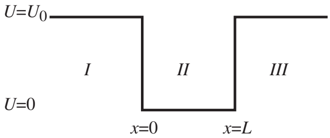
Finite square well (Serway 6.5)

- Region II: particle free to travel.
- Regions I and III: classically forbidden.

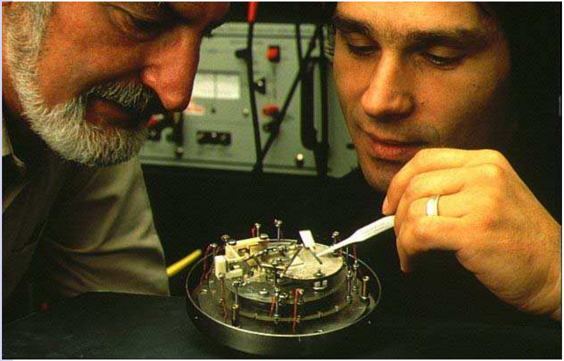


Walking through walls

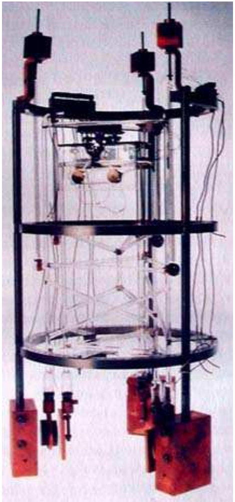
- When $E < U_0$, wavefunction ψ dies off to $1/e$ of its amplitude in a distance δ of $1/\alpha$, or
$$\delta = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(U_0 - E)}} \tag{1}$$
- The probability $\propto \psi^2$ will be attenuated by $\exp[-1] = \exp[-1/2]^2 = e^{-\left(\frac{1}{2}\right)^2} = 0.37$ when we have traveled a tunneling distance x_t of $\delta/2$.
- But perhaps nucleons can escape from the nucleus by tunneling! George Gamow, 1936: explanation for radioactivity. We'll get to this. . .
- Tunneling of an electron over a 5 eV gap:
$$\begin{aligned} x_t &= \frac{\hbar}{2\sqrt{2m(V-E)}} = \frac{1}{2\pi}\frac{hc}{2\sqrt{2mc^2(V-E)}} \\ &= \frac{1}{2\pi}\frac{1240\ \text{eV}\cdot\text{nm}}{2\sqrt{2\cdot 511\times 10^3\ \text{eV}\cdot 5\ \text{eV}}} = 0.044\ \text{nm} \end{aligned}$$
so for every 0.1 nm or 1 Å the current will be reduced by a factor of $\exp[-0.1/0.044] = 0.1$.

The scanning tunneling microscope

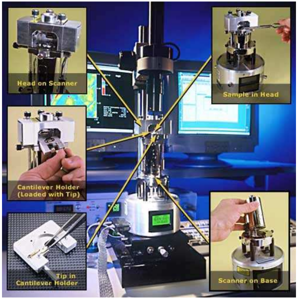
The first STM, with its inventors Heinrich Rohrer (b. 1933) and Gerd Binnig (b. 1947) at the IBM Zurich lab (they won the 1986 Nobel Prize):



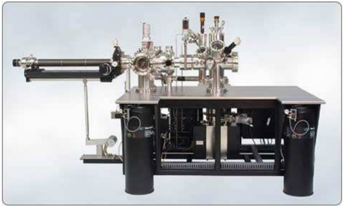
Binning and Rohrer's third STM:



Modern STMs

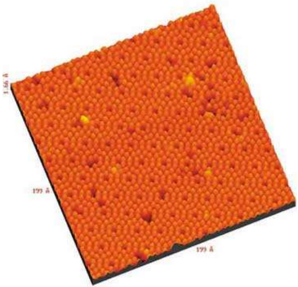


Veeco Instruments: an example of a system that can be run on a desk top.

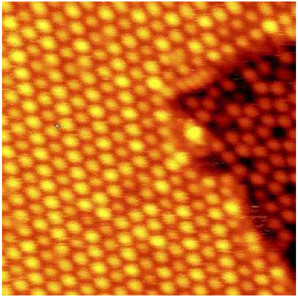


RHK Instruments: an example of an ultra high vacuum system for surface studies.

Example STM images



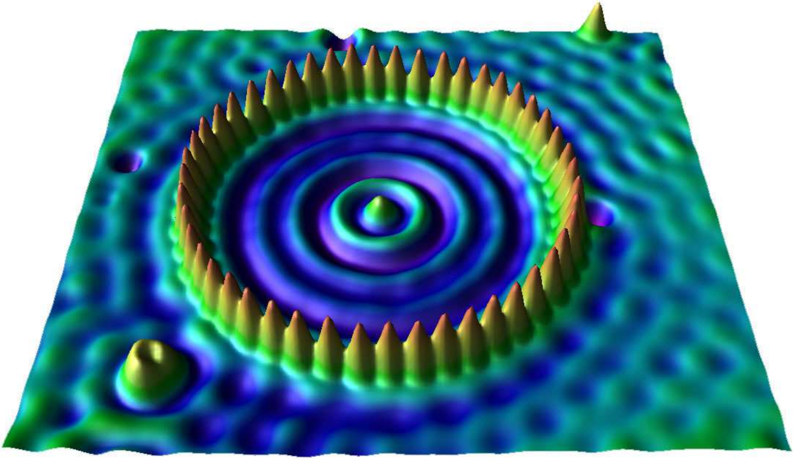
Silicon (111) surface, 7 × 7 reconstruction. Courtesy RHK Instruments.



Iron monolayer making FeSi on Si (111). Courtesy RHK instruments.

The Quantum Corral

Don Eigler's quantum corral:



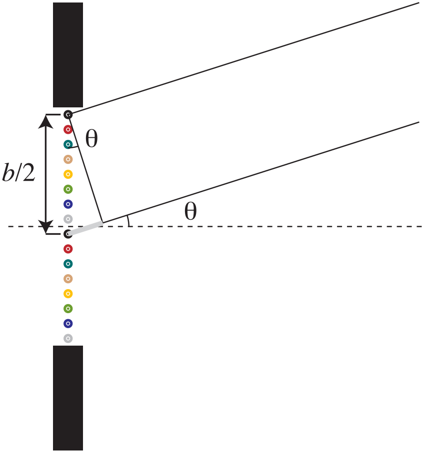
Diffraction from a slit

You've probably seen this construction in your first year physics course. Imagine dividing a slit up into many point sources. You can then pick, two-by-two, point sources that cancel each other when you meet the condition

$$\begin{aligned} \frac{b}{2}\sin\theta &= \frac{\lambda}{2} \\ \sin\theta &= \frac{\lambda}{b} \end{aligned}$$

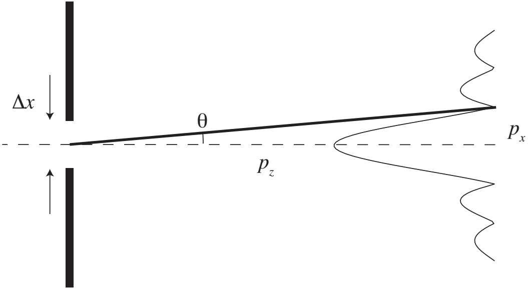
In the small angle approximation, minima are at

$$\theta \simeq \frac{\lambda}{b}$$



Uncertainty and slits

- Consider the act of trying to measure the $\hat{x}$ momentum of a particle passing through a defined position Δx:



- Because the particle is wavelike in its properties, it will be diffracted by the slit with a semi-angle θ of $\sin\theta = \lambda/\Delta x$.
- If the particle had a velocity v_z, we will now have an uncertainty in the $\hat{x}$ velocity of

$$\Delta p_x = p_z \sin\theta = \frac{h}{\lambda}\frac{\lambda}{\Delta x} = \frac{h}{\Delta x}$$

giving $\Delta p_x \Delta x = h$.

Heisenberg uncertainty relationship

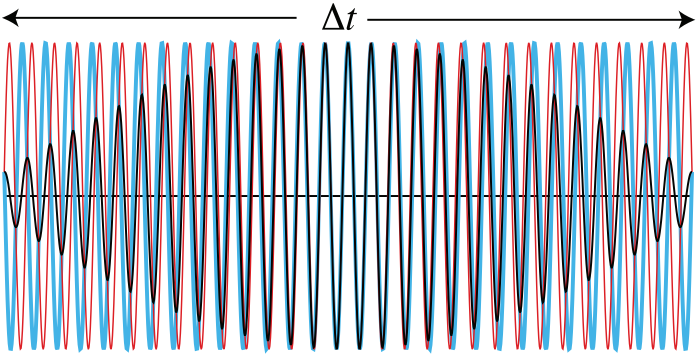
- Our relationship $\Delta p_x\,\Delta x = h$ was for the full slit width and the semi-opening angle. We can usually estimate the centroid a bit more accurately, but we can't be too exact about the fuzziness so there is a bit of wiggle room in the prefactor used! Heisenberg concluded (*cf.* Serway Eq. 5.31):

$$\Delta x\,\Delta p_x \simeq \frac{h}{4\pi} = \frac{\hbar}{2} \tag{2}$$

  in a paper in *Zeitschrift für Physik* **43**, 172–198 (1927).
- So particles in quantum mechanics are like many politicians, or overweight wrestlers: the more you try to pin them down, the squishier they get.
- The act of limiting a particle to a certain position inevitably means that you cannot predict its momentum exactly, and vice versa.

Counting uncertainty

- Let's count wave crests that go by in a time interval Δt.
- If the wave has a period T, we can only count $N = \Delta t/T$ waves.
- Therefore we can really only specify the period to plus or minus a wave, or $\Delta T \simeq T/N$.
- This is sometimes called the Fourier transform limit for reasons you'll see in PHY 300.



Energy-time uncertainty

- Again, we could only count $N = \Delta t/T$ waves.
- We could really only specify the period to plus or minus a wave, or $\Delta T \simeq T/N$.
- The product is

$$\Delta T\,\Delta t \simeq \left(\frac{T}{N}\right)(NT) \simeq T^2 \tag{3}$$

- Next, from $\omega = 2\pi/T$ we get $d\omega = (2\pi/T^2)\,dT$ or

$$\Delta T = \frac{T^2}{2\pi}\,\Delta\omega \tag{4}$$

- Now from Eqs. 3 and 4 we get

$$\begin{aligned} \Delta T\,\Delta t = \frac{T^2}{2\pi}\,\Delta\omega\,\Delta t &= T^2 \\ \Delta\omega\,\Delta t &= 2\pi \\ (\hbar\Delta\omega)\,\Delta t &= \frac{h}{2\pi}\,2\pi \\ \Delta E\,\Delta t &= h \qquad (5) \end{aligned}$$

- Again we can pin the centroid down a bit more so the convention is to say $\Delta E\,\Delta t \simeq \hbar/2$ (*cf.* Serway Eq. 5.34).

Confusion over uncertainty

- It will not fly if you write the following as your total solution to an exam problem: "According to Heisenberg, the answer is uncertain."
- The Heisenberg uncertainty relationship is widely abused. Some postmodernists say it means we can't know anything for certain in life, so all points of view are equally valid. This is a rather sweeping overgeneralization of the observation that matter behaves like de Broglie waves!
- Another overinterpretation is to say that this marks the death of classical physics, in the following argument:
  - With Newtonian mechanics, if we could measure the position and momentum of all particles in the universe, we could predict the future with perfect accuracy.
  - The Heisenberg uncertainty relationship means we can't know both, so we've lost the ability to predict the future (unless, of course, we are astrologers).
- In fact we can't even do it in classical mechanics. There are a great number of situations where a small change in initial conditions produces nonlinear changes in outcomes. These situations are *chaotic*, and they exist in classical mechanics.

Clarity over uncertainty

- So let's limit ourselves to things we can do experiments on, such as electron transitions in atoms. If an excited state has a lifetime of Δt, we can define the energy of its transition only as well as $\Delta E = \hbar / \Delta t$. Short-lifetime states have broad energy/wavelength distributions; long-lifetime states have well-defined energy/wavelength distributions. We can measure this in spectroscopy experiments!
- Another example we'll consider is the confinement of protons and neutrons to the nucleus, where we can gain insight into their momenta p and thus energy from their confinement distance Δx.

Expectation values I

- Imagine having a die (singular of dice): what's the average number you get? Well, it's $(1+2+3+4+5+6)/6 = 21/6 = 3.5$, which sort of makes sense. We can also get this result by constructing a table:

Die value x	1	2	3	4	5	6
Relative probability	1	1	1	1	1	1
Normalized probability $P(x)$	1/6	1/6	1/6	1/6	1/6	1/6

- Maybe if we multiply the thing we are trying to measure, which is x, by the probability $P(x)$ of each value we might get, we can calculate the average value? Let's call the average $\langle x\rangle$:

$$\begin{aligned} \langle x\rangle &= 1\cdot\frac{1}{6}+2\cdot\frac{1}{6}+3\cdot\frac{1}{6}+4\cdot\frac{1}{6}+5\cdot\frac{1}{6}+6\cdot\frac{1}{6} \\ &= (1+2+3+4+5+6)\frac{1}{6} = \frac{21}{6} = 3.5 \end{aligned}$$

Expectation values II

- So it looks like $\langle x\rangle = \int_{-\infty}^{\infty} x\,P(x)\,dx$ is a procedure that makes sense for getting averages (see Serway Eq. 6.31).
- Let's try a slightly less trivial situation, like a loaded die such that it comes up on the number 4 twice as often. What's the average number you get? Well, if we double-count the 4 we have seven possibilities:

Die value x	1	2	3	4	5	6
Relative probability	1	1	1	2	1	1
Normalized probability $P(x)$	1/7	1/7	1/7	2/7	1/7	1/7

- In this case we have

$$\langle x\rangle = 1\cdot\frac{1}{7}+2\cdot\frac{1}{7}+3\cdot\frac{1}{7}+4\cdot\frac{2}{7}+5\cdot\frac{1}{7}+6\cdot\frac{1}{7} = (1+2+3+8+5+6)\frac{1}{7} = 3.57$$

which sounds plausible.

Expectation values III

What if we want to measure the average value of x^2? Well, we could just multiply each of the possible values of x^2 by their relative probabilities, which would look like

Die value squared x^2	1	4	9	16	25	36
Relative probability	1	1	1	2	1	1
Normalized probability $P(x)$	1/7	1/7	1/7	2/7	1/7	1/7

It looks like we could generalize the procedure for any function of x like $f(x)$—which is x^2 in the above example—to have a rule (see Serway Eq. 6.32)

$$\langle f \rangle = \int_{-\infty}^{\infty} f(x)\, P(x)\, dx \tag{6}$$

Expectation values IV

- Now let's think about some uses for these expectation values. Obviously $\langle x\rangle$ tells us the average value, which we usually like to know.
- But averages don't always tell us the whole story! We could take a lot of precision ball bearings and determine their average diameter, and a collection of pumpkins from a field and determine *their* average diameter. But we know we're missing something in this simple calculation: the degree of uniformity around that average.
- So let's consider the standard deviation σ, which is the square root of the variance σ^2:

$$\sigma = \sqrt{\sigma^2} = \sqrt{\frac{\sum_{i=1}^{N}(x_i-\bar{x})^2}{N}} = \sqrt{\frac{\sum(x_i-\langle x\rangle)^2}{N}} \qquad (7)$$

- Why look at the square of the difference of each particular measurement x_i from the average $\bar{x}$? Because the average of the differences without squaring is zero; it's how we determine the average in the first place!

$$\bar{x} = \langle x\rangle = \frac{\sum x_i}{N} \qquad (8)$$

Expectation values V

- By the way, we're supposed to have $N-1$ in the denominator of Eq. 7 because it's only with $N=2$ measurements that we can see some variance. . .
- Let's expand out the calculation of the variance σ^2 using Eqs. 7 and 8:

$$\begin{aligned} \frac{\sum (x_i - \langle x \rangle)^2}{N} &= \frac{\sum (x_i)^2}{N} - 2(\langle x \rangle)\frac{\sum (x_i)}{N} + (\langle x \rangle)^2 \sum \frac{1}{N} \qquad (9) \\ &= \langle x^2 \rangle - 2(\langle x \rangle)(\langle x \rangle) + (\langle x \rangle)^2 = \langle x^2 \rangle - (\langle x \rangle)^2 \end{aligned}$$

so that the standard deviation is (Serway Eq. 6.34)

$$\sigma = \sqrt{\sigma^2} = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \qquad (10)$$

- What has this given us? A way to measure not only the average position of a particle in a particular quantum state, but also the width of its distribution.

Relates to uncertainty principle!

- The particle is no longer confined to being purely inside the box, even though classically it would be! The particle can “leak” some distance out of the box. Consider an electron with $(U_0 - E) = 1$ eV:

$$x_t = \frac{\delta}{2} = \frac{\hbar}{2\sqrt{2m(U_0 - E)}} = \frac{hc}{4\pi\sqrt{2mc^2(U_0 - E)}} \Rightarrow 0.09 \text{ nm.}$$

  or about the radius of one atom.

- We can compare this leakage distance with the de Broglie wavelength for a particle with an energy $E_\lambda = (U_0 - E)$:

$$\lambda = \frac{h}{p} = \frac{2\pi\hbar}{\sqrt{2mE_\lambda}} \qquad \text{leading to} \qquad x_t = \frac{\lambda}{4\pi}.$$

  This helps us (in a hand-waving way) to understand why the Heisenberg uncertainty principle is $(\Delta x)\cdot(\Delta p) = \hbar/2$ rather than $\hbar$.