

The Bohr model

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- Thomson and Millikan: discovery of the electron, its ratio q/m , and then its charge q . “Classical” radius: $r_e = 2.82 \times 10^{-15}$ m.
- Rutherford: all of an atom’s positive charge is in a very small nucleus, with $r \simeq 10^{-14}$ m.
- Bohr model (1913):
 - Rearrange centripetal=electrostatic force to find constants at atomic length scale, in expression with angular momentum.
 - Angular momentum ℓ is in units of Planck’s constant h .
 - Postulate $\ell = n\hbar$ with $\hbar = h/2\pi$.
 - Fantastic agreement with hydrogen spectra, and good agreement with Moseley’s law and the Franck-Hertz experiment!

$$r = \frac{n^2}{Z} a_0 \text{ with } a_0 = 0.053 \text{ nm} \quad (1)$$

$$E = -\frac{Z^2}{n^2} E_0 \text{ with } E_0 = 13.60 \text{ eV} \quad (2)$$

Bohr model: problems

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- The Bohr model is fantastically successful predicting the energies of 1-electron atoms and ions!
- It becomes less and less accurate when you take into account more and more electrons.
 - Bohr and others extend it: parabolic orbits, etc. . . But still not fully successful.
- By the mid-1920s, it is clear that while the Bohr model provides important insights, it is not complete and fully correct.
- The meaning of the Bohr model is also mysterious. *Why* is it that $\ell = n\hbar$?
- In 1924, Louis de Broglie provides an explanation: $\lambda = h/p$, so $\ell = n\hbar$ describes standing waves.
 - Wavelike nature of matter confirmed by Davisson and Germer in 1927.

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It all began when Volkswagen introduced the Quantum in the US market in 1982. Somebody needed to repair the things! Here's one that was for sale on EBay that *really* needed a Quantum mechanic:



Well. . . the *real* birth of quantum mechanics

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Max Born, “Quantum mechanics,” *Zs. f Phys.* **26**, 379–395 (1924); paper received June 13:

This paper contains an attempt to make a first step towards a quantum theory of coupling, which takes into account some of the more important properties of atoms (stability, resonance for transition frequencies, correspondence principle) and which also arises in a natural way from the classical laws. . . What we shall do is to bring the classical laws for the perturbation of a mechanical system, caused by internal couplings or external fields, into one and the same form, which would very strongly suggest the formal passage from classical mechanics to ‘quantum mechanics.’



Max Born
(1882–1970;
Nobel Prize
1954)

That was the labor. Here's the birth

Werner Heisenberg, "Quantum-theoretical reinterpretation of kinematic and mechanical relations," *Zs. Phys.* **33**, 879–893 (1925); received July 29:

It is well known that the formal rules which are used in quantum theory for calculating observable quantities such as the energy of the hydrogen atom may be seriously criticized on the grounds that they contain, as basic element, relationships between quantities that are apparently unobservable in principle, e.g., position and period of revolution of the electron. Thus these rules lack an evident physical foundation, unless one still wants to retain the hope that the hitherto unobservable quantities may later come within the real of experimental determination. This hope might be regarded as justified if the above-mentioned rules were internally consistent and applicable to a clearly defined range of quantum mechanical problems. Experience however shows that only the hydrogen atom and its Stark effect are amenable to treatment by these formal rules of quantum theory.

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Heisenberg's approach

- Treat electron states as harmonic oscillators with some friction and some anharmonicity. This will make more sense after you take PHY 303. . .
- From the [AIP history site](#):

Heisenberg looked first at the connection between the observable properties of the emitted light—its color (frequency) and the intensity—and the motion of the charged ball according to the classical mechanics of Newton. Then he considered the quantum properties of the observed light and reinterpreted the classical formulas for the motion in order to give the observed frequencies and intensities. This resulted in an unfamiliar rule for multiplying two amplitudes of the oscillation in order to obtain an intensity; normal multiplication gave the wrong result.

- Heisenberg's conclusion for position q and momentum p :

$$\sum_k p(n, k)q(k, n) - q(n, k)p(k, n) = -i\hbar \quad (3)$$

Heisenberg's matrix mechanics

- Max Born and Pascual Jordan, “On Quantum Mechanics,” *Zs. f. Phys.* **34**, 858–888 (1925); received Sep. 27:

The recently published theoretical approach of Heisenberg is here developed into a systematic theory of quantum mechanics (in the first place for systems having one degree of freedom) with the aid of mathematical matrix methods.

The package is really wrapped up in what is now called the “Driemännerarbeit” (work of three men) paper: Max Born, Werner Heisenberg, and Pascual Jordan, “On Quantum Mechanics II,” *Z. Phys.* **35**, 557–615 (1926); received Nov. 16, 1925.

- Using these matrix methods, Bohr's results for the spectrum of the hydrogen atom are reproduced, and by two people independently!
 - W. Pauli, Jr., “On the hydrogen spectrum from the standpoint of the new quantum mechanics,” *Zs. f. Phys.* **36**, 336–363 (1926); received Jan. 17.
 - P.A.M. Dirac, “Quantum mechanics and a preliminary investigation of the hydrogen atom,” *Proc. Roy. Soc. A* **110**, 561–569 (1926); received Jan. 22.

The idea of the matrix equations

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Matrix equation for non-commuting operators between momentum p and position q :

$$\begin{pmatrix} p(1,1) & \dots & p(1,k) \\ \vdots & & \vdots \\ p(n,1) & \dots & p(n,k) \end{pmatrix} \times \begin{pmatrix} q(1,1) & \dots & q(1,n) \\ \vdots & & \vdots \\ q(k,1) & \dots & q(k,n) \end{pmatrix} -$$
$$\begin{pmatrix} q(1,1) & \dots & q(1,k) \\ \vdots & & \vdots \\ q(n,1) & \dots & q(n,k) \end{pmatrix} \times \begin{pmatrix} p(1,1) & \dots & p(1,n) \\ \vdots & & \vdots \\ p(k,1) & \dots & p(k,n) \end{pmatrix} =$$

$$PQ - QP = -i\hbar$$

In 1926, Heisenberg realized that this carried the consequence of the uncertainty principle, but we'll get to that in a bit.

Meanwhile...

- Meanwhile de Broglie's 1924 PhD thesis with $\lambda = h/p$ is getting noticed. Hector-Lois Langevin passes a copy to Victor Henri with the suggestion that it go to Erwin Schrödinger in Zurich.
- Henri did not understand de Broglie's thesis, but gave it to Schrödinger. After two weeks, Schrödinger returned it, saying "That's rubbish!"
- Langevin hears of this, and tells Henri "I think that Schrödinger is wrong; he must look at it again."
- Peter Debye, head of the Zurich institute, asks Schrödinger to lead a discussion of de Broglie's thesis. Now that he is forced to look at it more carefully, he becomes enthusiastic.
- Debye remarks that if anything is ever going to come of it someone would need to write down a wave equation for matter, but how can that be?



Erwin
Schrödinger
(1887–
1961;
Nobel
Prize 1933)

Complex algebra for wave equations

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- Let $\psi = Ae^{i\varphi}$. A represents the magnitude, and φ represents the phase. Euler's equation:

$$Ae^{i\varphi} = A(\cos \varphi + i \sin \varphi)$$

- Intensity is $|\psi|^2 = \psi^\dagger \psi = A^2$
- Phase lets us keep track of whether we're at the max, zero, or min of the wavefield. [Look at the movie.](#)

Schrödinger's approach

- Schrödinger took two things along to Arosa in the Swiss Alps over his Christmas holiday in 1925:

- ① a mistress (it's not clear which one; for some years later on a mistress shared the house with his wife);
- ② thoughts of matter wave equations.

By the time he returned to Zurich in January 1926, he had a solution.

- Particles travel in straight lines so we expect matter to have a plane wave solution:

$$\psi(x, t) = \psi_0 e^{-i(\vec{k} \cdot \vec{x} - \omega t)}. \quad (4)$$

- If we take $\partial^2/\partial x^2$ we obtain

$$\frac{\partial^2 \psi}{\partial x^2} = \psi_0 e^{i\omega t} (-ik)^2 e^{-ikx} = -k^2 \psi_0 e^{-i(kx - \omega t)} = -k^2 \psi. \quad (5)$$

- Now $k \equiv 2\pi/\lambda$ is intrinsic to our choice of a plane wave solution. However, from de Broglie we have $\lambda = h/p$. Therefore,

$$k^2 = \left(\frac{2\pi}{\lambda}\right)^2 = p^2 \hbar^2. \quad (6)$$

Schrödinger's approach II

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- Note that $p^2/(2m)$ describes the kinetic energy of a nonrelativistic particle; we will denote kinetic energy as being the total energy E minus the potential energy U . We therefore have

$$k^2 = \frac{2m}{\hbar^2} \frac{p^2}{2m} = \frac{2m}{\hbar^2} (E - U). \quad (7)$$

- Inserting this into Eq. 5, we have (Krane Eq. 5.3)

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 \psi = -\frac{2m}{\hbar^2} (E - U) \psi \quad \text{or} \quad -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U \psi = E \psi \quad (8)$$

as the nonrelativistic, time-independent equation for a particle wave.

Schrödinger's approach III

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- Again, Eq. 8 gives

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U\psi = E\psi.$$

- Time derivative of the plane wave solution is

$$\frac{\partial \psi}{\partial t} = \psi_0 e^{-ikx} (i\omega) \frac{\partial}{\partial t} e^{i\omega t} = (i\omega)\psi. \quad (9)$$

Multiplying both sides by $-i\hbar$ gives

$$-i\hbar \frac{\partial \psi}{\partial t} = \hbar\omega\psi = E\psi, \quad (10)$$

where we have assumed $E = \hbar\omega$ for the energy of matter waves just as with photons.

- Now rewrite Eq. 8 as

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U\psi = -i\hbar \frac{\partial \psi}{\partial t}. \quad (11)$$

... and break out singing Handel's Hallelujah Chorus!

But what's waving?

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- We have a wave equation. What's waving? We will consider the hydrogen atom a few lectures for now. Suffice it to say that what we get are the orbitals you have probably already seen glimpses of.
- But that means the electron is really smeared out? Not consistent with small classical radius or other electromagnetic phenomena.
- So does the wave equation describe the particle, or something about the particle?

Heisenberg and Schrödinger

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- Heisenberg, writing to Wolfgang Pauli in 1926:

The more I think about the physical portion of Schrödinger's theory, the more repulsive I find it. . . What Schrödinger writes about the visualizability of his theory 'is probably not quite right'; in other words, it's crap.

- Schrödinger's perspective:

I knew of [Heisenberg's] theory, of course, but I felt discouraged, not to say repelled, by the methods of transcendental algebra, which appeared difficult to me, and by the lack of visualizability.

- Yet in May 1926 Schrödinger publishes a paper showing the equivalence of his wave mechanics with Heisenberg's operator theory. Schrödinger visits Heisenberg at Bohr's Institute in October 1926; vigorous discussions. . .

Particle in a box

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- Consider a particle in an infinite box.
- Let $U(x) = 0$ for $0 \leq x \leq L$ and $U \rightarrow \infty$ elsewhere.
- Looking at Eq. 8, we would have to have $E \rightarrow \infty$ to produce a wave that could satisfy $-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U\psi = E\psi$. Therefore $\psi = 0$ outside of box.
- Wave should be continuous, so it must be zero at the boundaries $x = 0$ and $x = L$. A sine function does this at $x = 0$, and also at $x = L$ if we require $kL = n\pi$. We therefore guess that the solution has the form $\psi = A \sin\left(\frac{n\pi x}{L}\right)$.

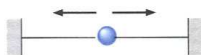
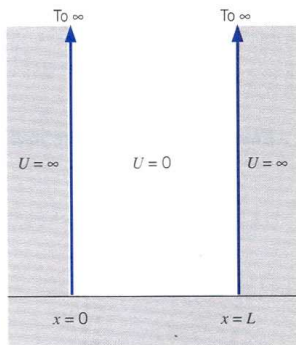


FIGURE 5.4 A particle moves freely in the one-dimensional region $0 \leq x \leq L$, but is excluded completely from $x < 0$ and $x > L$.

Particle in a box II

- Again, we have $U(x) = 0$ for $0 \leq x \leq L$ and $U \rightarrow \infty$ elsewhere.
- We guess $\psi = A \sin\left(\frac{n\pi x}{L}\right)$ with $kL = n\pi$.
- Inside the box with $U = 0$ we have

$$-\frac{\hbar^2}{2m} \frac{d}{dx} \left(\frac{d}{dx} A \sin\left(\frac{n\pi x}{L}\right) \right) = \frac{\hbar^2}{2m} \left(\frac{n\pi}{L}\right)^2 A \sin\left(\frac{n\pi x}{L}\right)$$

Putting this in the Schrödinger equation gives

$$\frac{\hbar^2}{2m} \left(\frac{n\pi}{L}\right)^2 A \sin\left(\frac{n\pi x}{L}\right) = E A \sin\left(\frac{n\pi x}{L}\right) \quad (12)$$

- Eq. 12 works only if we meet the following condition:

$$E_n = \frac{\hbar^2 \pi^2}{2mL^2} n^2. \quad (13)$$

That is, we can satisfy the Schrödinger equation only if we have discrete energy states! Recall the Bohr model? $E_n = -E_0 Z^2 / n^2$.

So... What's waving?

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- So we can solve for ψ in a simple example (and we'll soon do less simple examples).
- We can get the energies of quantum states.
- But what's waving? And how do we figure out the value of A in $\psi = A \sin(\frac{n\pi x}{L})$?
- Again, think of what

Heisenberg wrote to Wolfgang Pauli in 1926:

The more I think about the physical portion of Schrödinger's theory, the more repulsive I find it... What Schrödinger writes about the visualizability of his theory 'is probably not quite right'; in other words, it's crap.



What's waving? Electron waves!

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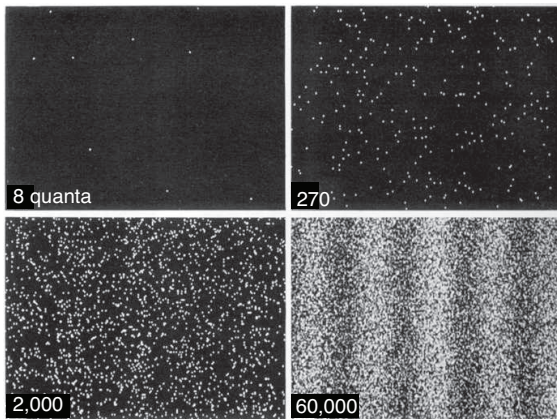
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From A. Tonomura, *Electron Holography* (Springer-Verlag, 1993), p. 14.

Born/Copenhagen interpretation

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- See Serway Sec. 6.1. The most commonly accepted interpretation arose from the work of Max Born, and also discussions in Niels Bohr's institute in Copenhagen.
- Matter waves ψ describe not the particle, but its probability amplitude.
- $\psi^\dagger\psi = |\psi|^2$ represents the probability. Therefore we realize that $\int |\psi|^2$ should be normalized to 1.



Max Born (1882–
1970; Nobel
Prize 1954)

Light and matter

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Property	Light	QM
Amplitude $\psi = Ae^{-i(kx-\omega t)}$	Electric field $E = \psi$	Probability amplitude ψ
Amplitude squared $ \psi ^2 = \psi^\dagger \psi$	Electric field squared gives irradiance (from the Poynting vector in classical E&M): $I = \sqrt{\epsilon/\mu} \langle E \rangle^2$.	Probability amplitude squared $ \psi ^2$ gives probability distribution.
Particle arrival	Individual photons arrive at particular locations, but with a probability given by the wave theory calculation of the irradiance $I \propto \psi ^2$.	Individual matter particles arrive at particular locations, but with a probability given by the wave theory calculation of the probability $ \psi ^2$.

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“One can even set up quite ridiculous cases. A cat is penned up in a steel chamber, along with the following device (which must be secured against direct interference by the cat): in a Geiger counter there is a tiny bit of radioactive substance, so small, that perhaps in the course of the hour one of the atoms decays, but also, with equal probability, perhaps none; if it happens, the counter tube discharges and through a relay releases a hammer which shatters a small flask of hydrocyanic acid. If one has left this entire system to itself for an hour, one would say that the cat still lives if meanwhile no atom has decayed. The ψ -function of the entire system would express this by having in it the living and dead cat (pardon the expression) mixed or smeared out in equal parts.”

Naturwiss. **23**, 807 (1935)

