PHYSICS TODAY.org



Member logoff

For a limited time, OriginLab is offering a 10-user Lab License for \$750. Offer expires on September 30, 2005. Please call for details.

<u>Welcome!</u> <u>Herbert</u>



Search

advanced search

Table of contents Past issues

Links to advertisers Products advertised Place an ad Buyers' guide

About us Contact us Submit press release

American Institute of Physics

The Industrial Physicist Computing in Science & Engineering Journals Virtual Journals

Articles

The Early History of Quantum Tunneling

Access profile

Molecular spectra, electron emission from metals, and alpha decay provided fertile ground in the 1920s for applying the new ideas of quantum mechanics.

Eugen Merzbacher

Among all the successes of quantum mechanics as it evolved in the third decade of the 20th century, none was more impressive than the understanding of the tunnel effect--the penetration of matter waves and the transmission of particles through a high potential barrier. Eventually, five Nobel prizes in physics were awarded for research involving tunneling in semiconductors and superconductors and for the invention of scanning tunneling microscopy. Tunneling occurs in all quantum systems. It is crucial for nucleosynthesis in stars, and it may also have played an essential role in the evolution of the early universe. From its beginning, recounted here, quantum tunneling has remained a hot topic, with myriad applications to this day.

In 1923, Louis de Broglie proposed that matter waves have a wavelength inversely proportional to their velocity. It must have been immediately realized that, in a manner analogous to optics, a particle of energy E incident on a region of potential energy V enters a refractive medium characterized by an index of refraction n that varies inversely with the wavelength. It is given by

$$n = \sqrt{\frac{E - V}{E}}.$$
 (1)

Ordinarily, when the particle energy E > V, so that n is real, the medium is dispersive, but in classically inaccessible regions where E < V and the kinetic energy is negative, the index of refraction is imaginary. In optics, the penetration of light through a thin reflecting metallic layer signals an imaginary index of refraction. A related phenomenon, unaccounted for by the laws of geometric optics, is the appearance of an evanescent light wave accompanying total internal reflection at the interface of two transparent media. In the less dense medium, the normal component of the propagation vector is imaginary, and the wave amplitude is exponential rather than oscillatory. If a second medium of higher refractive index is within range of the evanescent wave, an attenuated portion of the incident wave can be transmitted (a phenomenon termed frustrated total internal reflection).

In analogy with light waves, matter waves presumably would also penetrate and be transmitted through classically forbidden regions, albeit with attenuated amplitude. A quantitative analysis of the physical implications of this tunneling effect had to await Erwin Schrödinger's wave mechanics and Max Born's probability Also this month Sinks for Anthropogenic Carbon Superconducting Magnets above 20 Tesla The Early History

of Quantum

Tunneling

Request product info

COMPANY SPOTLIGHT



PHYSICS TODAY



- 85,000 unique visitors/month
- 400,000 page views/month

Find out more.



interpretation of the quantum wavefunction. Transmission of particles through a potential barrier of finite height and width is less easily visualized in the Heisenberg-Bohr formulation of quantum mechanics, which speaks of particles going over the top of the barrier with transient violation of conservation of energy. In both formulations, the language that permeates most descriptions of quantum transmission through a potential barrier has the anachronistic ring of Newtonian mechanics, with its underlying assumption that a particle always moves in a continuous orbit.

By 1927, quantum mechanics was in place, and a new generation of theoretical physicists went to work on its many applications in the microscopic domain, from condensed matter to nuclear physics. The history of the early days of the tunnel effect is set in a few centers of theoretical physics--Göttingen, Leipzig, and Berlin, Germany; Copenhagen, Denmark; Cambridge, both England and Massachusetts; Princeton, New Jersey; and Pasadena, California--with most of the active participants in their twenties or early thirties. Before tunneling became the standard term for the nonclassical transmission of particles through a potential barrier, ¹ the quantum mechanical process, either in German or English, was often referred to as penetration of, or leaking through, a barrier (or sometimes a potential hill).

Tunneling in atoms and molecules

Friedrich Hund (1896-1997) was the first to make use of quantum mechanical barrier penetration in discussing the theory of molecular spectra in a series of papers in 1927. The first of these² was submitted from Copenhagen in November 1926, acknowledging encouragement from Niels Bohr and Werner Heisenberg and support from the International Education Board (IEB), founded in 1923 by John Rockefeller Jr. The paper deals with an outer electron



<u>Figure 1</u>

(*Leuchtelektron*, or luminous electron, in Hund's words) moving in an atomic potential with two or more minima separated by classically impenetrable barriers (*Schwellen*, that is, sills or ridges). As illustrated in figure 1, Hund was primarily concerned with characterizing the electronic energy eigenfunctions in terms of the quantum numbers for the limiting cases of united and widely separated atoms, as the distance between the atoms is changed adiabatically from zero to infinity. He explained the sharing of an electron between the atoms represented by the potential wells--so fundamental for an understanding of covalent chemical binding-and discussed the distinction between classical orbits and quantum mechanical wavefunctions.

The third paper of Hund's series on molecular spectra³ was completed in Copenhagen and submitted from Göttingen in May 1927. Hund assumed the separability of the electronic motion from the vibration and rotation of the atoms, an approximation later made quantitative by Born and Robert Oppenheimer. He discussed the dynamics of the constituent atoms of a molecule and noted the omnipresence of reflection-symmetric potentials with classically impenetrable barriers. As shown in Hund's first paper, the stationary states for such potentials are even (symmetric) or odd (antisymmetric) functions of the relative coordinates that link the particles. The superposition of the even ground state and the odd first excited state (labeled *o* and *1* in figure 1b) yields a nonstationary state that shuttles back and forth, or tunnels, from one classical equilibrium position to the other. The beat period or reciprocal tunneling rate, *T*, is approximately given by 400,000 impressions/month--no production required! \$500/month. visit us online

Help the physics community displaced by Katrina:

<u>Katrina Affected</u> <u>Physics and</u> <u>Astronomy</u> <u>Community Bulletin</u> <u>Board</u>

U.S. Department of Energy Temporary Educational Matching Program

$$\frac{T}{\tau} \approx \sqrt{\frac{h\nu}{V}} \exp{\frac{V}{h\nu}}.$$
 (2)

Here t = 1/n is the period of oscillation in one of the harmonic potential wells when the atoms are far apart, and *V* is the height of the barrier between the wells. The exponential dominates the beat period; its argument, *V*/*h*n, approximately equals the product of the width of the potential barrier (or the interatomic distance) and the effective wavenumber for penetration into the classically forbidden region, $k = (2mV)^{1/2}/\frac{\pi}{2}$.



Assuming a typical infrared vibration period of $t = {}^{1}/{}_{3}$ ${}^{-10}$ s, Hund tabulated the beat or shuttling period *T* for a range of values of *V*/*h*n and displayed its extreme sensitivity to relatively small variations in the barrier height (see figure 2). He showed that transitions between chiral isomers--optically active left-

handed and right-handed molecular configurations--are extraordinarily slow and improbable for biological molecules, a conclusion that he found reassuring. (In contrast, the ammonia molecule is an example of a system for which T is comparable to t, and the beats are observable: The molecule's inversion spectrum falls in the microwave region.)

Tunneling into the continuum

While Hund worked out the tunnel effect for a system with only bound states and recognized its relevance for chemical binding and molecular dynamics, he did not consider barrier penetration for unbound states, with continuum energy eigenvalues. The next chapter in the tunneling story had to be the penetration of a barrier in the energy continuum. In 1927, in Cambridge, England, Lothar Nordheim (1899-1985) published a paper on the thermionic emission of electrons from a heated metal and the reflection of electrons from metals.⁴ Also assisted by IEB funding and acknowledging Ralph Fowler (1889-1944), Nordheim applied wave mechanics to Arnold Sommerfeld's electron theory of metals, which assumes an ideal Fermi gas for the electrons. He calculated the electron wavefunction across a steep potential rise or drop--a model for the surface barrier that confines electrons within a metal--and showed that, for particle energies near the top of the barrier, either reflection or transmission can occur with finite probabilities, although classically there would be only one or the other. The models he used for the potential U are all rectangular, composed of sections of constant height as sketched in figure 3. Nordheim's analysis is nowadays found in every quantum mechanics textbook. He estimated that, for energies in the electron volt range, the transmissivity for a thin barrier is negligible unless the barrier is no more than a few atoms thick, and he therefore thought that tunneling would be of little physical importance. However, he and Fowler soon realized that the emission of electrons from a metal in a strong electric field could be understood as a consequence of barrier penetration.

In the meantime, Oppenheimer (1904-67) published in *The Physical Review* of January 1928 a lengthy and important paper, submitted in August 1927 while he was a National Research Fellow at Harvard University, that notably



lacked any figures and acknowledgments.⁵ Using an early version of Paul Dirac's bra-ket

<u>Figure 3</u>

notation and delta-function normalization for the continuum energy eigenfunctions, Oppenheimer combined in his article three different topics, all related to the continuous portion of the energy spectrum of hydrogen (also called *aperiodic* orbits or states, as a reminder of their character in classical mechanics).

In the third section of the paper, Oppenheimer dealt with the ionization produced by exposing the electron in a hydrogen atom to a uniform electrostatic field (that is, a linear voltage drop). Following Dirac's lead, Oppenheimer developed a version of timedependent perturbation theory, including what we now call Fermi's Golden Rule for transition rates, and calculated perturbation matrix elements between discrete energy eigenstates of the unperturbed hydrogen atom and the continuum energy eigenstates of an electron in a linear potential. The continuum wavefunctions have analytic expressions in the form of Bessel or Hankel functions of fractional order, all well known from George Watson's famous mathematical treatise.⁶ Even if the energy is below the maximum of the potential energy curve, the matrix elements are nonzero, because the wavefunctions overlap in the classically inaccessible region. Rather than speaking of tunneling or barrier penetration, Oppenheimer used the phraseology of perturbation theory, with its transitions between stationary states.

Oppenheimer's discussion of the physics is sophisticated and provides a three-dimensional treatment instead of a onedimensional approximation. However, he expanded the wavefunction of the system in terms of linearly dependent unperturbed energy eigenfunctions, which thus raises questions about his interpretation of the expansion coefficients as probability amplitudes. Still, after many computational approximations, he arrived at a transition rate that has the correct exponential dependence on the electron energy and the barrier parameters, in qualitative agreement with the available results of measurements. In a short communication submitted to the *Proceedings of the National Academy of Sciences* on 28 March 1928 from Caltech, Oppenheimer applied his calculations to Robert Millikan's experiments on field emission from cold (that is, unheated) metals.^Z



Also in March 1928, Fowler and Nordheim submitted their paper on electron emission in intense electric fields to the *Proceedings of the Royal Society*.⁸ Referring to Oppenheimer's work, the authors commented that "the calculation can be shorn of irrelevancies and made so much simpler that it is worth while attacking the problem *de novo*."

They gave an exact treatment of the transmission of conduction electrons through a 1D triangular barrier, shown in <u>figure 4</u>, representing the application of a uniform static electric field perpendicular to the plane surface of a conductor. As in equation 2, the rate for transmission through the triangular barrier is controlled by an exponential. In the exponent is the expression

$$-\frac{\sqrt{2m(C-W)}}{\hbar} \times \frac{C-W}{F} \propto \frac{(C-W)^{3/2}}{F}, \quad (3)$$

where *W* is the kinetic energy of the conduction electrons inside the metal, *C* is the height of the potential barrier at the metal surface,

and *F* is the electric force experienced by the emitted electrons. The two factors on the left-hand side are the maximum effective wave number under the barrier and the width of the barrier penetrated by the conduction electrons. The dependence of the cold-emission current on the field strength F/e and on the work function C - W was found to be consistent with experiments. In the absence of a field, there is zero transmission, and the current increases dramatically at high field strengths. Fowler and Nordheim also estimated the effect of including thermionic emission and of more realistic, less abruptly discontinuous potentials. Here they applied Harold Jeffreys's 1924 *pre*-wave mechanics version of the WKB method (sometimes called the JWKB method).

The rotationally induced dissociation of a diatomic molecule from an excited state, observed through the broadening of infrared spectral lines, was first interpreted by Oscar Rice (1903-78) as a manifestation of tunneling from a potential "valley" through a "mountain" into the "plains." In a 1930 paper submitted to *The Physical Review* when he was a National Research Fellow in Leipzig and had consulted with Heisenberg, Felix Bloch, and Hendrik Kramers,⁹ Rice treated the theory of this breakup and stressed the analogy with alpha decay, in which the tunnel effect had scored its greatest triumphs.

Tunneling in nuclei

Roger Stuewer has given a full historical account of George Gamow's theory of alpha decay.¹⁰ Gamow (1904-68) popularized the story in his entertaining memoirs, *My World Line*,¹¹ and we have reports as well from other physicists who witnessed the remarkable events in 1928. Over the years, the history of Gamow's theoretical discovery has become colorfully embellished, because the mischievous Gamow never made it easy to separate fiction from fact. It appears, however, that he almost immediately saw an opportunity for applying quantum mechanics to the nucleus, when, on arriving in Göttingen from the Soviet Union, he read Ernest Rutherford's 1927 article in the *Philosophical Magazine* about the puzzle surrounding Hans Geiger's 1921 experiments on scattering alpha particles from uranium.

The dilemma that Rutherford confronted was stark: Scattering experiments with alpha particles from radioactive thorium C (nowadays known as polonium-212) confirmed the validity of the repulsive Coulomb potential in uranium up to a height of at least 8.57 MeV. On the other hand, uranium-238 was known to emit alpha particles of less than half that energy (4.2 MeV), which posed a conundrum if the particles had to pass over the top of the Coulomb barrier to emerge from the nuclear interior. The tortured theories that had been proposed to account for this paradox vanished almost overnight when Gamow, on 29 July 1928, and, independently, Ronald Gurney (1898-1953) and Edward Condon (1902-74), on the next day, submitted their quantum mechanical explanations based on the tunnel effect. Publishing in the Zeitschrift *für Physik*,¹² Gamow thanked Born for his hospitality in Göttingen, and his friend N. Kotschin for help with some tricky integrals. Gurney and Condon published their first note in *Nature*, ¹³ followed by a longer exposition in *The Physical Review* in February 1929;¹⁴ both papers were sent from Princeton University. A poignant personal account by Condon of Gurney's underappreciated role in proposing the quantum theory of alpha decay was published posthumously.¹⁵ (For more on Condon's own life, see Jessica Wang's article, "Edward Condon and the Cold War Politics of Loyalty," in Physics Today, December 2001, page 35.*)

The new quantum mechanical theories could account for two important features of alpha decay: Because probabilities occur naturally in quantum mechanics, it became easy to understand the observed statistical character of alpha radioactivity, with its constant transition rate (as in the Golden Rule of perturbation theory) and exponential decay; and the theories yielded a functional relationship between the decay rate (or the nuclear half-life) and the energies of the emitted alpha particles that was in semiquantitative agreement with experiment.

The three theoreticians who solved the puzzle posed by radioactive alpha-particle emission at surprisingly low energies were familiar with the earlier work of Oppenheimer, Nordheim, and Fowler, and patterned their calculations on those models. Gurney and Condon also cited Hund's work as a precursor. They even carried out a calculation now well known to students of quantum mechanics: If a particle is in the ground state of a harmonic oscillator potential, what is the probability of finding it outside the classically allowed region? (Answer: 15.7%.)

Gurney and Condon as well as Gamow recognized that a stationary state with sharp energy, as in bound-state problems or in the time-independent method for calculating scattering cross sections, is inadequate to predict the decay process. The continuity equation for the probability density r and the current density **j**,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0, \qquad (4)$$

does not permit a stationary state to represent a current of particles that is only outgoing from an interior region. Yet the three authors also understood that the smallness of the decay constant compared with the nuclear energies implies a very small current and an alpha-particle state that is *nearly* stationary. They



<u>Figure 5</u>

all drew on the experience with simple rectangular 1D potential barriers, such as in <u>figure 5</u>, for which exact results for transmission rates could be obtained.



In the nuclear case, the strong attractive forces inside the nucleus-still of mysterious origin in 1928-and the external Coulomb repulsion combine to form the potential barrier. Sketched in <u>figure 6</u>, this barrier was, of course, quite unlike a rectangular barrier or even the triangular barrier of <u>figure 4</u> used for field emission, and the calculation had to be appropriately modified. The critically important

exponent in the formula for the transmission coefficient was expressed as the phase (or action) integral in units of Planck's constant,

$$\frac{1}{\hbar} \int_{r_1}^{r_2} \sqrt{2m \left[V(r) - E \right]} \, \mathrm{d}r \,, \quad (5)$$

where the limits r_1 and r_2 are the inner and outer classical turning points for an alpha particle with energy *E*. The integral was an obvious generalization of Hund's formula and of Nordheim's result for a rectangular barrier, but it also had a more rigorous justification in the theory of the WKB approximation, familiar to the theorists from Gregor Wentzel's 1926 paper.¹⁶ Gurney and Condon evaluated the integral graphically, but Gamow--although averse to complex mathematical analysis--produced an excellent analytic approximation. The resulting formula for the transmission coefficient, or barrier penetrability,

$$\exp\left(-\frac{2\pi Z_1 Z_2 e^2}{hv}\right) \equiv e^{-2G} \qquad (6)$$

for a particle of charge $Z_1 e$ emitted with final velocity v from a nucleus of atomic number Z_2 , defines the Gamow factor G.

The alpha decay rate 1 is proportional to the exponential function e^{-2G} , with a prefactor that depends on the alpha-particle wavefunction inside the nucleus and has only a minor influence on the energy dependence of the decay rate. As shown in figure 7, the tunneling theories of 1928 reproduced remarkably well the empirical relationship, established





by Geiger and John Nuttall in 1912, between the decay rate and the energy of the emitted alpha particle, and at last provided firm evidence for the validity of quantum mechanics in the nuclear domain.

Many theoretical derivations of alpha decay have subsequently found their way into the literature. Most assume that the alpha particle is somehow preformed inside the nucleus and can be treated as existing in a nearly bound state before being emitted. The methods used can be sorted into a few categories:

- With his strong physical intuition, Gamow assumed a quasistationary state solution of the Schrödinger equation; he allowed for a small imaginary contribution to the energy and a correspondingly small source term in the continuity equation that expresses conservation of probability. That strategy gave a good approximation for the decay rate. As a solution of the time-dependent Schrödinger equation, the quasi-stationary and nearly bound decaying state represents a wavepacket that models the decay process.
- Gurney and Condon applied a less consistently quantum mechanical treatment to the problem. They reasoned that in the classically accessible regions--inside the nucleus and outside the barrier--the alpha particle could be supposed to perform periodic and aperiodic classical motions, respectively, although the discrete energy of the nearly bound alpha-particle state should in principle be determined by quantum mechanics. In their first announcement in *Nature*, Gurney and Condon concluded, "Much has been written of the explosive violence with which the a-particle is hurled from its place in the nucleus. But from the process pictured above, one would rather say that the a-particle slips away almost unnoticed."
- A fundamentally more consistent method is to construct a wavepacket that is initially confined to the inside of the nucleus. This nonstationary state is a superposition of a narrow band of truly stationary states, with energies centered around an almost discrete quasi-bound state and extending over a narrow range of energies with width of order $G = \frac{1}{2}$. As time progresses, the stationary states that make up this wavepacket interfere to produce precisely Gamow's decaying

state, with a wavefront that spreads out from the nucleus. It was soon realized that the decay can also be pictured as the final stage in the scattering of a sharply defined wavepacket with a mean energy that corresponds to a narrow, and thus long-lived, resonance.

• As an alternate approach, it is natural to apply a version of first-order time-dependent perturbation theory to the problem. This treatment is akin to Oppenheimer's theory of field ionization of an atom and thus subject to the same criticism. Born developed the theory along these lines in 1929, regarding the decay as a transition between a discrete stationary state and a set of continuum states.¹⁷ The characteristic exponential energy dependence of the decay rate arises in this theory from the transition matrix elements between stationary-state eigenfunctions that extend into the classically forbidden region and overlap there.

In summary, quantum mechanics explains alpha decay as a resonance phenomenon, represented by wavefunctions with large amplitude inside and small amplitude outside the nucleus. Between the sharp, narrow resonances lie extended energy regions that correspond to an exponential attenuation of the external wavefunction continued smoothly under the potential barrier. At those energies, alpha-particle scattering is essentially Coulombic without significant modification by the nuclear forces.

Before the advent of quantum mechanics, Rutherford had devised an ad hoc explanation for the emission of alpha particles from heavy nuclei based on the assumption that two electrons could attach themselves to a helium nucleus and then get stripped off once the particle has passed out of the parent nucleus. In a similar vein, the cold emission of electrons from metal surfaces exposed to an electric field had been attributed by the leading experimentalists-especially Millikan--to some unusual quality of the conduction electrons, which would be distinct from the electrons that leave the metal surface in thermionic emission. In both instances, wave mechanics provided a straightforward, unifying, and convincing account of the observed phenomena.

Contrary to the popular view of quantum mechanics, the tunnel effect reveals smoother and more continuous features than the abrupt behavior found in the corresponding classical description. Between 1926 and 1929, the theoretical developments described here proved unequivocally--if any such demonstration was still needed--that there could be no substitute for quantum mechanics, with its astonishing explanatory power in the microscopic domain.

I owe thanks to Hans Frauenfelder, who suggested this study, and to Harry Lustig, Peter Price, and Roger Stuewer for their valuable help.

References

- 2. F. Hund, Z. Phys. 40, 742 (1927).
- 3. F. Hund, Z. Phys. 43, 805 (1927).
- 4. L. Nordheim, Z. Phys. 46, 833 (1927).
- 5. J. R. Oppenheimer, Phys. Rev. 31, 66 (1928).
- 6. G. N. Watson, Theory of Bessel Functions, Cambridge U. Press,

^{1.} In a talk given in 1931 and published in *Phys. Z.* **32**, 833 (1931), Walter Schottky referred to the *wellenmechanische Tunneleffekt* (wavemechanical tunnel effect) at the metal-semiconductor interface. I found the first English use of the term "tunnel effect" in J. Frenkel, *Wave Mechanics, Elementary Theory*, Clarendon Press, Oxford, UK (1932). To this day, Frenkel's rarely cited textbook provides one of the most comprehensive theoretical accounts of quantum tunneling.

7. J. R. Oppenheimer, Proc. Natl. Acad. Sci. USA 14, 363 (1928).
8. R. H. Fowler, L. Nordheim, Proc. R. Soc. London, Ser. A 119, 173 (1928).
9. O. K. Rice, Phys. Rev. 35, 1538 (1930).
10. R. H. Stuewer, in The Kaleidoscope of Science, vol. 1, E. Ullmann-Margalit, ed., D. Reidel, Hingham, Mass. (1986), p. 147. See also J. Mehra, H. Rechenberg, The Historical Development of Quantum Theory, vol. 6, part 1, Springer-Verlag, New York (2000), p. 639.
11. G. Gamow, My World Line: An Informal Autobiography, Viking Press, New York (1970).
12. G. Gamow, Z. Phys. 51, 204 (1928).
13. R. W. Gurney, E. U. Condon, Nature 122, 439 (1928).
14. R. W. Gurney, E. U. Condon, Phys. Rev. 33, 127 (1929).
15. E. U. Condon, Am. J. Phys. 46, 319 (1978).

16. G. Wentzel, Z. Phys. **38**, 518 (1926).

17. M. Born, Z. Phys. 58, 306 (1928).

London (1922).

Eugen Merzbacher is Keenan Professor Emeritus of physics at the University of North Carolina at Chapel Hill and author of a popular textbook on quantum mechanics.

Physics Today References December 2001, page 35

© 2003 American Institute of Physics

<u>About Physics Today</u> <u>Contact Us</u> <u>FAQ</u> <u>Disclaimer</u> <u>Terms and Conditions</u> <u>Privacy Policy</u>