CHAPTER 3.8

What happened to the Bohr-Sommerfeld elliptic orbits in Schrödinger's wave mechanics?

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SCI.DAN.M. I · ONE HUNDRED YEARS OF THE BOHR ATOM: PROCEEDINGS FROM A CONFERENCE
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Abstract

Heisenberg and Pauli, two of the great pioneers of quantum mechanics, declared that in the domain of atoms and molecules the Bohr-Sommerfeld elliptic orbits disappears. But Bohr's correspondence principle requires that for large quantum numbers, quantum mechanics leads to classical mechanics. It is shown how this correspondence takes place.

1. Introduction

According to Felix Bloch, when he was a physics student in 1926 in Zurich, Peter Debye asked Erwin Schrödringer to give a seminar on Louis de Broglie's association of a wave with the motion of an electron. De Broglie had proposed the relation $p = h/\lambda$, where p is the momentum of the electron, and λ is its wavelength, extending the relation $e = \hbar v$ between the energy e and the frequency v, proposed by Einstein for the photon. At the seminar, Schrödinger gave "a beautiful and clear account" of how to obtain the Bohr quantization rules by demanding that an integral number n of waves can be fitted along a stationary orbit, i.e., $\int dq/\lambda = n$. This condition corresponds to $\int pdq = nh$, which later was introduced as a quantization

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rule by Sommerfeld. At the end of Schrödringer seminar, Debye remarked that to deal properly with waves one had to have a wave equation, and only a few weeks later, after a vacation with his mistress at a winter resort in Austria, Schrödringer gave another seminar announcing: "my colleague Debye suggested that one should have a wave equation; well I have found one!"[1]. But the meaning of the solution of this equation, the wave function ψ, was not clear, as revealed by a verse that Bloch and his fellow students composed at the time:

Erwin with his psi can do
Calculations quite a few.
But one thing has not been seen:
Just what does psi really mean?[2]

In Schrödinger's wave mechanics for the atom,[3] the Bohr-Sommerfeld quantized classical elliptic orbits appeared to have vanished. The demise of classical orbits in the atomic realm had already been emphasized by Pauli and by Heisenberg, who a year earlier had developed the matrix formulation of quantum mechanics that dispensed with this concept.[4] Indeed, there does not appear to be any obvious connection between elliptic orbits, and the canonical solutions of Schrödinger's equation for the hydrogen atom, although for large quantum numbers the existence of such orbits are required by Bohr's correspondence principle. Actually, shortly after publishing his seminal paper, Schrödringer addressed this problem in an article entitled "The transition from Micro- to Macromechanics,"[5], where he treated the one-dimensional harmonic oscillator, and obtained a solution consisting of a time dependent Gaussian wave packet which travels without spreading along the classical trajectory. At the end of his paper he wrote:

1. Bloch (1976).
2. Bloch (1976).
3. Schrödinger (1926a).
4. Heisenberg (1925). The paper was received 29 July 1925.
5. Schrödinger (1926b)

... One can foresee with certainty that similar wave packets can be constructed which will travel along Keplerian ellipses for high quantum numbers; however technical computational difficulties are greater than in the simple example given here ...[6]

Schrödinger sent his paper in manuscript form to Lorentz, with whom he had been corresponding about his new wave mechanics.[7] But due to "technical computational difficulties," he did not solve the problem that he had posed for wave packets that travel along Kepler's elliptical orbits. In another letter to Lorentz written on June 6, 1926, he wrote:

Allow me to send you, in an enclosure, a copy of a short note in which something is carried through for the simple case of an oscillator which is also an urgent requirement for all the more complicated case ... . You see from the text of the note, which was written before I received your letter, how much I too was concerned about the "staying together" of these wave packets. I am very fortunate that now I can at least point to a simple example where, contrary to all reasonable conjectures, it still proves right. I hope that this is so, in any event for all those cases where ordinary mechanics speaks of *quasi-periodic* motion.[8]

Then a surprising statement followed:

Let us accept this as secured or conceded for once; there still always remains the difficulty of the completely *free* electron in a completely field-free space. Would you consider it a very weighty objection against the theory if it were to turn out that the electron is incapable of existing in a completely field free space? ...[9]

Lorentz promptly responded that,

6. Schrödinger (1926b).

7. Przibram (1967), pp. 43-75.

8. Przibram (1967), p. 58.

9. Przibram (1967), p. 59.

> ... with your note ... you have given me a great deal of pleasure, and as I read it, a first thought came upon me: with a theory which resolves a doubt in such a surprising and beautiful way, one has to be on the right path. Unfortunately my pleasure was soon diminished; namely I cannot see, for example, how in the case of the hydrogen atom you can construct wave packets (I am thinking now of the *very high* Bohr orbits which travel like the electron...)[10]

Earlier Lorentz[11] had written to Schrödinger that,

> Your conjecture that the transformation which our dynamics will have to undergo will be similar to the transition from ray optics to wave optics sounds very tempting, but I have some doubts about it. If I have understood you correctly, then a "particle", an electron for example, would be comparable to a wave packet which moves with the group velocity. But a wave packet can never stay together and remain confined to a small volume in the long run. The slightest dispersion in the medium will pull it apart in the direction of propagation, and even without that dispersion it will always spread more and more in the transverse direction. Because of this unavoidable blurring, a wave packet does not seem to me to be very suitable for representing things to which we want to ascribe a rather permanent individual existence ...[12]

Lorentz had correctly pointed out that the association of a wave packet with the charge density of an electron, as Schrödinger had proposed, was not tenable if this wave packet dispersed. Later, this dilemma was resolved by Born's interpretation of the absolute square of Schrödinger's wave function as the probability function for finding the electron at a given position and time.[13] But Schrödinger did not accept this interpretation, and as late as 1946 he wrote to Einstein that,

10. Przibram (1967), p. 69.
11. Przibram (1967).
12. Przibram (1967), p. 47.
13. Born (1926a), (1926b).

> God knows I am no friend of the probability theory, I have hated it from the first moment our dear friend Max Born gave it birth. For it could be seen how easy and simple it made everything, in principle, every thing ironed out and the true problems concealed ... .

Schrödinger's misunderstanding, which persists in some quarters up to the present time, was due to the association of a quantum wave packet with a single classical trajectory, rather than with an appropriate ensemble of such trajectories as Born had pointed out; a situation that contributed also to Einstein regarding quantum mechanics as an *incomplete* description of physical reality. But Born concluded that,

> It is misleading to compare quantum mechanics with deterministically formulated classical mechanics; instead one should first reformulate the classical theory, even for a single particle, in an indeterministic, statistical manner. Then some of the distinctions between the two theories disappear, others emerge with great clarity ... . The essential quantum effects are of two kinds: the reciprocal relation between the maximum of sharpness for coordinate and velocity in the initial and consequently in any later state (uncertainty relations), and the interference of probabilities whenever two (coherent) branches of the probability function overlap. For macro-bodies both these effects can be made small in the beginning and then remain small for a long time; during this period the individualistic description of traditional classical mechanics is a good approximation. But there is a critical moment t_c where this ceases to be true and the quasi-individual is transforming itself into a genuine statistical ensemble.[14]

2. Recent developments

Following Born's admonition, it can be readily shown that the dispersion of a Gaussian wave packet describing the motion of a free particle is *exactly* the same as that of a classical Gaussian ensemble of such particles, provided that the *initial* mean square deviation in coordinate and momentum satisfies Heisenberg's uncertainty relation

14. Born (1955).

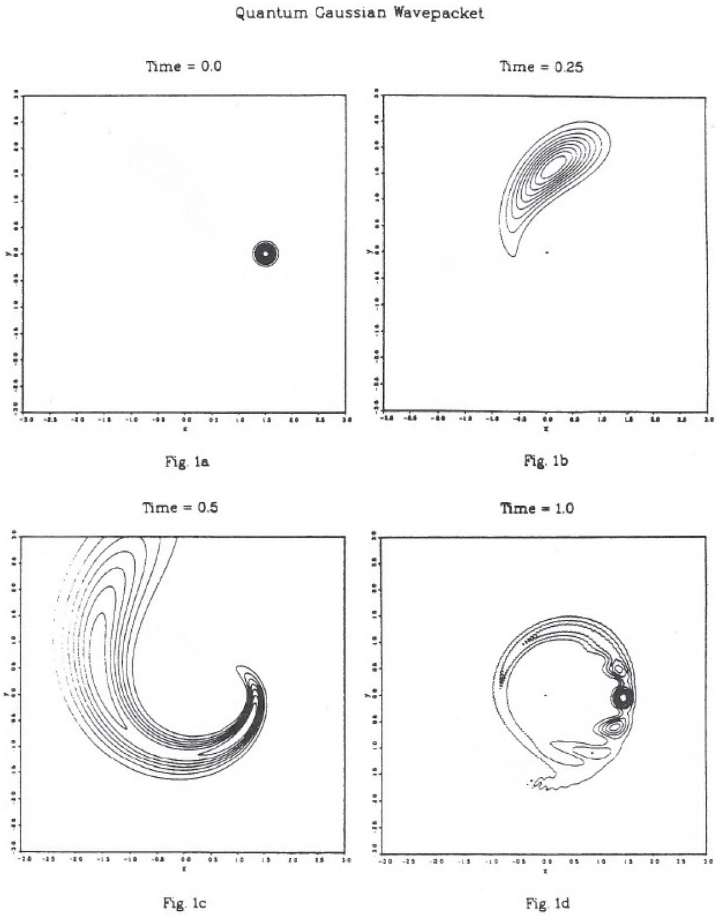

Figure 1: Contours of the the absolute square of a Gaussian wave packet in a Coulomb field. The initial mean momentum p and coordinate q correspond to a particle on a circular orbit with Bohr radius for the principal quantum numer $n = 40$. The evolution of this wavepacket is shown for times t =0,.25,.50, and 1.0 in units of the Kepler period for this orbit.

$\Delta p \Delta x = \hbar/2$.[15] Hence, the concern Schrödinger expressed to Lorentz, that a free electron *is incapable of existing in a completely field free space*, turned out to be unfounded, after Born's correct interpretation of

15. Nauenberg (2000).

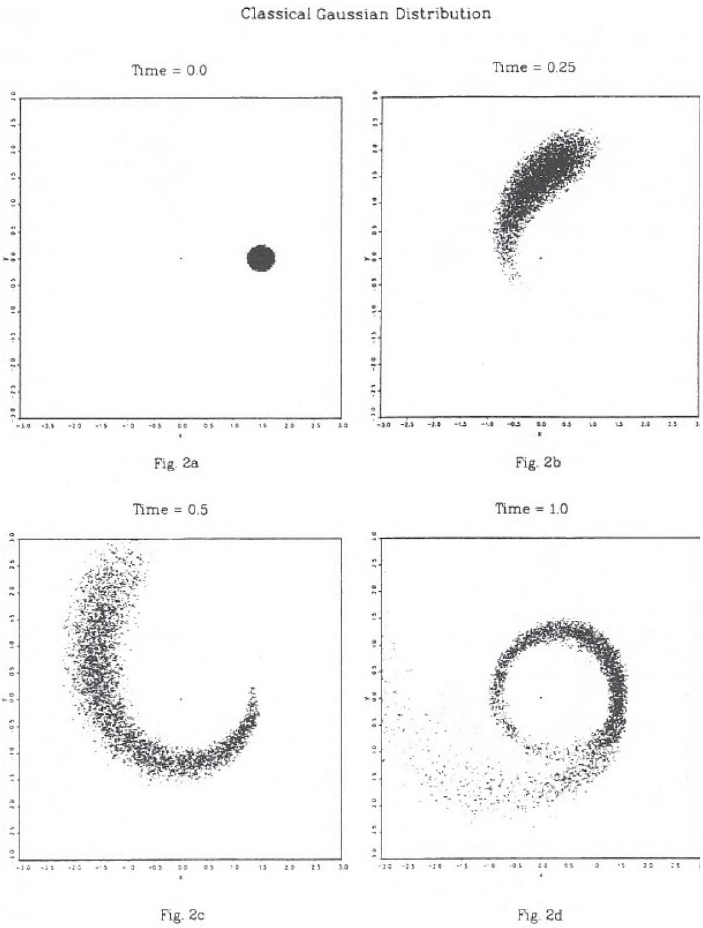

Figure 2: Classical evolution of 6000 particles initially distributed in phase space according to the Wigner distribution associated with the Gaussian wavepacket in Figure 1. The coordinates of these particles are shown at times t =0,.25,.50 and 1.0 in units of the Kepler period.

$|\psi|^2$ as a probability distribution.[16] Indeed, for localized wave packets, the quantum and classical distributions also remain the same for orbits in the present of a gravitational or electromagnetic potential, until the head of the wave packet catches up with its own tail, see Figures 1 and 2. Then, in the quantum case, wave interference

16. Born (1926).

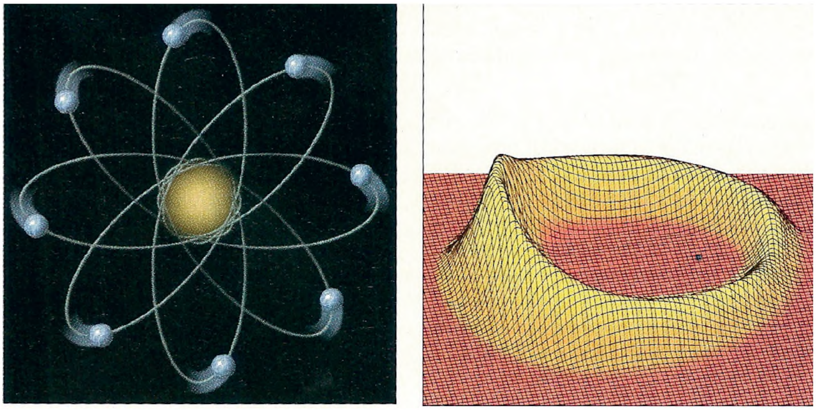

Figure 3: Left figure - Elliptic orbits in the Bohr-Sommerfeld model for an electron orbiting around a proton located at the focus of these ellipses. Right figure - Probability distribution for finding the electron in a stationary quantum elliptic state for a mean principal quantum number $n = 40$.

phenomena occur when the *two coherent branches of the probability function overlap*, see Figure 1d, for which there is no analogy in the classical case, see Figure 2d.[17]

Finally, in 1989 Schrödinger's "technical computational difficulties" with the Kepler problem were surmounted, and the probability distribution for a stationary ensemble of particles on a Keplerian elliptic orbit were calculated.[18] Moreover, such orbits have been created experimentally in Rydberg atoms were a single electron is excited to high quantum numbers.[19] The right side of Figure 3 shows the absolute square of a wave function representing the probability distribution for finding an electron in such an orbit for a principal quantum number $n = 40$, mean angular momentum $L = 32\hbar$, and eccentricity $\epsilon = 0.6$, satisfying the classical relation $\epsilon = \sqrt{1 + 2E_n L^2/me^4}$, where $E_n = -e^4 m/2n^2\hbar^2$ is the Bohr energy.[20] Such Keplerian wave functions are well defined linear superposi-

17. Nauenberg and Keith (1991).
18. Nauenberg (1989); Gay, Delande, and Bommier (1989).
19. Nauenberg, Stroud, and Yeazell (1994). For a discussion of Rydberg atoms in the Bohr model, see Kragh (2015).
20. Nauenberg (1989).)

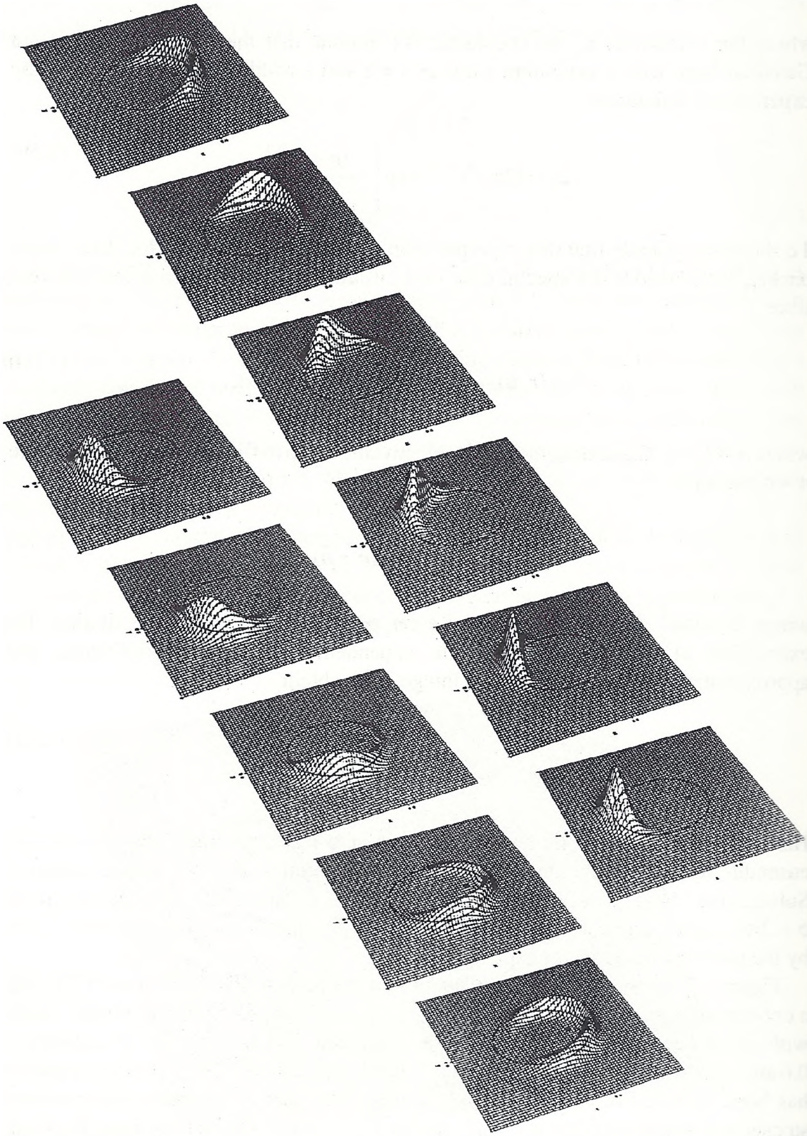

Figure 4: A wavepacket during one Kepler period representing an electron rotating counterclockwise (from top right to left bottom) around a proton located at the focus of an elliptical orbit (black dot).

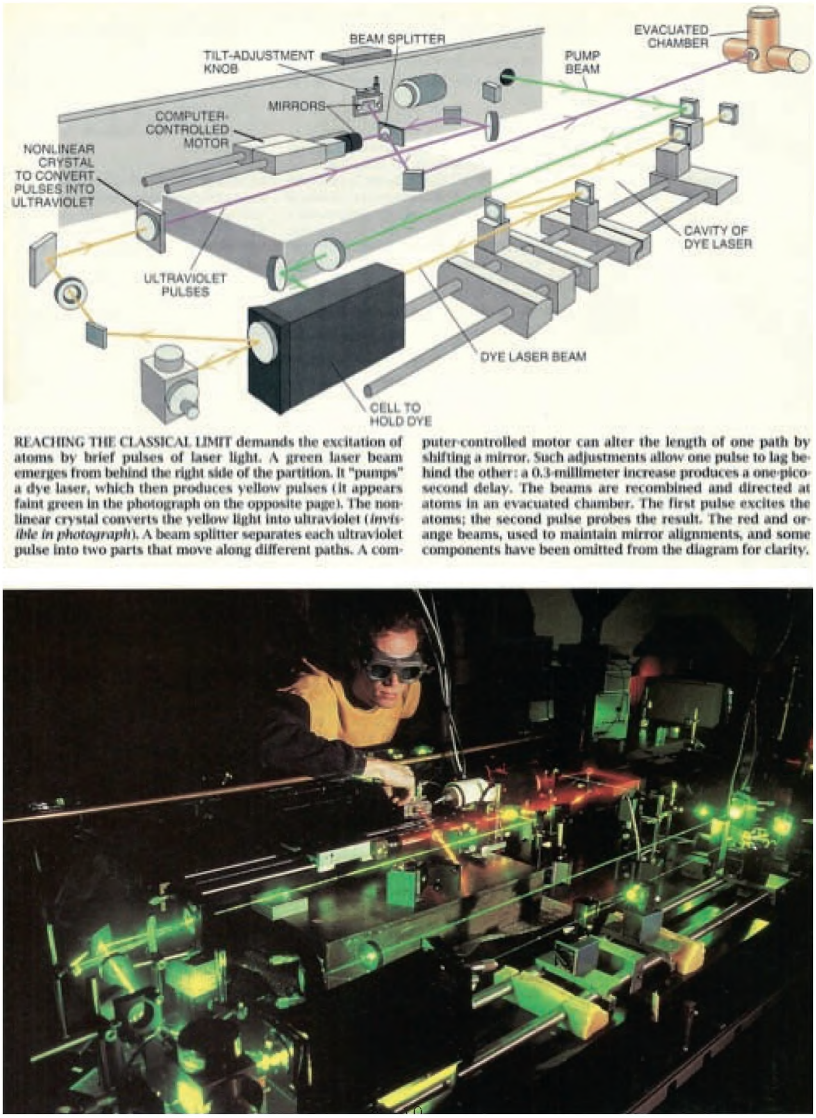

Figure 5: A "pump-probe" experiment to demonstrate the elliptic orbit of an electron in a Rydberg atom as shown in Scientific American, June 1994.

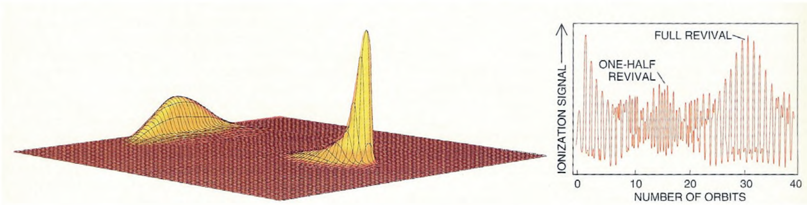

Figure 6: Left figure shows a revival of the initial wave packet into two wave packets. Right figure shows the observed ionization signal for the one-half revival, seen as a doubling of the oscillation frequency, and a subsequent full revival of the initial wave packet.

tions of degenerate energy eigenstates with angular momentum $l = 0, 1, \dots, n-1$.[21] As expected, the maximum probability of finding the electron occurs when it is farthest from the center of force, where the classical velocity is at a minimum, while the minimum probability occurs when the electron is at the opposite location, where the velocity is a maximum.

Solutions were also obtained for the time dependent Schrödinger equation for particles that travel on elliptic orbits with the classical Kepler period τ_n with mean principal quantum number n, by forming an appropriate superposition of these time independent solutions multiplied by $exp(-E_n t/\hbar)$, where $\tau_n = h/2E_n$.[22] In Figure 4, the evolution of such a wave packet is shown during one Kepler period τ_n at equal time intervals $\tau_n/10$. While the wave packet returns to its initial position, it also has dispersed as can be seen by comparing the initial and final shape of the wave packet. After a time interval $t = (n/3)\tau$, the head of the wave packet has caught up with its tail, and interference phenomena occur,[23] leading to revivals that do not have any classical counterpart.[24]

21. The energy degeneracy of the hydrogen atom is due to an invariance in addition to rotation symmetry, for Newton's $1/r^2$ force, which fixes the direction in space of the major axis of an ellipse. Then a rotation of the circular $l = n - 1$ state, in an abstract O(3) subspace of the O(4) symmetry group of the hydrogen atom by an angle θ, where $\sin(\theta) = \epsilon$, gives rise to the elliptic states. Nauenberg (2000).

22. Nauenberg (1989).

23. Averbukh and Perelman (1989).

24. Nauenberg (1990).

These predictions have been verified experimentally in Rydberg atoms by R. Stroud and his collaborators. In Figure 5 their experimental set up is described, and Figure 6 shows an ionization signal as a function of time in units of the Kepler period, providing experimental evidence for a one-half revival after 15 orbits (see the theoretical description of the corresponding distribution on the left side of Figure 6), and and a full revival after 30 orbits.[25]

For macroscopic bodies, like the planets rotating around the sun, the principal mean quantum number n associated with the Keplerian ellipse is enormous due to the very small value of Planck's constant $\hbar$. Our quantum mechanical solution of Newton's planetary problem answers the perennial question posed by Einstein: " is the moon there when no one is looking", with a resounding *yes*. It also demonstrates, at least in this particular case, that a so called *quantum-classical divide* that continues to be debated up to the present time, does not exist.

BIBLIOGRAPHY

Averbuch, I.S., and N.F. Perelman (1989). "Fractional revivals: Universality in the long-term evolution of quantum wave packets beyond the correspondence principle dynamics." *Physics Letters A* 139, 449-453.

Bloch, F. (1976). "Heisenberg and the early days of quantum mechanics." *Physics Today* 29 (December), 23-27.

Born, M. (1926a). "Zur Quantenmechanik der Stossvorgänge." *Zeitschrift für Physik* 37, 863-865.

Born, M. (1926b). "Quantenmechanik der Stossvorgänge." *Zeitschrift für Physik* 38, 803-827.

Born, M. (1955). "Continuity, determinism and reality." *Det Kongelige Danske Videnskabernes Selskab. Matematisk-fysiske Meddelelser*. 30: 2.

Gay, J.C., D. Delande and A. Bommier (1989), "Atomic quantum states with maximum localization on classical elliptical orbits." *Physical Review* A 39, 6587-6590.

Heisenberg, W. (1925). "Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen." *Zeitschrift für Physik* 33, 879-893.

Kragh, H. (2015). "The many faces of the Bohr atom." This volume.

25. Nauenberg, Stroud, and Yeazell (1994).

Nauenberg, M. (1989) "Quantum wavepackets on Kepler elliptical orbits." *Physical Review* A 40, 1133-1136.

Nauenberg, M. (1990). "The transition from quantum to classical mechanics in atomic physics." *Comments in Atomic and Molecular Physics* 25: 1-3, 151-157.

Nauenberg, M. (2000). "Wave packets: Past and present." 1-29 in *The Physics and Chemistry of Wave Packets*, J.A. Yeazell and T. Uzer, eds. New York: Wiley and Sons.

Nauenberg, M., and A. Keith (1991), "Negative probability and the correspondence between classical and quantum physics." 265-272 in *Quantum Chaos—Quantum Measurement*, P. Cvitanović, I. Percival and A. Wirzba, eds. Copenhagen: Kluwer Academic Publications.

Nauenberg, M., C. Stroud and J. Yeazell (1994). "The classical limit of an atom." *Scientific American* 270 (June), 44-49.

Przibram, K., ed. (1967). *Letters on Wave Mechanics: Schrödinger, Planck, Einstein, Lorentz*. Translated from the German with an introduction by Martin J. Klein. New York: Philosophical Library.

Schrödinger, E. (1926a). "Quantisierung als Eigenwertproblem (Erste Mitteilung." *Annalen der Physik* Series 4, 79, 361-376.

Schrödinger, E (1926b). "Der stetige Übergang von der Mikro- zur Makromechanik." *Die Naturwissenchaften* 14, 664-666.