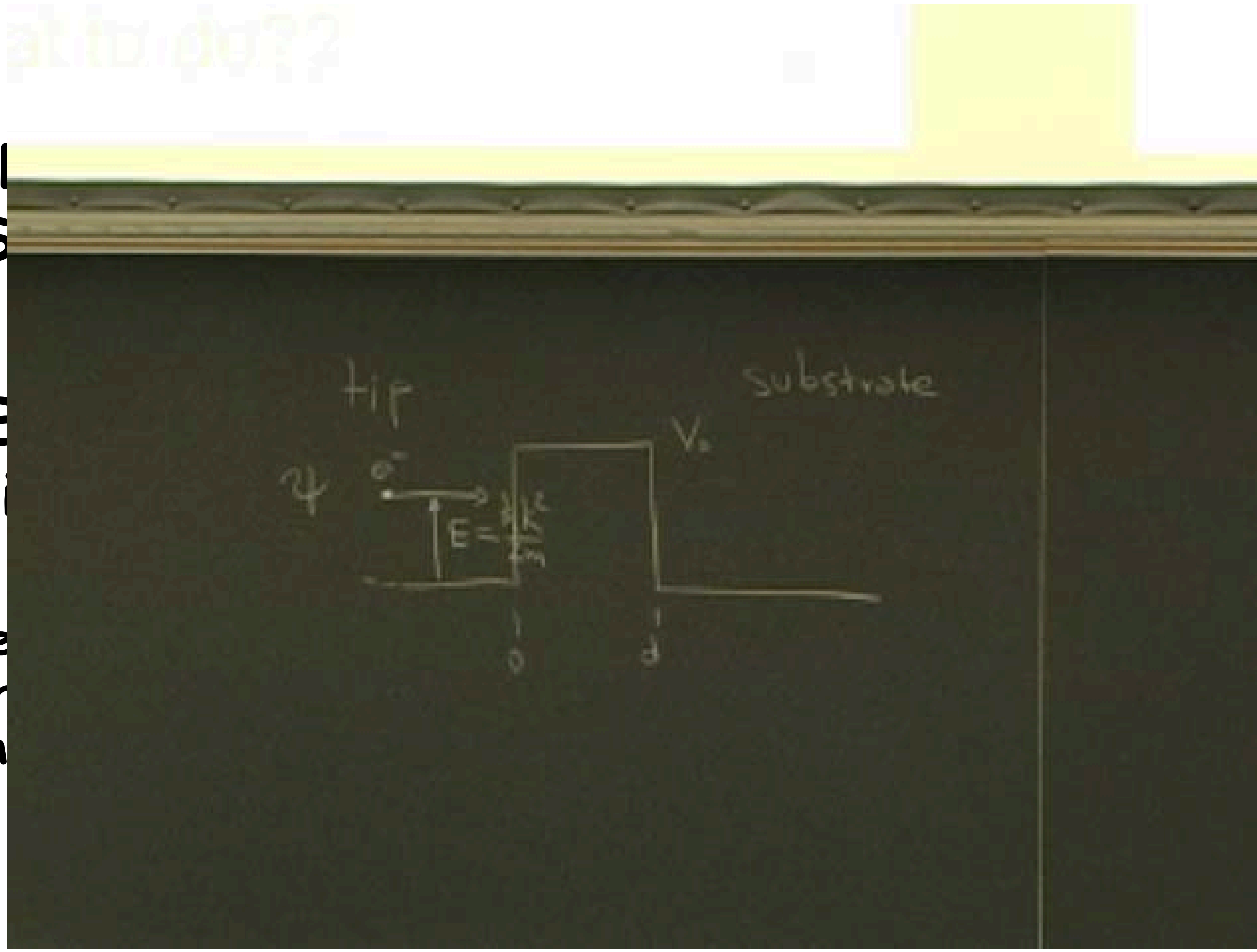
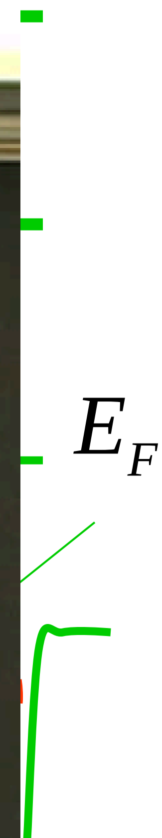
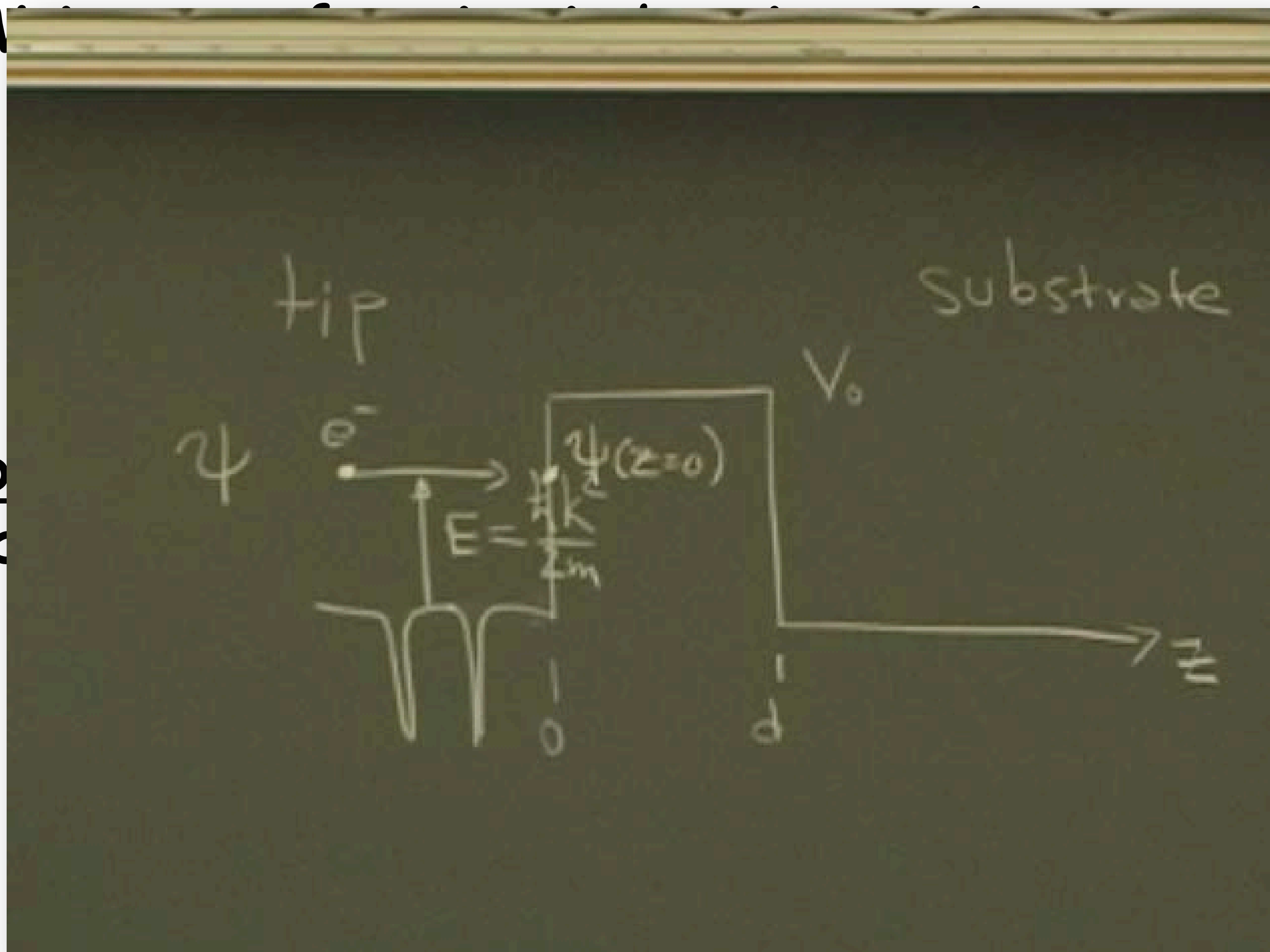




What to do??

Use insights gained from square barrier problem

W

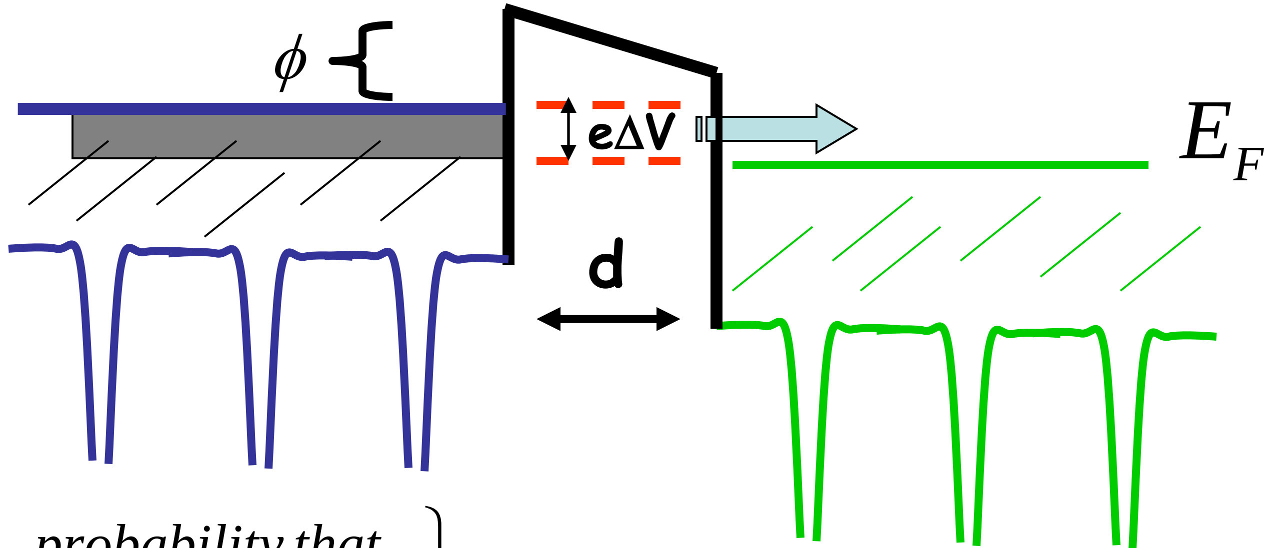


Probab e

z will b

very similar in form to T calculated earlier

To make current flow, apply bias voltage ΔV



$$I \propto \left\{ \begin{array}{c} probability\ that \\ electrons\ in\ shaded \\ region\ get\ to\ z=d \end{array} \right\} = \sum_{E_F - e\Delta V}^{E_F} \left| \psi_n(0) \right|^2 e^{-2\alpha_n d}$$

Useful to define the Local Density of States (LDOS):

$$\boxed{\rho(z,E) \equiv \frac{1}{\varepsilon} \sum_{E-\varepsilon}^{E} \left| \psi_n(z) \right|^2}$$

ρ(z,E) measures

$$\frac{\#\ \text{electrons/volume}}{\text{energy interval}}$$

at a GIVEN distance z from substrate
and at a GIVEN energy E

The LDOS has a few nice features:

- It is independent of the volume of metal
- It is a number (for given z & E) that reflects the energy band structure of metal
- It can be used to obtain an expression for the current that flows

Note that:

$$\rho(0,E) \equiv \frac{1}{\varepsilon}\sum_{E-\varepsilon}^{E} \left|\psi_n(0)\right|^2$$

$$= \frac{1}{e\Delta V}\sum_{E-e\Delta V}^{E} \left|\psi_n(0)\right|^2$$

so

$$I \propto probability\ of\ tunneling = \sum_{E_F-e\Delta V}^{E_F} \left|\psi_n(0)\right|^2 e^{-2\alpha_n d}$$

$$= e\Delta V\, \rho(0,E_F)\, e^{-2\alpha d} \quad where\ e\Delta V \to 0$$

LDOS Calculations

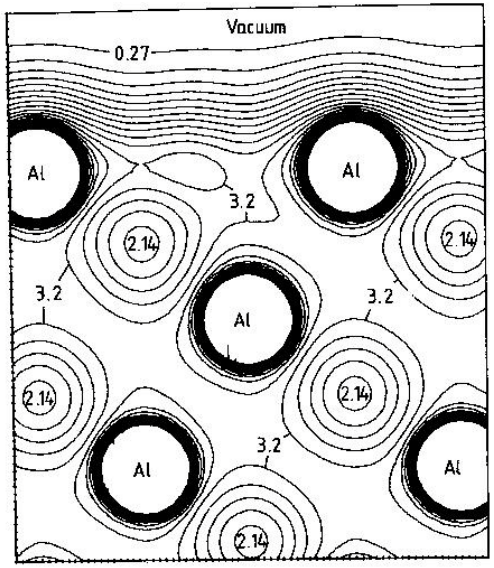


Figure 12. Contours of charge density at Al (111) surface (Wang *et al* 1981).

contours of constant charge density (proportional to LDOS)

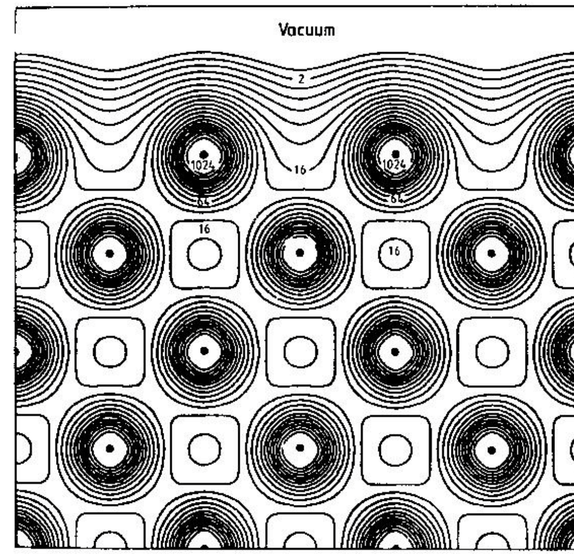
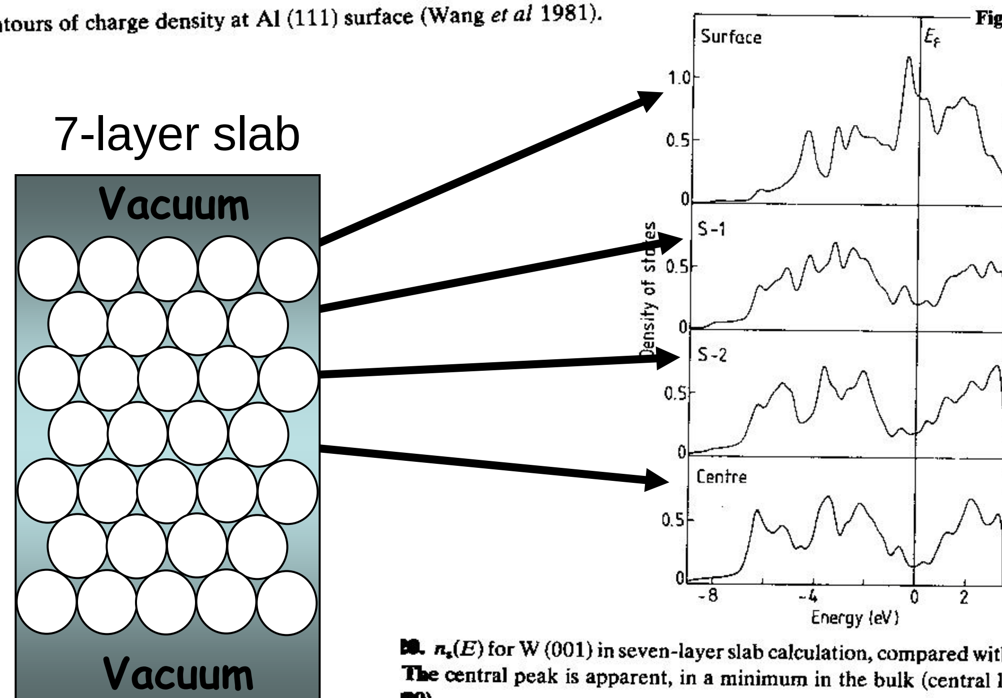


Figure 29. Contours of charge density at Ni (001) surface (Arlinghaus *et al* 1980

7-layer slab



LDOS

10. $n_s(E)$ for W (001) in seven-layer slab calculation, compared with densities of states on sub-surface The central peak is apparent, in a minimum in the bulk (central layer) density of states (Posternak 80).

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Journal of Physics and Chemistry of Solids 60 (1999) 681–688

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OF SOLIDS

Cluster-model density functional study of a W–Cu(1 0 0) STM junction

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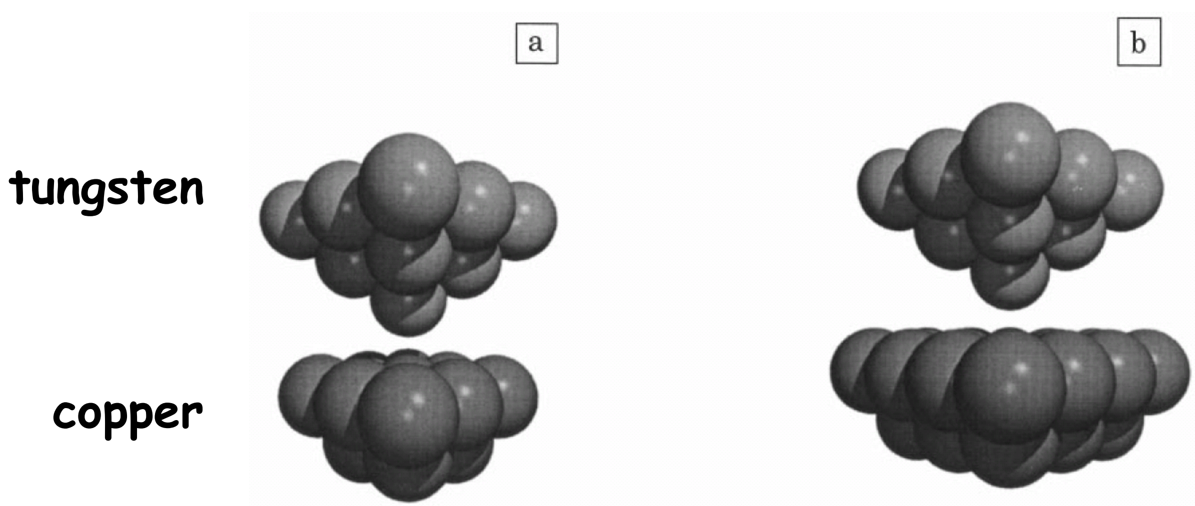


Fig. 1. Geometries of the W–Cu interacting clusters: (a) W_{14}–Cu_{13}; (b) W_{14}–Cu_{25}.

Total:

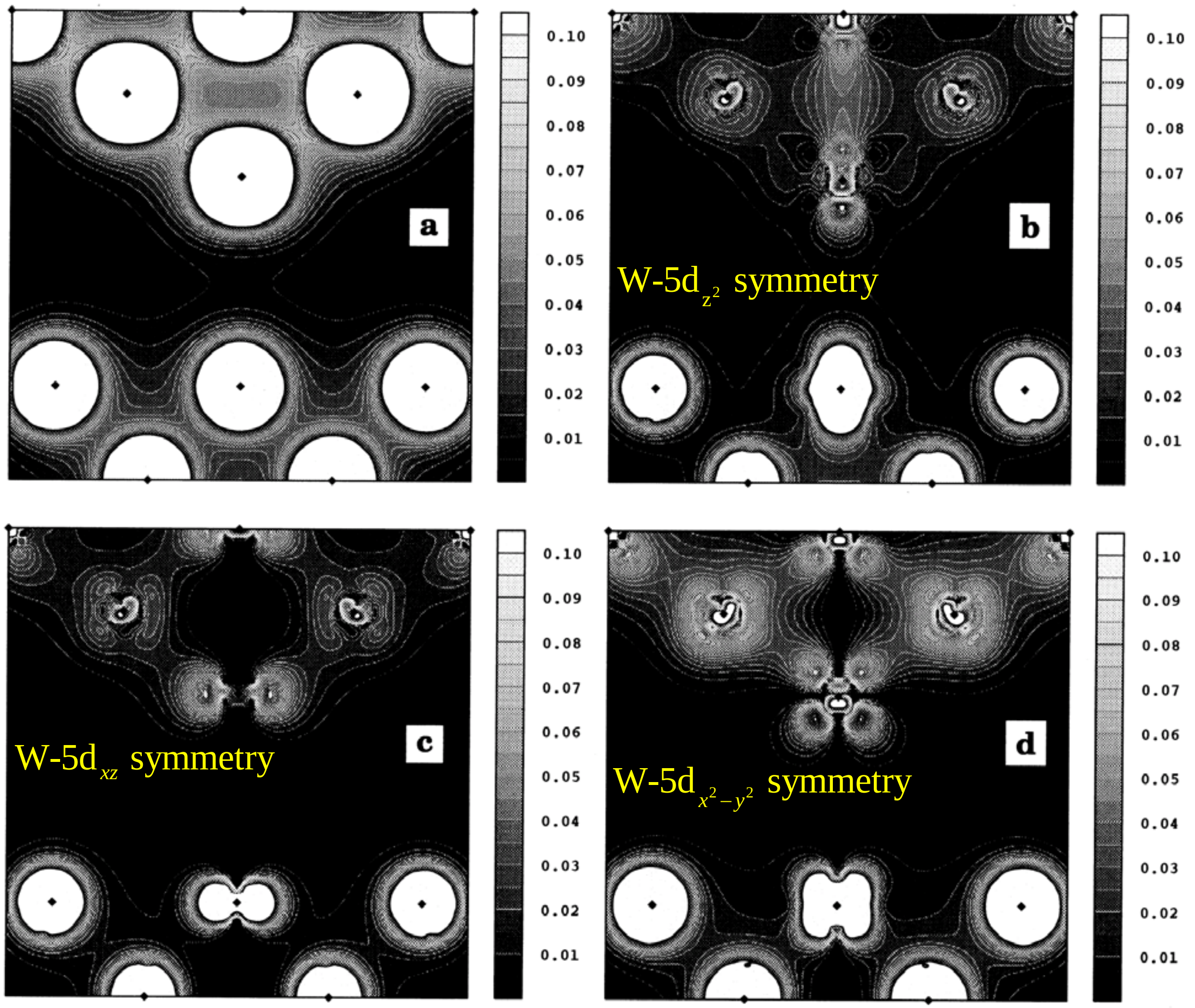


Fig. 5. Contour maps of the total and symmetry-projected electronic valence density of W_{14}–Cu_{13} cluster for a tip–sample separation of 4 Å: (a) total density (including core states); (b) A1-density; (c) B1-density; (d) E-density. Black diamonds indicate the atomic positions.

W electron configuration: 1s2, 2s2, 2p6, 3s2, 3p6, 3d10, 4f14, 5s2, 5p6, 5d4, 6s2

5d: n=5,l=2,m=0,±1,±2

Typical values

Element	Al	Au	Cu	Ir	Ni	Pt	Si	W
Φ (in eV)	4.1	5.4	4.6	5.6	5.2	5.7	4.8	4.9
α (nm^{-1})	10.3	11.9	10.9	12.1	11.6	12.2	11.2	11.2

$$\alpha(in\ m^{-1}) \equiv \sqrt{\frac{2m\left(V_o - E\right)}{\hbar^2}}$$

$$\alpha(in\ nm^{-1}) = 5.1\sqrt{\varphi\ (in\ eV)} \quad \left[convenient\ units\right]$$

$$I(z) = I(0)e^{-2\alpha z}$$

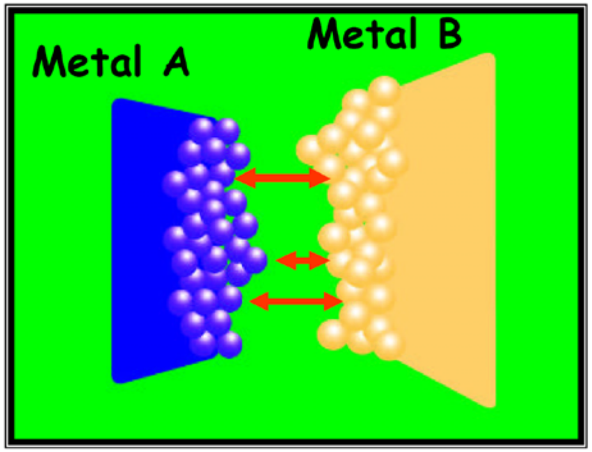
$$I(z + 0.1nm) = I(0)e^{-2\alpha(z+0.1)} = I(z)e^{-2\alpha(0.1)}$$

$$for\ \varphi = 5.09\ eV \Rightarrow \alpha = 11.51\ nm^{-1},\ then$$

$$I(z + 0.1\,nm) = 0.1\,I(z)$$

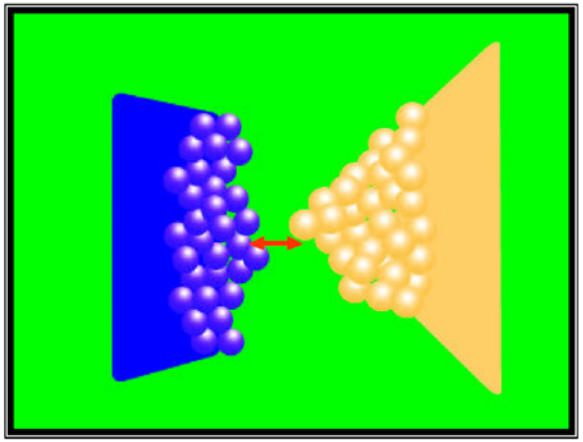
Table from C. Julian Chen, *Introduction to Scanning Tunneling Microscopy, 2nd Edition* (Oxford University Press, Oxford) 2008.

How to achieve a controllable small vacuum gap?



What's d?

Binnig and Rohrer, 1981



Using tip geometry,
d might be well
defined!

Does $I(z) \sim e^{-2ad}$??

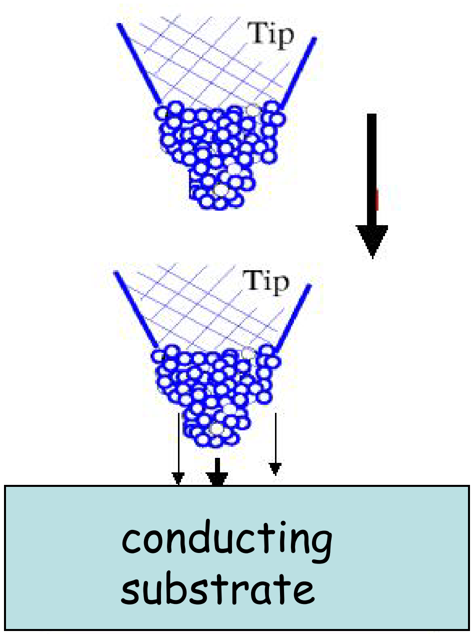
Tunneling through a controllable vacuum gap

G. Binnig, H. Rohrer, Ch. Gerber, and E. Weibel
IBM Zurich Research Laboratory, 8803 Rüschlikon-ZH, Switzerland

(Received 30 September 1981; accepted for publication 4 November 1981)

We report on the first successful tunneling experiment with an externally and reproducibly adjustable vacuum gap. The observation of vacuum tunneling is established by the exponential dependence of the tunneling resistance on the width of the gap. The experimental setup allows for simultaneous investigation and treatment of the tunnel electrode surfaces.

PACS numbers: 73.40.Gk



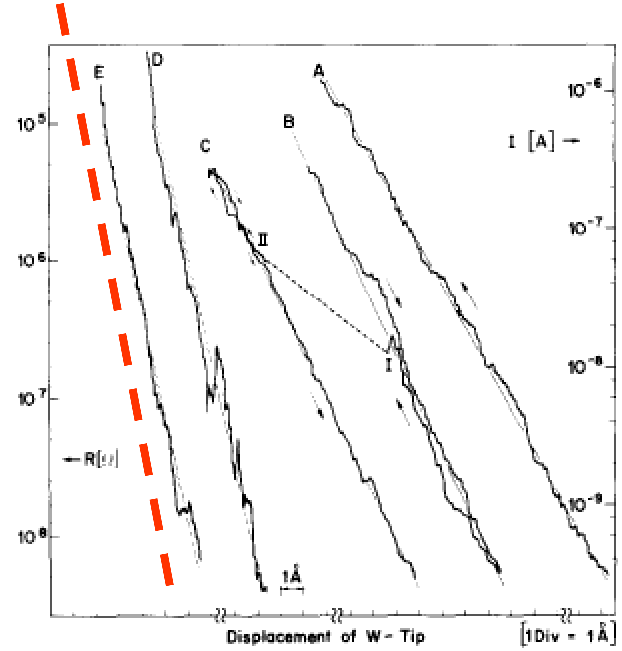
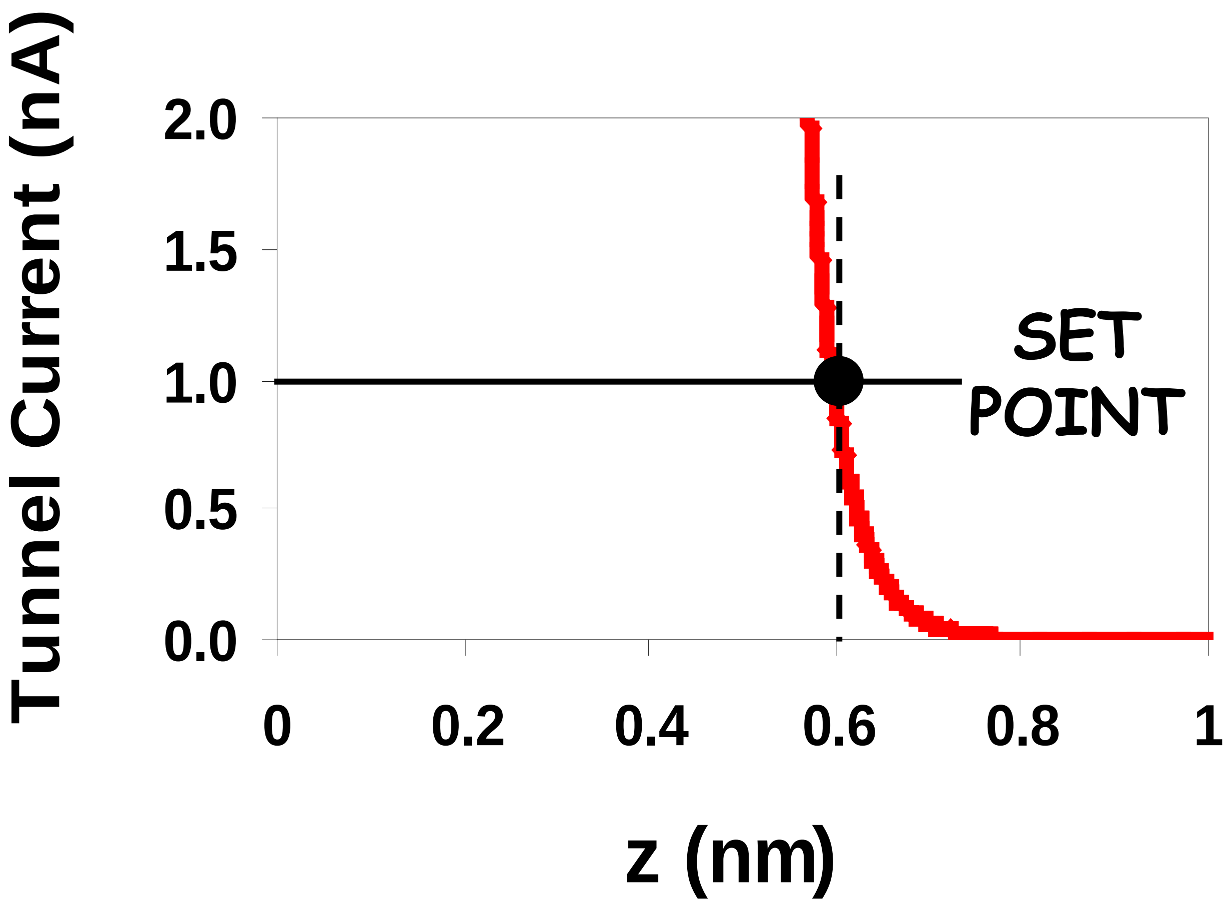


FIG. 2. Tunnel resistance and current vs displacement of Pt plate for different surface conditions as described in the text. The displacement origin is arbitrary for each curve (except for curves B and C with the same origin). The sweep rate was approximately 1 Å/s. Work functions $\phi = 0.6$ eV and 0.7 eV are derived from curves A, B, and C, respectively. The instability which occurred while scanning B and resulted in a jump from point I to II is attributed to the release of thermal stress in the unit. After this, the tunnel unit remained stable within 0.2 Å as shown by curve C. After repeated cleaning and in slightly better vacuum, the steepness of curves D and E resulted in $\phi = 3.2$ eV.

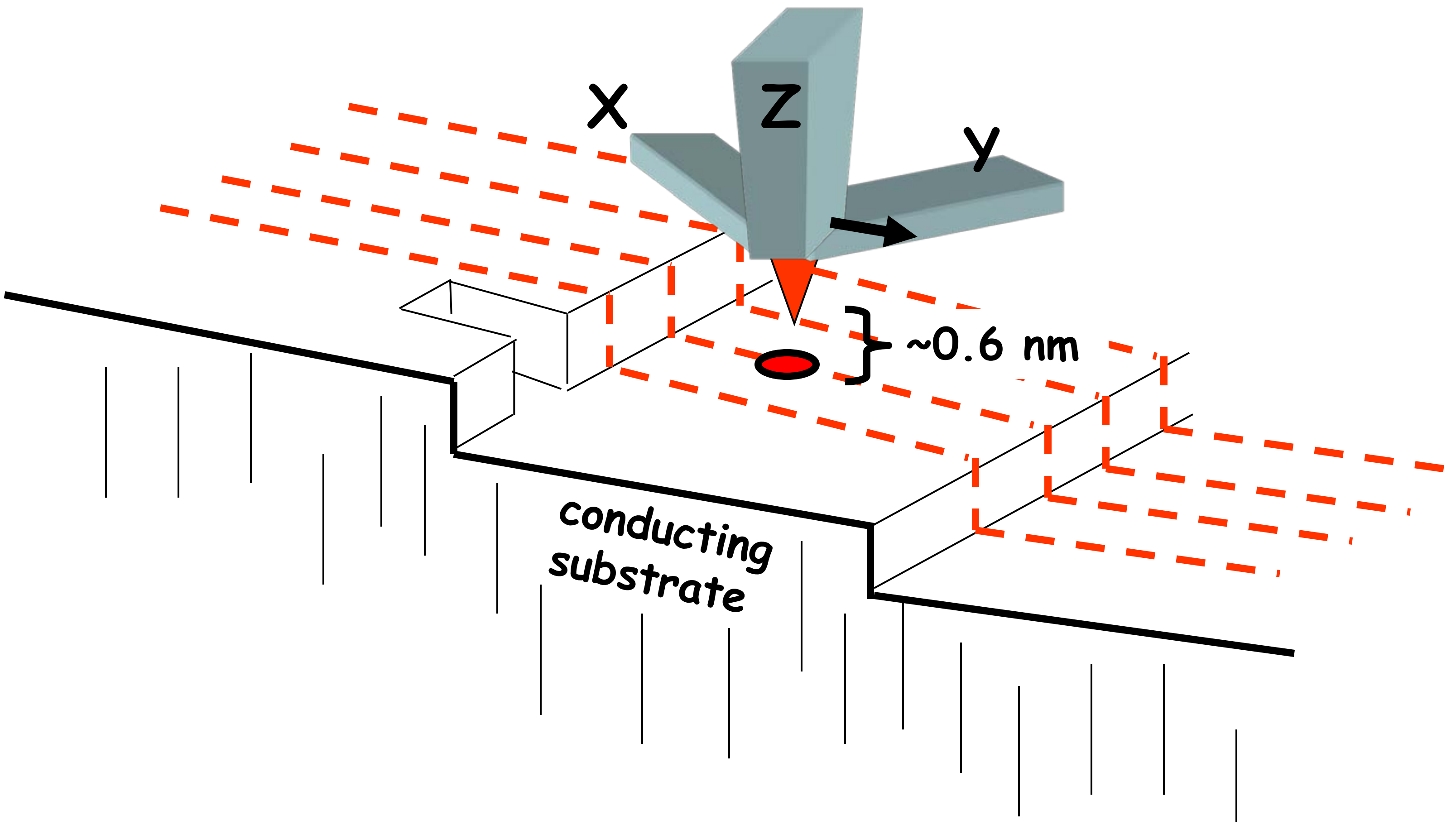
Appl. Phys. Lett., Vol. 40, No. 2, 15 January 1982

Use the tunnel current as a height monitor!



The Scanning Tunneling Microscope

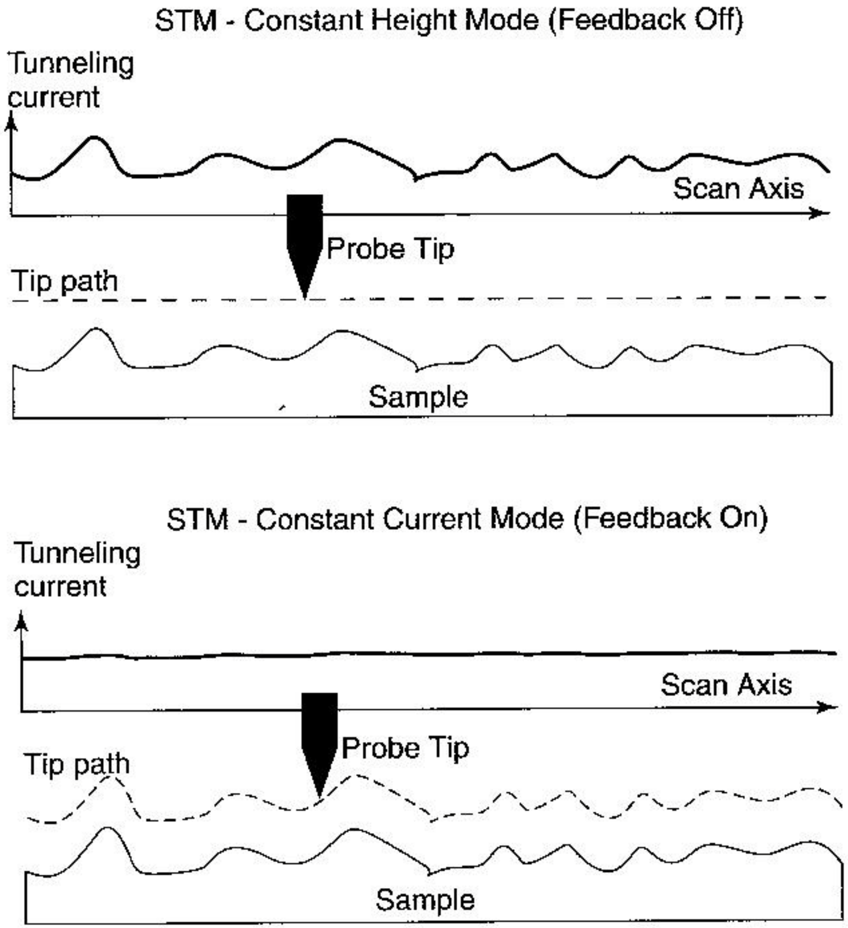
$I(x,y) = e\Delta V \rho(z=0.6\ \mathrm{nm}, x, y; E_F)$



Since gap is tunable, maintain <u>constant</u> current by continuously adjusting tip height.

If tip scanned in controllable way → a microscope!

A z-height microscope!



tip path constant

current constant

Figure 2.18. Constant-height (top sketch) and constant-current (bottom sketch) imaging mod of a scanning tunneling microscope. (From T. Bayburt, J. Carlson, B. Godfrey, M. Shaw Retzlaff, and S. G. Sligar, in *Handbook of Nanostructured Materials and Nanotechnolog* H. S. Nalwa, ed., Academic Press, Boston, 2000, Vol. 5, Chapter 12, p. 641.)