Title

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

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Abstract

According to Heisenberg and Pauli, two of the great pioneers of quantum mechanics, in the domain of atoms and molecules the Bohr-Sommerfeld elliptic orbits disappear. But Bohr's correspondence principle requires that for large quantum numbers, quantum mechanics corresponds to classical mechanics. It is shown here how this correspondence, generally ignored in physics textbooks, takes place.

Historical Remarks

According to Felix Bloch, who was a student in 1926 at the E.T.H 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 corresponds to the wavelength, extending a relation previously proposed by Einstein for the photon. At the seminar, Schrödinger gave "a beautiful and clear account" how to obtain the Bohr-Sommerfeld quantization rules by demanding that an integral number of waves fitted along a stationary orbit, i.e. $\int dq/\lambda = n$, which corresponds to $\int pdq = nh$. At the end of this 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 started another seminar announcing:

"my colleague Debye suggested that one should have a wave equation; well I have found one!"[1], [2]. But the meaning of his wave function ψ was not clear, as revealed by a popular verse 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?* [1]

In Schrödinger wave mechanics for the atom [3], the Bohr-Sommerfeld quantized classical elliptic orbits appear 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 Macro Mechanics* [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 that

> *...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 [6], but apparently he never solved the problem he had posed for wave packets that travel along Kepler's elliptical orbits. In a 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. [6]

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?...[6]

Lorentz promptly responded that,

...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 can not 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...) [6]

Earlier Lorentz [6] 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 remained confined to a small volume in the long run. The slightest dispersion in the medium will pull it apart in the direction

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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... [6]

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 [8]. But Schrödinger did not accept this interpretation, and as late as 1946 he wrote to Einstein that,

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...[6]

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

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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.[6]

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, provided that the *initial* mean square deviation in coordinate and momentum satisfies Heisenberg's uncertainty relation $\Delta p \Delta x = \hbar/2$ [7] (see Appendix A). Hence, the concern that 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 the Schrödinger wave function as a probability amplitude [8]. In fact, 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 Figs. 1 and 2. Then, in the quantum case, wave interference phenomena occurs when the *two coherent branches of the probability function overlap*, see Fig.1d, as Born already had pointed out, for which, of course, there is no analog in the classical case, see Fig. 2d [9].
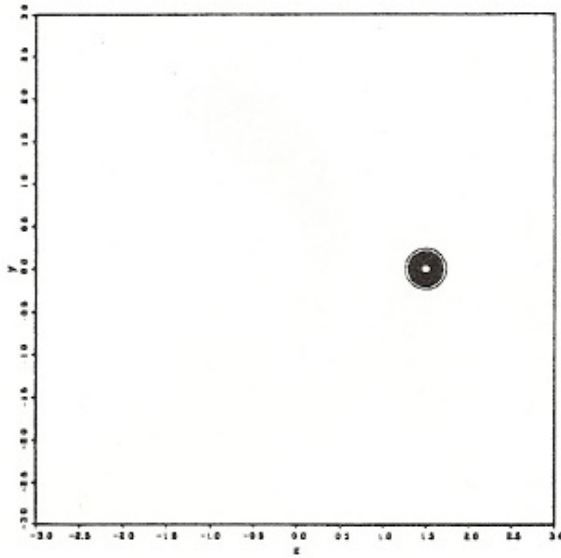
Quantum Gaussian Wavepacket
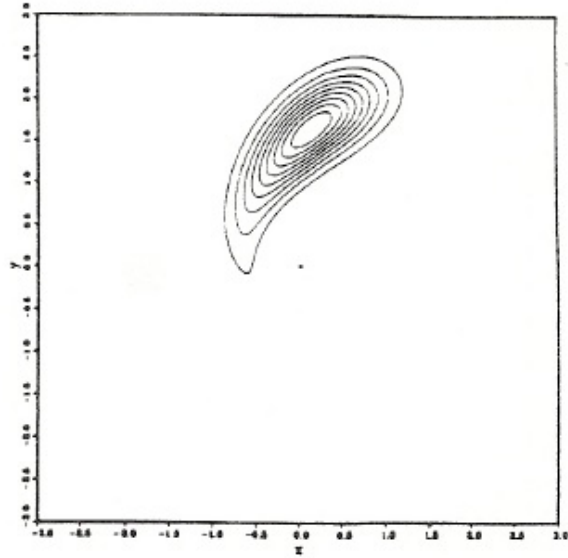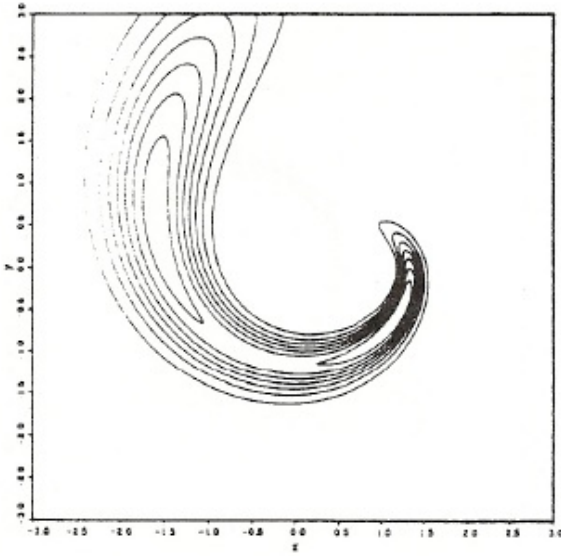
Time = 0.0

Fig. 1a

Time = 0.25

Fig. 1b
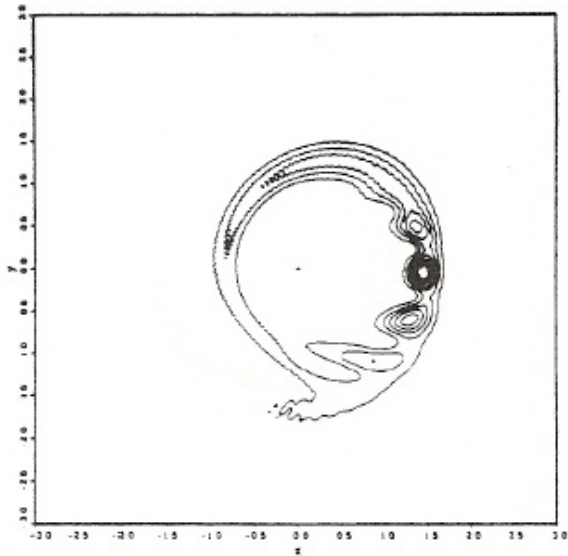
Time = 0.5

Fig. 1c

Time = 1.0

Fig. 1d

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

Classical Gaussian Distribution

Time = 0.0

Fig. 2a

Time = 0.25

Fig. 2b

Time = 0.5

Fig. 2c

Time = 1.0

Fig. 2d

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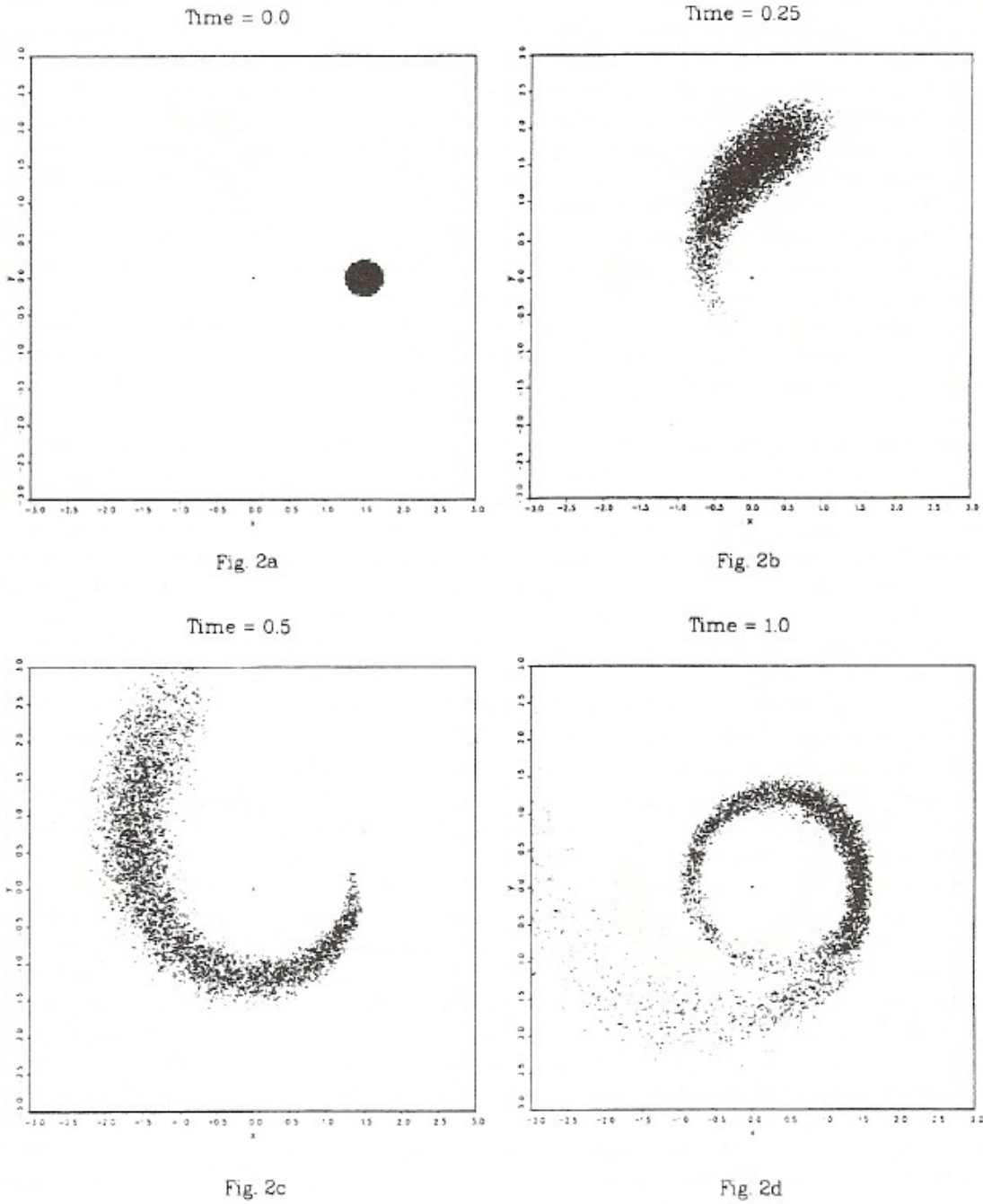
Figs. 2a-2d Classical evolution of 6000 particles which have been initially distributed
in phase space according to the Wigner distribution associated with the Gaussian
wavepacket in Figs. 1a. The coordinate of these particles are shown at times t=0.
.25 .50 and 1.0 in units of the Kepler period.

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 (see Appenix B) [10], [11]. Moreover, such orbits have beem created experimentally in Rydberg atoms were a single electron is excited to high quantum numbers [12]. On the right side of Fig. 3 we show 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 [10]. Such Keplerian wave functions are well defined linear superpositions of degenerate energy eigenstates with angular momentum $l = 0, 1, ...n - 1$ [13]. As expected, the maximum probability of finding the electron occurs at apastron, where the classical velocity is a minimum, while the minimun probability occurs at periastron, 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 $\tau_n = h/2E_n$ [10]. In Fig.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 occurs, leading to revivals that do not have any classical counterpart [14].

These predictions have been verified experimentally in Rydberg atoms by R. Stroud and his collaborators. In Fig. 5 their experimental set up is described, and Fig. 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 Fig. 6), and and a full revival after 30 orbits[12].

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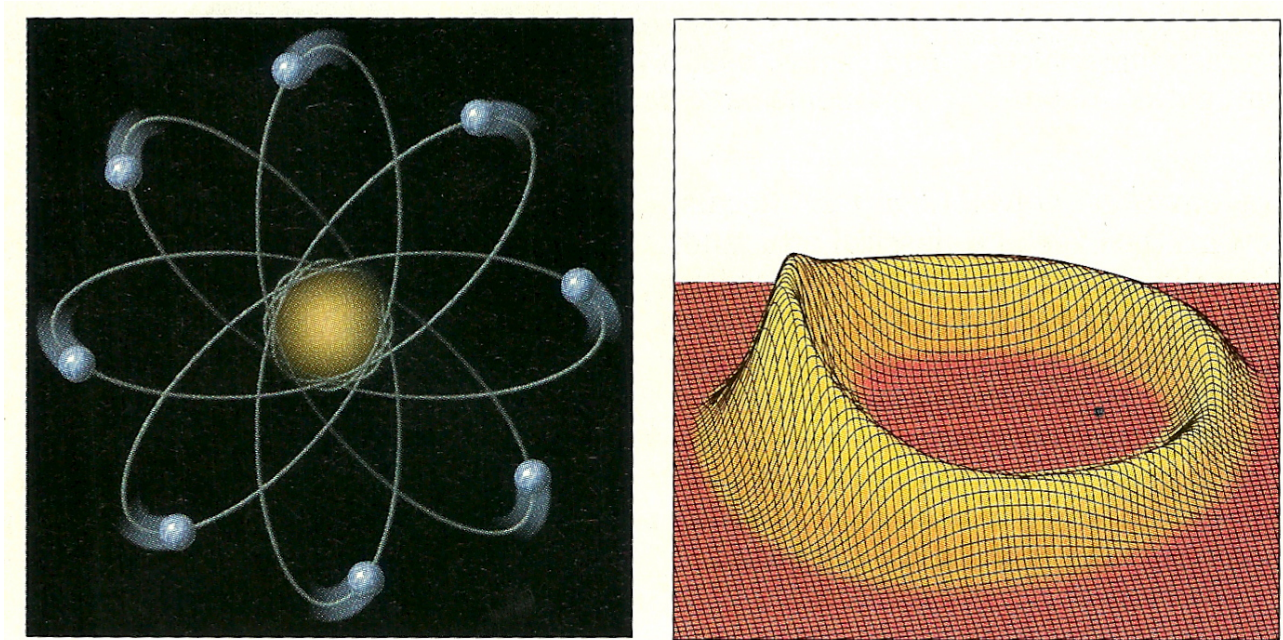
Figure 3: Left figure - Elliptic orbits in the Bohr-Sommerfeld model for an electron orbiting around a proton located at the focus of these ellipses. Right figure - Probability distribution for finding the electron in a stationary quantum elliptic state for a mean principal quantum number $n = 40$.

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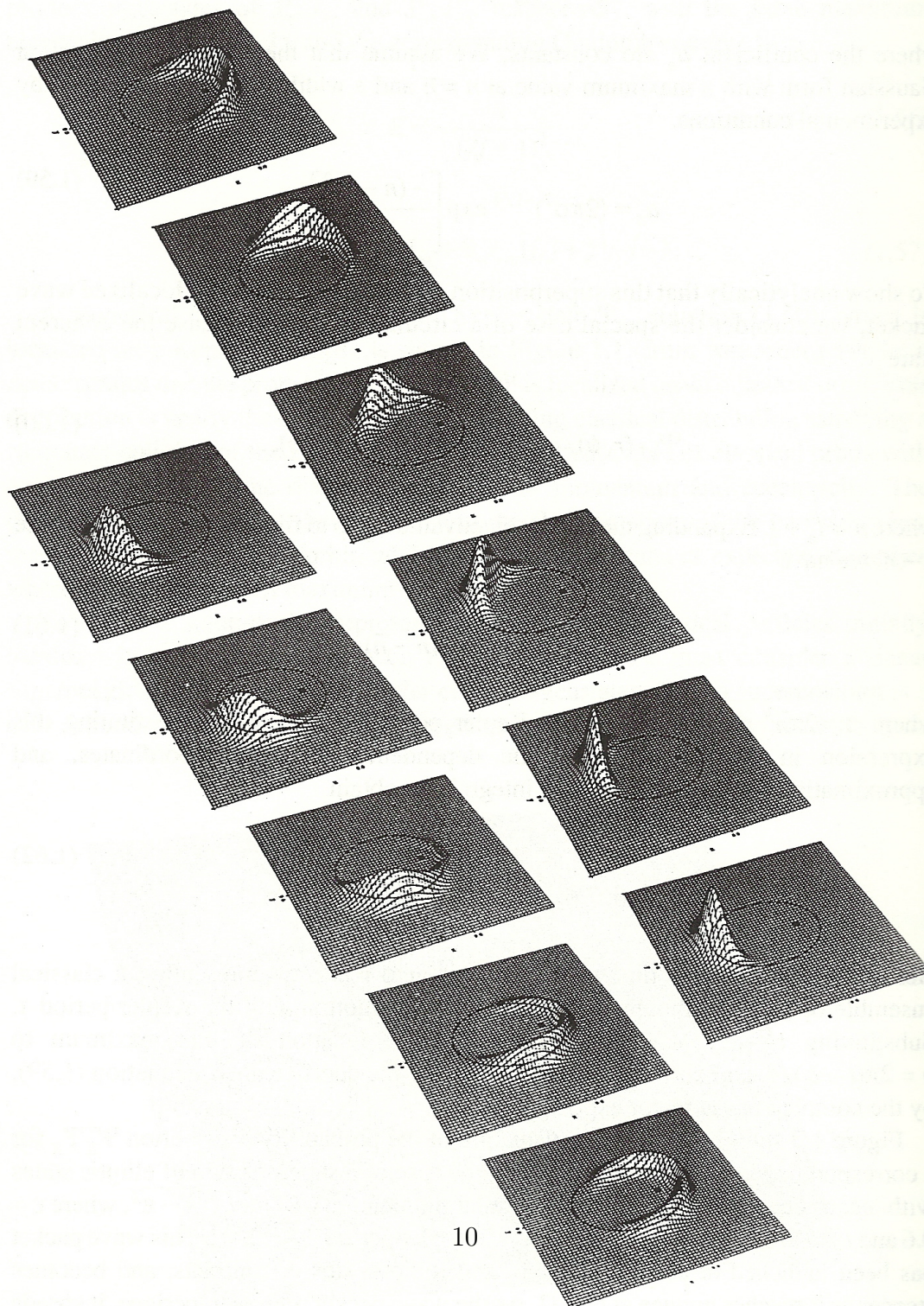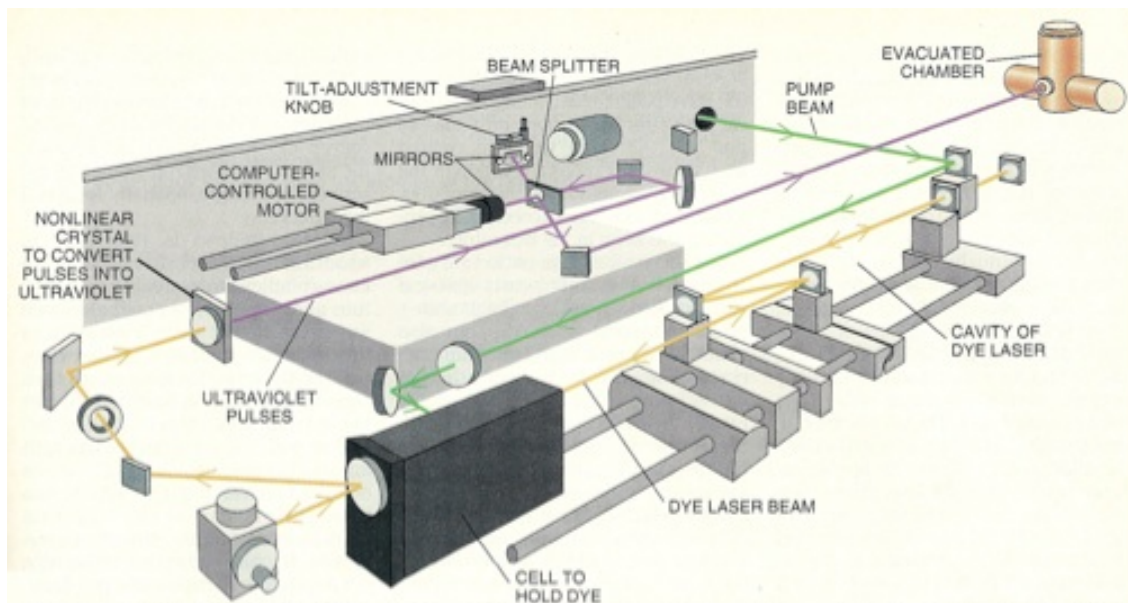
Figure 4: A wavepacket during one Kepler period representing an electron rotating counterclockwise (from top right to left bottom) around a proton located at the focus of an elliptical orbit (black dot).

REACHING THE CLASSICAL LIMIT demands the excitation of atoms by brief pulses of laser light. A green laser beam emerges from behind the right side of the partition. It "pumps" a dye laser, which then produces yellow pulses (it appears faint green in the photograph on the opposite page). The nonlinear crystal converts the yellow light into ultraviolet (*invisible in photograph*). A beam splitter separates each ultraviolet pulse into two parts that move along different paths. A computer-controlled motor can alter the length of one path by shifting a mirror. Such adjustments allow one pulse to lag behind the other: a 0.3-millimeter increase produces a one-picosecond delay. The beams are recombined and directed at atoms in an evacuated chamber. The first pulse excites the atoms; the second pulse probes the result. The red and orange beams, used to maintain mirror alignments, and some components have been omitted from the diagram for clarity.
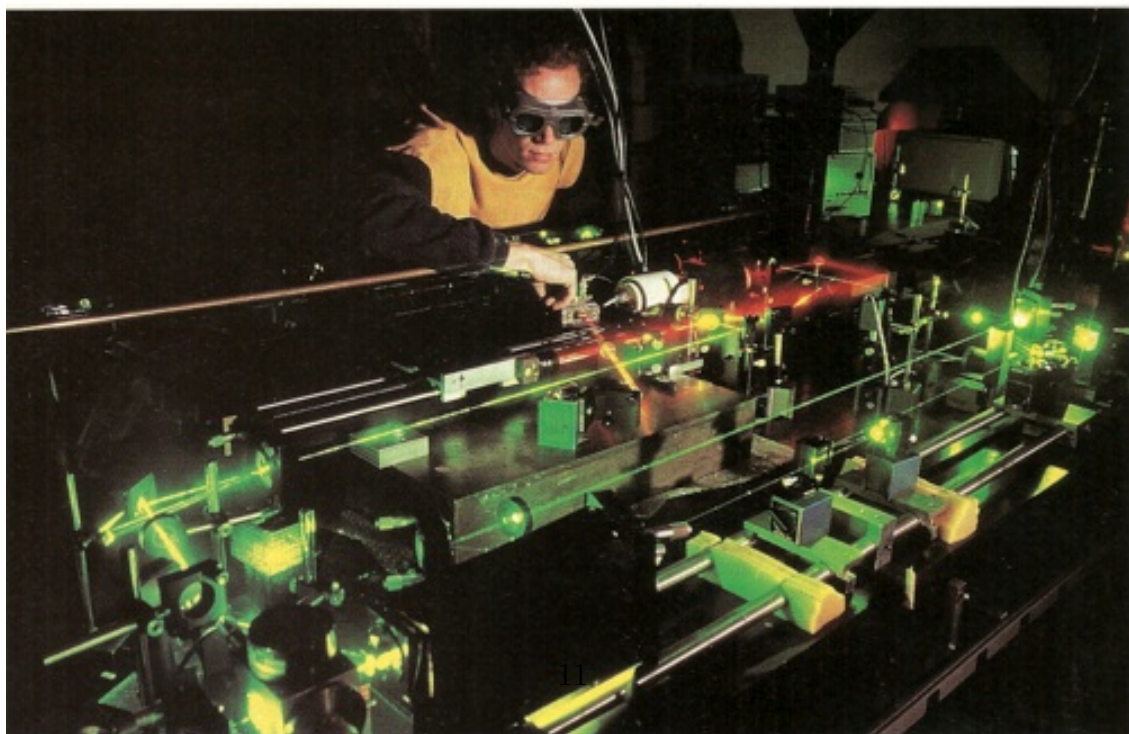
Figure 5: A "pump - probe" experiment to demonstrate the elliptic orbit of an electron in a Rydberg atom as shown in Scientific American, June 1994.
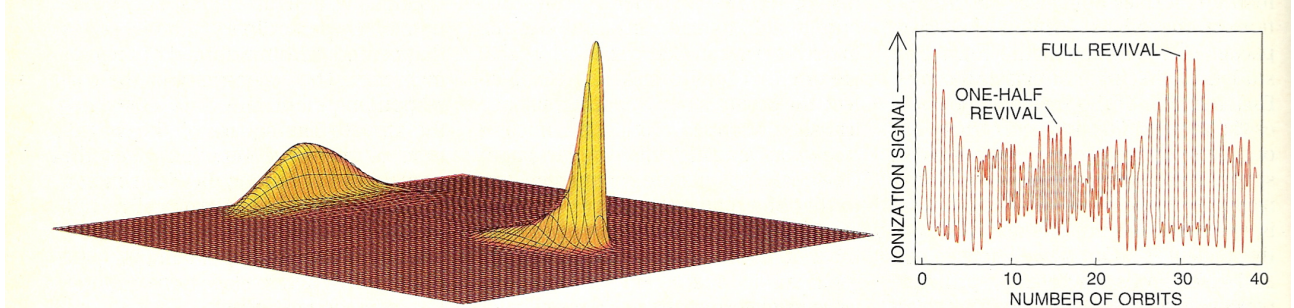
Figure 6: Left figure shows a revival of the initial wave packet into two wave packets. Rigth figure shows the observed ionization signal for the one-half revival, seen as a doubling of the oscillation frequency, and a subsequent full revival of the initial wave packet.

Appendix A, Wave Packet for a Free Particle

To illustrate some of the basic ideas about coherent quantum wave packets and to show how these wave packets illuminate the fundamental relation between quantum and classical motion, we consider in some detail the simple problem of the motion of a free particle in one dimension. Suppose that the particle has a mean momentum $\bar{p}$ and that it is initially localized near the origin of coordinates at $x = 0$. In quantum mechanics the initial state can be represented by a Gaussian wavefunction

$$\psi(x,0) = (2\pi\sigma^2)^{-1/4} exp(i\bar{p}x/\hbar - x^2/4\sigma^2) \tag{1}$$

where σ is the width representing the uncertainty in the initial position position of the particle. At a later time the wavefunction is obtained by solving the time dependent Schrödinger equation

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} \tag{2}$$

subject to the initial condition Eq.1. For mathematical convenience we will now set Planck's constant $\hbar$ and the mass m of the particle equal to unity (one can recover these parameters in the subsequent equations by the replacement $p \to p/\hbar$ and $t \to t\hbar/m$. We obtain

$$\psi(x,t) = N(t) exp[i\bar{p}x - i\bar{p}^2 t/2 - (x - \bar{p}t)^2/(4\sigma^2 + 2it)] \tag{3}$$

where $N(t) = (2\pi\sigma^2)^{-1/4}(1+it/2\sigma)^{-1/2}$. Hence the probability of finding the particle in the interval $(x, x + dx)$ at time t is given by $|\psi(x,t)|^2 dx$ where

$$|\psi(x,t)|^2 = \frac{1}{\sqrt{2\pi}\Delta(t)}exp[-(x-\bar{p}t)^2)/2\Delta^2(t)] \tag{4}$$

where $\Delta(t) = \sqrt{\sigma^2 + t^2/4\sigma^2}$ is the time dependent width of the wave packet.

We now consider a corresponding ensemble of free particles in classical mechanics which is described initially by a Gaussian distribution in both momentum and coordinate space, localized near $p = \bar{p}$ and $x = 0$, with corresponding widths σ_p and σ_x,

$$P_c(x,p,0) = \frac{1}{2\pi\sigma_x\sigma_p}exp[-(p-\bar{p})^2/2\sigma_p^2 - x^2/2\sigma_x^2], \tag{5}$$

where $P_c(x, p, t)$ is the probability distribution for such an ensemble. At later times it must satisfy the the Liouville equation for free particles

$$\frac{\partial P_c(x,p,t)}{\partial t} + p\frac{\partial P_c(x,p,t)}{\partial x}. \tag{6}$$

where we have set $m = 1$ (to recover the dependence on m in the classical equations replace $t \to t/m$). It can be easily verified that the solution of this equation is given by

$$P_c(x,p,t) = \frac{1}{2\pi\sigma_x\sigma_p}exp[-(p-\bar{p})^2/2\sigma_p^2 - (x-pt)^2/2\sigma_x^2]. \tag{7}$$

To compare the classical and quantum mechanical probability distributions in coordinate space we now integrate P_c over momentum space to obtain

$$\int P_c(p,q,t)dp = \frac{1}{\sqrt{2\pi}\Delta_c(t)}exp[-(x-\bar{p}t)^2/2\Delta_c^2(t)] \tag{8}$$

where $\Delta_c(t) = \sqrt{\sigma_x^2 + \sigma_p^2 t^2}$. This expression has the same form as the quantum mechanical probability, Eq. 4. Furthermore, if we equate the classical and quantum widths in coordinate space, $\sigma_x = \sigma$, and require that σ_p satisfy the minimum quantum mechanical uncertainty relation

$$\sigma_p = \frac{1}{2}\frac{\hbar}{\sigma} \tag{9}$$

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we obtain the remarkable result that the time evolution of the classical and the quantum mechanical probability distributions are *identically* the same in coordinate space. In quantum mechanics this relation between σ_p and σ_x can be obtained directly by evaluating the Fourier transform $\phi(p, t)$ of $\psi(x, t)$ which determines the probability distribution in momentum space. It turns out that the Gaussian wave packet corresponds to the minimal uncertainty relation, Eq. 9, which is allowed by the quantum mechanical commutation relations $[x, p] = i\hbar$. Integrating $P_c(x, p, t)$ over the position coordinate x gives the momentum distribution of the classical ensemble which for free particles is independent of time and is equal to $|\phi(p, 0)|^2$ if we identify the classical momentum width in accordance with the uncertainty relation, Eq. 9. It can also be verified that in this special case the classical distribution $P_c(x, p, t)$ is given by the Wigner distribution

$$P_c(x, p, t) = \int \frac{dq}{2\pi} \psi^*(x + q/2, t) \psi(x - q/2, t) \ exp(ipq) \qquad (10)$$

Thus, we have shown that the main distinction between quantum and classical mechanics for free particles is that quantum mechanics imposes a constraint on the minimal uncertainty, Eq. 9, with which the initial position and momentum of the particle can be determined. Actually this quantum-classical correspondence is exact only for Gaussian distributions, but for large quantum numbers this is also a very good approximation for other distributions which are sharply peaked near mean values of the initial position and the momentum. However, this correspondence breaks down when there is a force or potential acting on the particle. For example, if the quantum wave packet reaches a potential barrier or well part of the incident wave can be reflected producing interference effects which have no correspondence in classical mechanics. We shall see in the next section that it is precisely such interference phenomena which determines the onset for the breakdown of the quantum- classical correspondence. Other well known phenomena such as quantum mechanical tunneling through a barrier also does not have a correspondence in classical mechanics, but this topic will not be discussed further here.

Appendix B, Wave packet for a Particle in a Coulomb Potential

The Hamiltonian for the Coulomb potential in atomic units ($m = \hbar = e^2 = 1$) is

$$H = \frac{p^2}{2} - \frac{1}{r} \tag{11}$$

where $\vec{p}$ is the momentum, and r is the radial distance. This Hamiltonian is rotationally invariant and therefore it commutes with the angular momentum operator $\vec{L} = \vec{r} \times \vec{p}$. From classical mechanics we expect that there exists an additional operator which also commutes with H. This is an operator associated with the the Laplace vector

$$\vec{A} = \vec{p} \times \vec{L} - \frac{\vec{r}}{r}, \tag{12}$$

which is a conserved quantity in classical mechanics. For an elliptic orbit the magnitude of this vector is equal to its eccentricity e, and its direction is along the major axis of this ellipse. This can be readily seen by multiplying Eq. (12) by $\vec{r}$, which gives the equation of a conic section in polar coordinates,

$$r = \frac{L^2}{1 + cos(\theta)}, \tag{13}$$

where r is the radial coordinate and θ is the angle between $\vec{r}$ and $\vec{A}$.

In 1926 Pauli, who had been urged by Heisenberg to solve the hydrogen spectrum with his newly developed matrix mechanics, extended the Laplace vector to a matrix operator in quantum mechanics and anti-symmetrizing the cross-product of $\vec{p}$ and $\vec{L}$. Applying the Heisenberg- Born-Jordan commutation relations for the components of momentum $\vec{p}$ and position $\vec{r}$, he then obtained the commutation relations for the components of $\vec{L}$ and $\vec{A}$,

$$[L_i, L_j] = i\epsilon_{ijk}L_k, \tag{14}$$

$$[L_i, A_j] = i\epsilon_{ijk}A_k, \tag{15}$$

$$[A_i, A_j] = -i2H\epsilon_{ijk}L_k. \tag{16}$$

Setting $\vec{A} = \sqrt{(-2H)}\vec{M}$ for the bound states of the Hamiltonian H, the components of $\vec{L}$ and $\vec{M}$ satisfy the commutation relation of the generators

of the O(4) symmetry group. The Hamiltonian H can then be expressed in terms of these operators in the form

$$H = -\frac{1}{2(L^2 + M^2 + 1)} \qquad (17)$$

and in this way one obtains the spectrum of the hydrogen atom.

To simplify our discussion we restrict these relations to a two dimensional space, which reduces the symmetry to the rotation group O(3) with the commutation relations

$$[L_z, M_x] = iM_y, \qquad (18)$$

$$[L_z, M_y] = -iM_x, \qquad (19)$$

$$[M_x, M_y] = iL_z, \qquad (20)$$

and

$$H = -\frac{1}{2(L^2 + M^2 + 1/4)}. \qquad (21)$$

Since the components of the operators $\vec{L}$ and $\vec{M}$ do not commute it is not possible to obtain eigenstates of H which are simultaneous eigenstates of these operators. The conventional eigenstates of the Coulomb Hamiltonian found in most quantum mechanics textbooks are chosen to be eigenstates of L^2 and L_z, and for such states the expectation value of the Laplace vector vanishes. This is the fundamental reason why these states do not manifest the properties of classical elliptic orbits even in the correspondence limit of large quantum numbers. For a bound state an angular momentum eigenstate corresponds in the classical limit to an ensemble of elliptic orbits with a fixed value of the angular momentum, but with a uniform distribution of the direction of the major axis. Alternatively, one may consider eigenstates of components of the Laplace vector, but in this case the mean value of the angular momentum vanish. Hence, to represent a state in quantum mechanics that is related to an elliptic orbit in classical mechanics with fixed values of both the angular momentum and the Laplace vector, we must regard them as mean values in quantum mechanics, and minimize the quantum fluctuations of these operators.

The commutation relations Eqs. 18 -20 suggests that as a starting point we define coherent states Ψ for the Coulomb potential [10] which exhibit the properties of Keplerian orbits as bound eigenstates of H which have

fixed mean values of $\vec{L}$ and $\vec{M}$ and minimize the product $\Delta M_x \Delta M_y$ of the quantum fluctuations of M_x and M_y, where

$$(\Delta M_{x,y})^2 = <(M_{x,y} - <M_{x,y}>)^2 > \tag{22}$$

and $< .. >$ refers to the expectation value with respect to the state Ψ. Introducing the auxiliary state

$$\Phi = [M_x - <M_x> + i\delta(M_y - <M_y>)]\Psi, \tag{23}$$

where Ψ is an arbitrary state and δ is a real parameter, we have

$$0 \leq (\Phi, \Phi) = (\Delta M_x)^2 + \delta^2(\Delta M_y)^2 - \delta <L_z> . \tag{24}$$

Minimizing the right hand side of this equation with respect to δ, we obtain

$$\delta = \frac{<L_z>}{2(\Delta M_y)^2}, \tag{25}$$

and substituting this expression for δ in Eq. 24 we find that

$$\Delta M_x \Delta M_y \geq \frac{1}{2} <L_z> . \tag{26}$$

The minimum value of the product of these fluctuations is obtained when $\Phi = 0$, which implies that the state Ψ is a solution of the eigenvalue equation

$$(M_x + i\delta M_y)\Psi = \eta\Psi, \tag{27}$$

where $\eta = <M_x> + i <M_y>$. Hence the required states Ψ are simultaneous eigenstates of H and the nonhermitian operator $M_x + i\delta M_y$ with eigenvalue η. These eigenstates satisfy the relation

$$<(M_x - <M_x>)^2> = -\frac{1}{2}i\delta <[M_x, M_y]> \tag{28}$$

and applying the commutation relation Eq. 20 we obtain

$$(\Delta M_x)^2 = \frac{\delta}{2} <L_z> . \tag{29}$$

Likewise we find that

$$(\Delta M_y)^2 = \frac{1}{2\delta} <L_z> . \tag{30}$$

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To solve the eigenvalue problem Eq. (27), we introduce the raising and lowering operator $G_\pm$, where

$$G_\pm = \delta M_x + i M_y \mp \sqrt{(1 - \delta^2)} L_z, \tag{31}$$

which have the desired property that these operators satisfy the commutation relation

$$[M_x + i\Delta M_y, G_\pm] = \pm\sqrt{(1 - \delta^2)} G_\pm. \tag{32}$$

Hence if Ψ is an eigenstate with eigenvalue η, then $G_\pm\Psi$ is an eigenstate with eigenvalue $\eta \pm \sqrt{(1 - \delta^2)}$. In particular, there exists eigenstates $\Psi_\pm$ such that

$$G_\pm\Psi_\pm = 0, \tag{33}$$

which have real eigenvalues $\eta_\pm = \pm l_n\sqrt{(1 - \delta^2)}$, where l_n is an integer. It can be shown that these eigenstates minimize the quantum fluctuation sum

$$(\Delta M_x)^2 + (\Delta M_y)^2 + (\Delta L_z)^2, \tag{34}$$

which in this case is equal to l_n, which implies that $\Psi\pm$ are the optimal quantum states to represent classical behavior. Since the eigenvalues η are real it follows from Eq. 27 that for these states

$$< M_x >= \pm l_n\sqrt{(1 - \delta^2)}, \tag{35}$$

and

$$< M_y >= 0, \tag{36}$$

Hence, according to Eq. 33

$$< L_z >= \pm l_n\delta, \tag{37}$$

and applying Eq 34 we obtain

$$(\Delta L_z)^2 = \frac{l_n}{2}(1 - \delta^2). \tag{38}$$

The mean value of the eccentricity for a bound state of energy E_n is $< A_x >= \epsilon = \sqrt{(-2E_n)} < M_x >$, where $E_n = -1/2(l_n + 1/2)^2$. Hence for large l_n, $\epsilon \approx \sqrt{(1 - \delta^2)}$, and substituting for δ Eq. 37 we obtain

$$\epsilon \approx \sqrt{(1 + 2E_n < L_z >^2)}. \tag{39}$$

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This relation corresponds to the well known classical relation between eccentricity, angular momentum and energy of a Keplerian orbit, confirming the validity of our criteria for the construction of a coherent wave packet which exhibits classical properties. The coherent Kepler states can be represented as a linear superposition of the conventional eigenstates $\psi_{n,l}(r, \phi)$ of the Hamiltonanian H and angular momentum operator L_z,

$$\Psi_{\delta,n} = \sum_{l=-l_n}^{l=l_n} c_{n,l}^\delta \psi_{n,l}(r, \phi), \tag{40}$$

where the coefficients $c_{n,l}^\delta$ are determined from recurrence relations [10] obtained by applying Eqs. (27) and (33) to this expansion. We find that

$$c_{n,l}^\delta = \frac{1}{2^{l_n}} \sqrt{\frac{(2l_n)!}{(l_n + 1)!(l_n - 1)!}} (1 - \delta^2)^{l_n/2} [(1 + \delta)/(1 - \delta)]^{l/2} \tag{41}$$

For large quantum numbers l_n these coefficients are well approximated by a Gaussian function

$$c_{n,l}^\delta \approx [\frac{\pi}{2} l_n (1 - \delta^2)]^{1/4} exp[-(1 - \delta l_n)^2 / l_n (1 - \delta^2)] \tag{42}$$

Notice that this expression is of the form

$$c_{n,l}^\delta \propto exp[-(l - < L_z >)^2 / 2(\Delta L_z)^2], \tag{43}$$

where the mean value $< L_z >$ and the root mean square deviation ΔL_z are given by Eqs. (37) and (38) respectively. One of the most interesting and non-trivial results of our analysis is that Eq. 38 determines this width of the Gaussian to be proportional to the mean eccentricity ϵ and to the square root of the principal quantum number of the state. In particular for a circular orbit $\epsilon = 0$, and in this case the sum for the coherent Coulomb state reduces to a single state of maximum value $l = \pm l_n$.

These coherent states can also be obtained by rotations in the O(3) symmetry group of the Coulomb Hamiltonian. By combining Eqs. 27 and 31 we find that

$$(\sqrt{1 - \delta^2} M_x + \delta L_z)\Psi = l_n \Psi. \tag{44}$$

Hence setting $\delta = cos(\theta)$,

$$L_z' = exp(-iMy\theta) L_z exp(iM_y\theta) = M_x sin(\theta) + L_z cos(\theta), \tag{45}$$

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and
$$M'_x = exp(-iMy\theta)M_x exp(iM_y\theta) = M_x cos(\theta) - L_z sin(\theta), \qquad (46)$$

where θ corresponds to a rotation angle about the y-axis, the equation for a coherent state can be written in the equivalent form

$$L'_z\Psi = l_n\Psi \qquad (47)$$

It follows that
$$\Psi = exp(-iM_y\theta)\Psi_c, \qquad (48)$$

is a general solution of these equations, where Ψ_c is an eigenstate of H and L_z which satisfies the condition

$$exp(iM_y\theta)G_{\pm}exp(-iM_y\theta)\Psi_c = (M_x \pm iM_y)\Psi_c = 0 \qquad (49)$$

Hence Ψ_c is a circular eigenstate of H and L_z In three dimensional space, the coherent Kepler states can also be obtained from circular states by corresponding rotations within a SO(3) subgroup of the SO(4) symmetry group of the Coulomb Hamiltonian, as discussed by Bombier, Delande and Gay [11].

References

[1] F. Bloch, *Heisenberg and the early days of quantum mechanics*
Physics Today **29** December 23-27

[2] W. Moore, *Schrödinger, Life and Thought*
(Cambridge University Press, 1989) p. 192

[3] E. Schrödinger, *Quantisierung als Eigenwertproblem*
Annalen der Physik (4) Bd. **79** (1926) 361-376

[4] W. Heisenberg, *Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen.* Z. Phys. **33** 879, received July 29, 1929.

[5] E. Schrödinger, *Der stetige Übergang von der Mikro-zur Macro-m*echanik
Naturwissenchaften **14** (1926) 664.

[6] K. Przibram, *Letters on Wave Mechanics* (Philosophical Library, NY, 1967)

[7] M. Nauenberg, *Wave Packets : Past and Present*, in The Physics and Chemistry of Wave Packets,
edited by J. A. Yeazell and T. Uzer (Wiley and Sons, New York 2000) pp. 1,29

[8] M. Born, Z. Physik **37** (1926) 863; **38** (1926) 803. See also,*Continuity, Determinism and Reality* Dan. Mat. Fys. Medd. **30** nr. 2 (1955)

[9] M. Nauenberg and A. Keith, *Negative Probability and the Correspondence between Classical and Quantum Physics*
In Quantum Chaos-Quantum Measurement, edited by P. Cvitanović, I Percival and A. Wirzba (Kluwer Academic Publications Copenhagen 1991) pp. 265-272

[10] M.Nauenberg, *Quantum Wavepackets on Kepler Elliptical Orbits*,
Physical Review **A 40** (1989) 1133.

[11] J.C. Gay, D. Delande and A. Bommier, Phys. Rev. A **39** (1989) 6587

[12] M. Nauenberg, C. Stroud and Yeazell, *The Classical Limit of an Atom*,
Scientific American June 1994 pp. 44-49

[13] 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 [7].

[14] M. Nauenberg, *The Transition from Quantum to Classical Mechanics in Atomic Physics*,
Comments in Atomic and Molecular Physics, vol. **25**, Nos. 1-3, (1990) pp. 151-157