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TECHNICAL NEWSLETTER

SCHRÖDINGER'S HOPE

CARLOS STROUD

JULY 1993

THE INSTITUTE OF OPTICS
UNIVERSITY OF ROCHESTER
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U.S. ARMY RESEARCH OFFICE
ATTN: AMXRO-RT-IPL
BOX 12211
RESEARCH TRIANGLE PARK, NC 27709

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Abstract Recent work at the University of Rochester that was supported by the Army Research Office through the University Research Initiative Program has been featured in a recent book *Taming the Atom* by Hans Christian von Baeyer. This report contains an excerpt from that book that shows that the work in Rochester is the realization of Erwin Schrödinger's hope in the earliest days of quantum theory that a solution to his equation could be found in the form of a localized wave packet moving along the elliptical orbit predicted by classical theory. In a series of calculations and experiments the group in Rochester has shown that a short laser pulse can be used to excite such a wave packet state and that as the wave packet moves many times around the orbit it undergoes a complicated time evolutions in which it spreads all the way around the orbit, and then repeatedly relocalizes in the form of a single wave packet or a series of identical sub-wave packets equally spaced around the orbit. This work sheds new light on the boundary between microscopic quantum systems and macroscopic classical systems.

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The Army Research Office through the University Research Initiative Program and the Joint Services Optics Program has supported a research program at the Institute of Optics in Rochester that has recently received a great deal of attention. The work by Carlos Stroud and his group has been exploring the boundary between classical and quantum mechanics by using a short laser pulse to excite a single atom into a state that closely approaches the classical ideal of a planetary system with a well-localized electron wave packet traveling in a classical Kepler orbit. This work was featured in a recent book *Taming the Atom* by Hans Christian von Baeyer published by Random House in 1992. The book was reviewed by Phillip Morrison in the April 1993 issue of *Scientific American* where he praises the book and particularly emphasizes the work at the University of Rochester.

We will reprint here, with permission from the author, an excerpt from the book describing the work in Rochester and putting it into context.

> The transition from classical mechanics to quantum mechanics is ... murky. In spite of the best efforts of physicists since 1925, no general relationship like the simple connection between mechanics and relativity has yet been discovered. The quantum-classical boundary is a no-man's land that physicists navigate more by intuition born of experience than by reason, using quantum mechanical results where they fit, and classical mechanics where it seems more appropriate. There is only a small handful of special circumstances in which the demarcation between the two descriptions of nature can be studied in an orderly manner.
>
> A hydrogen atom excited to a very high level of energy provides one such example. From the point of view of Bohr's old theory, the electron would move slowly around the nucleus at a large distance, and there, like a distant planet, follow a well-defined elliptical trajectory. In this orbit its motion would be described according to classical Newtonian mechanics like that of the electrons in J. J. Thomson's tube and Hans Dehmelt's trap. However, in quantum mechanics terms the atom looks very different. The wave function for the electron in this high energy level is very well known—a college junior can compute and plot it. It represents a probability map that is spread out over the entire atom, and a graph of its magnitude resembles the pattern of ripples caused by a raindrop falling on a pond, except that the higher crests would be near the outer rim of the atom, rather than in the center. Schrödinger hoped that the reconciliation of this view with Bohr's particulate conception would help to clear up the relationship between quantum and classical mechanics.
>
> To achieve such an accommodation, he searched for a compromise, a phenomenon that is fundamentally wavelike but also displays some of the features of a particle. ... He thought that at the edge of the atom a number of quantum waves might interfere with each other and conspire to form a single tight wave packet, which would travel

around the nucleus in a Newtonian elliptical orbit. Such a packet constructed from the waves described by his equation would represent a marriage of the old mechanics with the new: Waviness would reside in the fundamental description of the atom, and particulateness in the isolated wave packets, which revolve around the nucleus like planets.

As soon as Schrödinger had finished the formidable task of developing his version of quantum theory in June 1926, he wrote a letter about his wave-packet conjecture to the Dutch professor Hendrik Lorentz, who had shared the 1902 Nobel Prize in physics for his explanation of how magnets affect atoms and at seventy-three years of age was regarded as the dean of theoretical physicists. Schrödinger emphasized the urgent need for a theoretical construction of "wave groups (or wave packets), which...mediate the transition to macroscopic mechanics." But he despaired of ever pinning them down because of the "great computational difficulties" he was encountering. Wouldn't it be nice, he added wistfully, if a calculation could be carried out not just for the hydrogen atom but for all quantum waves in general? But he knew that this was a hopeless wish, at least for the moment.

The problem, as Lorentz replied immediately, is that the mathematical form of the Schrödinger equation dictates that all conceivable atomic wave packets inexorably spread out with time. They may move along a definite trajectory temporarily, but they soon disperse and lose their shape and cohesiveness. And once dispersed, Lorentz continued, you could hardly expect them to reassemble again into tight bundles. Wave packets behave, in other words like normal waves.

And there the matter rested until Schrödinger's death in 1961, and for another generation after that. Most physicists regarded the wave function as a magical recipe for predicting probabilities that happened to facilitate the design of better electronic devices and faster lasers. Graduate students were taught Born's probability interpretation of the wave function — that the wave function determines the likelihood of an electron being found at a given spot—as revealed gospel, and were told that the transition to classical physics, while not fully understood, is a technical detail without practical consequences. Such phrases as wave-particle duality were declared obsolete relics of bygone days, and although a few die-hards kept alive Schrödingers's dream of finding a picturesque description of the atomic interior to replace Heisenberg's dry catalog of numbers, little progress was made. Success lulled physicists into pragmatic acceptance of the received doctrine.

Now, in the final decade of the twentieth century, more than sixty-five years after Schrödinger's miraculous spring of 1926, two new techniques are reviving interest in the subject of wave packets and their role in atoms. Theory is benefiting from the power of high-speed computers, and fast-pulsed lasers are beginning to make a new class of experiments possible. Again, just as in he case of organic dye lasers that record the birth of organic molecules and superconducting rings that monitor macroscopic quantum effects, the technological offspring of quantum theory are pressed into service to help uncover the meaning of their own roots.

The modern computers that have begun to generate pictures of wave packets within hydrogen atoms would have been a delight to Schrödinger. In 1988 a team headed by Carlos R. Stroud, Jr. at the University of Rochester reported that it had used Schrödinger's own solutions of the wave equation and combined them to produce a series of computer images. The difference between this accomplishment and Schrödinger's own abortive efforts is simple: computation power. Adding hundreds of complicated terms, and repeating the process over and over to follow the packets hypothetical motion around the nucleus, is child's play for a computer; displaying the results in graphical form for visual impact is routine. Even a computer-generated movie of a wave packet in action would not be difficult to make and would be a helpful guide for our imagination. [See page 8 for a reproduction of these computer-generated pictures.]

According to the new computer images, Schrödinger's hope was justified: The wave packet does follow a planetary trajectory. Like a heap of water, the tightly packed lump of probability begins at some point far away from the nucleus and, without losing its shape, pursues an elliptical path traveling at the same speed that an ordinary particle would have under similar circumstances. Studying that wave's orbit around the atom restores one's faith in the unity of physics: Newton's celestial mechanics, Bohr's old-fashioned but graphic theory of the hydrogen atom, and Schrödinger's revolutionary quantum mechanics come together and agree with each other in a most satisfying way.

In the end, choosing between the two images–the cloudy blur of waves or the miniature solar system—simply depends on how the system is prepared. Treat an electron like a particle, and it will produce a dot on a photographic plate. Manipulate it as though it were a wave, and it will leave the telltale marks of interference. The appearance of the inside of an atom is determined by how you look at it.

Until recently the tools available for reaching into the atom, such as Wineland's ultraviolet light beams that induce quantum jumps and Rutherford's alpha particles that penetrate all the way to the nucleus, have been blunt instruments that either revealed little detail or mangled the delicate structure of the atomic interior beyond recognition. The issue wasn't so much a matter of overbearing force—the intensity of a lamp can be turned down to feeble levels—as of insufficient speed. Electrons whirl around inside the atom at speeds approaching the speed of light, so any device designed for imaging them has to be quick about it. The watchmaker who holds his screwdriver in the gears is sure to ruin the mechanism, but if he delicately touches a wheel here and a spring here for a fraction of a second, he may uncover the secrets of the watch without destroying it. Picosecond laser pulses are proving to be the deft pointers that allow us to probe the interior of the atom.

They were the experimental tools Carlos Stroud used in order to explore the same wave packets in real atoms that he had simulated in a computer. First he and his team raised an atom of sodium into a very high state of excitation by means of a finely tuned burst of microwaves. The other most electron was thus carried into an orbit that is thousands of times larger than it would normally be. At that distance the electrical force of attraction to the nucleus is very weak, so the electron moves much more slowly than usual—just as the outermost planet, Pluto, moves only one sixth as fast in its orbit as Earth.

In the second step of the experiment Stroud's team hit the atom with a fast laser pulse. The pulse fixed the location of the electron at a particular spot in its distant orbit and reorganized its enormous, complicated wave function into a small wave packet centered at that spot. The process resembled an act of measurement: When an electron is detected, say at a particular point on a TV screen, the wave function, and thereby the probability of finding the electron, collapses to that point. The wave packet that Stroud actually created by use of the laser corresponded to one that his computer had previously generated by adding a large number of ordinary atomic wave functions.

After the atom had been prepared in this way, it was left to its own devices for a fraction of a microsecond. During this interval it can be described in two equivalent ways: In the language of classical mechanics, the electron revolves at a snail's pace on a huge elliptical path around the nucleus in a course of motion that could have been determined by Isaac Newton. The second description requires a digital computer to follow each of the constituent quantum waves, all of which spread over the entire miniature solar system of the sodium atom. At the beginning they all add up to a single small wave packet at the location of the electron. Then each one evolves on its own according to the Schrödinger equation. Step by tiny step the computer follows the twists and wiggles of each undulation in a sequence of intricate mathematical operations that would be impossible to duplicate by hand. Finally, when all the waves have been put together again, most of the troughs and crests miraculously cancel each out, leaving only a little packet where it should be at the advanced position of the electron in its orbit.

In the final step of the experiment Stroud tore the electron out of its atom by means of an external electric field. Since it is held in place by the force of its attraction to the nucleus, it can be removed by an opposing electrical force applied by letting the atom pass near a positively charged metal plate. The ease with which this could be accomplished revealed the approximate position of the electron in its orbit at the moment of ejection: At perigee, when its is closest to the nucleus, it is much more tightly attached than at the apogee, when it is farthest away. Lacking a microscope which he could follow the wave packet directly, Stroud resorted to this trick to determine its final position indirectly.

The agreement of the data with the predictions of both the Newtonian and the quantum mechanical theories vindicated Schrödinger's hunch and at the same time revived Bohr's picture of the atom, sixty-five years after it had been declared obsolete. In Stroud's experiment the classical picture of the electron speeding around the nucleus is mathematically equivalent to the quantum mechanical fuzzy clouds, but in practice far more efficient. As Schrödinger had predicted, a single wave packet moving like a planet can indeed replace the combined development of a large number of quantum waves. Schrödinger's conjectured compromise between classical and quantum physics has at long last received experimental confirmation.

But this belated corroboration of Schrödinger's physical intuition does not resolve the wave-particle paradox. Bohr's model has been reinstated only as a helpful calculational shortcut in one special circumstance, not as a general theory of the atom. At the very outset of his calculations Schrödinger had convinced himself, and Lorentz had agreed, that wave packets in atoms cannot cohere indefinitely but must inevitably disperse—and they were right. In Stroud's laser experiment the wave packet followed its elliptical path for only a fraction of a revolution but in his computer simulations the same wave packet was followed through many successive trips around the nucleus. And indeed, after a few revolutions it begins to disintegrate. A dozen revolutions later it has lost its original shape, and the probability of finding the electron is spread evenly around the entire orbit. The atom has reverted spontaneously to its wavelike aspect, and it is almost as if we have seen the transformation of a particle into a wave before our very eyes.

For a realistic space-time description of the atom this is bad news, for it emphasizes one more that a wave, or even a tight packet of waves, cannot really *be* the electron, as Schrödinger had hoped. But the disintegration of the wave packet is not the end of the story. The computer that followed the process continued grinding on hour after hour in calculations that for sheer volume far surpass human capability. The sequence of pictures published by Stroud's team look like photographs of water waves in a ring-shaped channel. It begins with an image of a tall, narrow wave packet launched on its course like Russell's solitary wave, but after a dozen revolutions nothing much is left of it but a few evenly dispersed ripples. Then, by the time the particle would have made many more revolutions, the motion of the wave becomes violent. Mysterious peaks suddenly crop up and travel around at the original speed of the packet, only to subside again just as quickly. At a time corresponding to just over a hundred circuits, the wave begins to gather its strength and to regroup in one place. And then the original wave packet, only slightly broadened, appears again at the right place and speed, as if nothing had happened in between. In the words of the authors, the wave packet has decayed and revived, in direct contradiction to Lorentz's intuitive expectation.

Although the original wave packet does not recover perfectly, and each subsequent revival is less sharply delineated than its predecessor until eventually there is no trace of a wave packet left, the regular sequence of decays and revivals is an exciting discovery. That the electron, like a platypus, has a dual nature has been evident since the birth of quantum theory, but heretofore we have seen only one or the other of its two faces at a time. Stroud's electron, on the other hand, switches back and forth between its two personalities, revealing one, then the other, before finally settling down. It is a signal that we have reached the threshold between particle and wave.

In the fall of 1989 Professor Stroud's team actually crossed it. In a paper entitled "Observation of the Collapse and Revival of an ... Electronic Wave Packet," they reported on a refinement of their first experiment in which they managed to follow an electron through a large number of revolutions and found the unmistakable imprint of the electron's vacillating nature. The original wave packet disappears, so that the physicist trying to follow the atom's evolution must resort to a quantum mechanical description, but then it regroups in such a way that classical mechanics can take over again.

This work goes beyond an illumination of the missing rung between quantum theory and classical mechanics; it represents a progression from observation to experimentation, from anatomy to surgery. When ultraviolet light illuminates a mercury atom in David Wineland's trap, it promotes internal electrons to higher levels of energy. Their wave functions acquire different forms, which are dictated by nature, not by the experimenter, so the experiment amounts to a passive observation. In Stroud's experiments, on the other hand, pulsed light rearranges the appearance of the wave function in a predetermined way. It is as though we have learned to mold wave functions like clay and watch their slithering gyrations. In this forcing of natural phenomena lies the difference between modern physics and medieval philosophy. When Sir Francis Bacon extolled the power of nascent scientific method in the beginning of the seventeenth century, he defined its aim as "putting nature to the question," by which he meant torturing her into giving up her secrets. The formation of wave packets by means of laser pulses represents the extension of this method to the hidden world inside the atom and promises a rich harvest of insights yet to come.

Stroud's experiments have opened up a new phase in atomic research. Picosecond pulses will inevitably be followed by femtosecond pulses, and supercomputers by hypercomputers. The manipulation of atoms will make way for the manipulation of atomic constituents—and not in isolation, as heretofore, but in vivo, as it were. Eventually the interior of the atom will become tamed in the same way that the atom as a whole is becoming familiar by means of Paul traps and scanning tunneling microscopes.

The work by Stroud's group that is discussed here is reported in a number of reprints:

"Coherence and Decay of Rydberg Wave Packets," Phys. Rev. Lett. **56**, 716–719 (1986), J. Parker and C. R. Stroud, Jr.

"Excitation of High Angular Momentum Ryd erg States," J. Phys. B **19**, L461–465 (1986), W. A. Molander, and J. A. Yeazell and C. R. Stroud, Jr.

"Rydberg Wave Packets and the Classical Limit," Phys. Scripta **T12**, 70–75 (1986), J. Parker and C. R. Stroud, Jr.

"Rydberg-Atom Wave Packets Localized in Angular Variables," Phys. Rev. A **35**, 2806–2809 (1987), John A. Yeazell and C. R. Stroud, Jr.

"Transient Theory of Cavity Modified Spontaneous Emission," Phys. Rev. A **35**, 4226–4237 (1987), J. Parker and C. R. Stroud, Jr.

"Transient Absorption by a Rydberg Atom in a Resonant Cavity," Phys. Rev. A **38**, 4765–4768 (1988), M. Mallalieu and J. Parker and C. R. Stroud, Jr.

"Observation of Spatially Localized Atomic Electron Wave Packets," Phys. Rev. Lett. **60**, 1494–1497 (1988), John A. Yeazell and C. R. Stroud, Jr.

"Classical Periodic Motion of Atomic Electron Wave Packets," Phys. Rev. A **40**, 5040–5043 (1989), J. Yeazell, M. Mallalieu and J. Parker and C. R. Stroud, Jr.

"Population Trapping in Short Pulse Laser Ionization," Phys. Rev. A **41**, 1602–1608 (1990), J. Parker and C. R. Stroud, Jr.

"The Production and Detection of Spatially Localized Atomic Electron Wave Packets," in *Coherence and Quantum Optics VI* (Plenum Press, New York, 1990), edited by J. H. Eberly, L. Mandel, pp. 1259-1263 J. Yeazell and C. R. Stroud, Jr.

"Classical Atoms and Quantum Mechanical Wave Packets," Acta. Phys. Polon. **A78** 253-261 (1990), J. Yeazell and C. R. Stroud, Jr.

"Observation of the Collapse and Revival of a Rydberg Electron Wave Packet," Phys. Rev. Lett. **23** 2007-2010 (1990), J. Yeazell, and M. Mallalieu and C. R. Stroud, Jr.

"Classical and Quantum Mechanical Dynamics of Quasiclassical State of a Hydrogen Atom," Phys. Rev. A **42**, 6308-6313 (1990), Z. Dačić Gaeta and C. R. Stroud, Jr.

"Behavior of Zone-Center, Subband Energies in Narrow, Strongly Coupled Quantum Wells," Appl. Phys. Lett. **58** 505-507 (1991), Mark L. Biermann and C. R. Stroud, Jr.

"Observation of Fractional Revivals in the Evolution of a Rydberg Wave packet," Phys. Rev. A **43**, 5153-5156 (1991), J. Yeazell and C. R. Stroud, Jr.

"Wave Packets in a Semiconductor Superlattice," Appl. Phys. Lett.**58**, 2279-2281 (1991), M. L. Biermann and C. R. Stroud, Jr.

"A Wave Packet Theory of Coherent Carrier Dynamics in a Semic nductor Superlattice," Phys. Rev. B **47**, 3717-3727 (1993), M. L. Biermann and C. R. Stroud, Jr.

Copies of these papers can be obtained by writing to Professor Stroud at Institute of Optics, University of Rochester, Rochester, NY 14627, or by contacting him by email at Stroud@optics.rochester.edu.

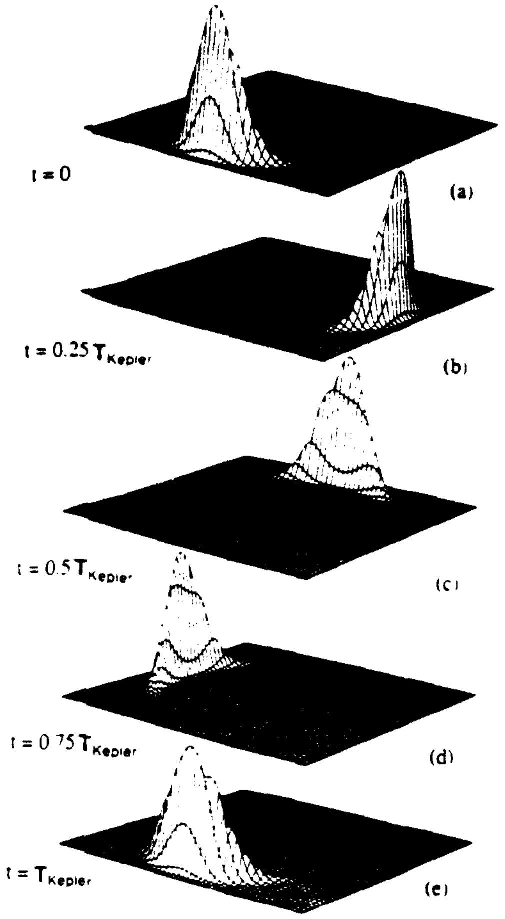

FIG. 1. (a)–(e) The initial stage of the evolution of the circular-orbit wave packet ($\bar{n}=320$, $\sigma_n=2.5$) at times 0, $\frac{1}{4}$, $\frac{1}{2}$, $\frac{3}{4}$, and 1 (in units of T_{Kepler}).

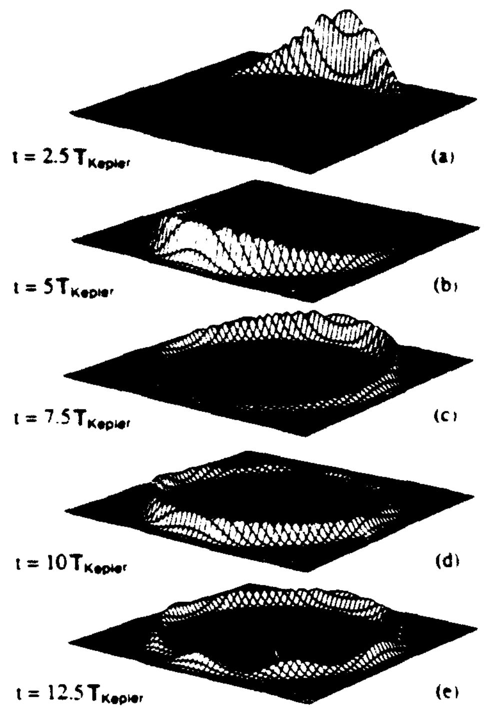

FIG. 2. (a)–(e) Spreading of the circular-orbit wave packet ($\bar{n}=320$, $\sigma_n=2.5$). The wave packet is depicted at times 2.5, 5, 7.5, 10, and 12.5 (in units of T_{Kepler}).

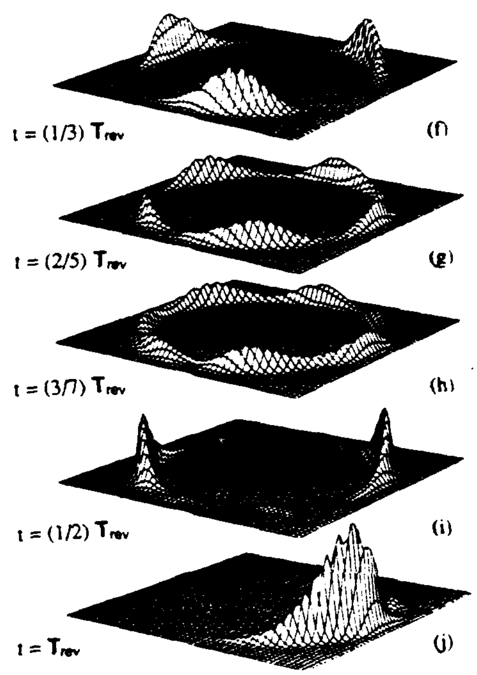

FIG. 3. (a)–(j) Fractional revivals of the circular-orbit wave packet ($\bar{n}=320$, $\sigma_n=2.5$) at times $\frac{1}{7}$, $\frac{1}{6}$, $\frac{1}{5}$, $\frac{1}{4}$, $\frac{2}{7}$, $\frac{1}{3}$, $\frac{3}{7}$, $\frac{2}{5}$, $\frac{1}{2}$, and 1 (in units of T_{rev}).

These figures are reproduced from Gaeta and Stroud (1990). They show the computer simulation of the electron wave packet moving along the classical Kepler orbit. The packet decays but has a strong revival some nanoseconds later as shown in FIG. 3(j). This complicated behavior was experimentally verified by Yeazell and Stroud (1991).