Wave packets - past and present

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> There was a time when the newspapers reported that only twelve men understood Einstein's theory of relativity. I do not believe that there was ever such a time.... On the other hand, it is safe to say that no one understands quantum mechanics. *R. Feynman* (1967)

> After half a century the relation between quantum mechanics and classical mechanics is still not fully understood. Uncertainty extends even to the foundations. *M. Berry* (1981)

Introduction

Since the time when the above quotations were made, considerable progress has been made in understanding more fully the relation between quantum and classical mechanics, but this correspondence remains an outstanding problem in physics. In classical mechanics the time evolution of a system is determined by Newton's equation of motion, while in quantum mechanics the corresponding evolution is described by a probability distribution given by the modulus square of a wavefunction satisfying Schrödinger's equation. Which of these two mechanics is relevant is usually assumed to depend on whether the system is macroscopic (planets, tennis balls), or microscopic (atoms, molecules, elementary particles), although there are exceptions, e.g. super fluids and super conductors which are macroscopic but obey quantum mechanical laws. However, recently physicists and chemists have been investigating an increasingly large number of systems of intermediary size called mesoscopic systems, where this distinction of size is no longer valid. Moreover, we believe that quantum mechanics is a fundamental theory which should apply to physical systems regardless of size. The key idea to relate these seemingly disparate points of view is the concept of a coherent wave packet in quantum mechanics, which will be elaborated in this book. Such a wave packet gives a probability distribution which can be related in the correspondence limit to an ensemble of orbits in classical mechanics [1]. This connection is fundamental but, as we shall see, it was not understood by some of the main founders of quantum mechanics, and subsequent confusion concerning the relation between quantum and classical mechanics persists even to the present.

Already at the birth of quantum mechanics, Schrödinger tried to explain the connection between his wave equation and classical mechanics by discussing the case of a particle moving in a harmonic oscillator potential [2]. Unfortunately Schrödinger's example, which is most often quoted in the literature, is somewhat misleading because it appears that the evolution of this wave packet describes a single orbit in classical mechanics. A more characteristic example is the case of a free particle which we will discuss in further detail below. In this case the motion in quantum mechanics can be represented by a Gaussian wave packet which is initially confined in space. This wave packet will move along a classical trajectory but spread in position as a function of time. It has been argued that this spreading is an effect which distinguishes quantum from classical behavior, which was the basis for an early criticism by H.A. Lorentz of Schrödinger's equation. However, a more careful examination indicates that the spreading is actually related to classical mechanics. This quantum-classical connection becomes clear if the correspondence is not made with a single classical trajectory , which is deterministic, but with an appropriate ensemble of orbits. Actually it was pointed out already some time ago by M. Born [3] that a single orbit is not an appropriate description for the motion of a particle in classical mechanics. Born concluded that determinism in classical mechanics was " a false appearance" because in practice initial conditions are known only approximately. For example, if the initial velocity for a free particle is determined with an uncertainty δv then the appropriate description of the motion is given by an ensemble of orbits with a distribution of velocity determined with this initial uncertainty. As a consequence, at later times there will be a spread in the position x of the particles given by $\delta x = \delta v\ t$ which increases linearly with time. In fact, we will show that when the initial classical position and velocity uncertainties are described by a Gaussian distribution, the time dependence of the classical and the quantum probability distributions are identically the same, provided there is an appropriate relation between the initial widths of the classical Gaussian distributions. Hence, the spreading of a wave packet is an effect which can be understood classically once the appropriate correspondence with quantum mechanics has been made.

Then where does the essential difference between quantum and classical mechanics appear? In quantum mechanics there is a constraint in the minimum value of the product of the root mean square deviation in position, δx, and in momentum, δp, which is determine by Planck's constant $\hbar$. This constraint is Heisenberg's uncertainty relation, $\delta x \delta p \geq \hbar/2$, while in classical mechanics there are no constraints on the magnitude of these deviations. Moreover, if there are any obstacles or slits, or if an external force acts on the particle, which lead to classical trajectories that are curved in space, then it is possible to have interference effects between separate portions of he wave packet. Such interference effects do not have any analog in classical mechanics, and it is at the time when these interference effects first occur that the quantum-classical correspondence fails, and phenomena which is characteristic of quantum mechanics emerges. Finally there are tunneling effects through potential barriers which do not occur in classical mechanics.

A fundamental problem, which already confounded Schrödinger during the early development of his wave mechanics, is to understand how the Bohr orbits in atomic physics or the corresponding Keplerian orbits in planetary physics emerged from wave mechanics. Over the past years there have been many attempts [4]- [7] to overcome the technical difficulties which Schrödinger first encountered to obtain a coherent wave packet which corresponds to classical motion in the Coulomb potential. However, a complete solution to this problem was obtained only recently [8] [9]. In the following sections coherent wavefunctions which are localized on classical Keplerian ellipses are introduced. It will be shown that the linear superposition of these wavefunctions form coherent wave packets which travel on ellipses with the classical Kepler period t_K, while spreading initially along the orbit, as had been argued originally argued by H.A. Lorentz. Initially this spreading is in accordance with the behaviour of a corresponding ensemble of orbits in classical mechanics [10]. However when the head of the wavepacket catches its own tail interference effects occur, and the quantum-classical correspondence ceases to be valid. Moreover, instead of continuing to spread indefinitely into the future, as had been generally conjectured, the initial wave packet reappears after a definite period t_r [9] [11]- [14]. This recurrence time, which is of purely quantum mechanical origin, depends on the mean principal quantum number n of the wave packet, and $t_r = [n/3]\tau_K \pm 1/2$ where τ_K is the Kepler period. In addition more subtle recurrences occur at rational fractions of this period which do not have any classical analogs. These results have been confirmed experimentally by exciting an electron in alkali atoms to a narrow band of Rydberg states with short pulsed lasers [17]-[19]. We will discuss the dynamics of these coherent wave packets in the presence of weak electromagnetic fields. These fields can be shaped to create and manipulate coherent wave packets in Rydberg atoms, and during the past few years this has become a very active theoretical and experimental field [20]-[23]. We conclude with a new semiclassical time dependent theory of wave packet propagation which demonstrate how the physical origin of the quantum revivals can be understood from the old Bohr quantization of the classical orbits.

Historical Remarks

To describe the stability of atoms and its discrete spectrum of emitted radiation, Niels Bohr postulated in 1913 a quantization rule for Rutherford's classical model of the atom [24]. This model consisted of electrons moving in circular classical orbits about a heavy central charged nucleus, and Bohr's quantization rule, which actually had been proposed a year earlier by J.W. Nicholson [25], required that the angular momentum of the electrons be quantized in units of the Planck's constant $\hbar$. Bohr introduced also a correspondence principle that for a large number of units of $\hbar$ an atomic system should exhibit classical behavior. However, when Schrödinger developed his wave mechanics of the atom Bohr's quantized classical orbits disappeared.

This point was emphasized by both Heisenberg and Pauli who believed that such classical concepts as orbits should be eliminated from the atomic realm . Indeed, there does not appears to be any obvious connection between Keplerian orbits and a typical solution of Schrödinger's equation for the hydrogen atom. Actually, Schrödringer [2] already addressed this problem in 1926 in an article entitled *The transition from Micro- to Macro-Mechanics*, where he treated the harmonic oscillator, and obtained a solution consisting of time dependent Gaussian wave packet which travels without *spreading* along a 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...

Schrödinger sent his paper in manuscript form to Lorentz, with whom he had been corresponding about his new wave mechanics [26]. In a letter 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.

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?...

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...

Earlier Lorentz [26] had written to Schrödinger

> 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 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...

Lorentz pointed out correctly that the association of the wave packet with the charge density of an electron as Schrödinger had proposed, was not tenable if the wave packet dispersed. This dilemma was resolved by Born's introduction of the probability interpretation, but Schrödinger did not accept it, and as late as 1946 he wrote to Einstein that [27]

> 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..

In the next section we will consider the wave packet for a free particle which resolves the difficulty Schrödinger and Lorentz had in understanding the quantum-classical correspondence. Their misunderstanding, which persists to the present, is due to the association of a quantum wave packet with a single classical trajectory rather than an appropriate ensemble of such trajectories; a situation which led Einstein to regard quantum mechanics as an *incomplete* description of physical reality. As Born concluded [28]

> 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.

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

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

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 $|\psi(x,t)|^2dx$ 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

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

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

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

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.

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,

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

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

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

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

$$[L_z, M_x] = iM_y, \tag{18}$$

$$[L_z, M_y] = -iM_x, \tag{19}$$

$$[M_x, M_y] = iL_z, \tag{20}$$

and

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

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 [9] 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

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

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

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

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

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

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,

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

where the coefficients $c^{\delta}_{n,l}$ are determined from recurrence relations [9] obtained by applying Eqs. (27) and (33) to this expansion. We find that

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

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

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

Notice that this expression is of the form

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

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 $\delta = cos(\theta)$,

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

and

$$M'_x = exp(-iMy\theta)M_x exp(iM_y\theta) = M_x cos(\theta) - L_z sin(\theta), \tag{46}$$

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

$$L'_z \Psi = l_n \Psi \tag{47}$$

It follows that

$$\Psi = exp(-iM_y\theta)\Psi_c, \tag{48}$$

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

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

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 [8]. Define

$$\vec{J}_{\pm} = \frac{1}{2}(\vec{L} \pm \vec{M}) \tag{50}$$

Then J satisfies the commutation relations

$$[J_{\pm i}, J_{\pm j}] = i\epsilon_{ijk} J_{\pm k} \tag{51}$$

and

$$[J_{+}, J_{-}] = 0 \tag{52}$$

In particular,

$$\vec{J}_{+}^{2} + \vec{J}_{-}^{2} = \frac{1}{2}(\vec{L}^{2} + \vec{M}^{2}), \tag{53}$$

and the Hamiltonian has the form

$$H = -\frac{1}{(2(\vec{J}_{+}^{2} + \vec{J}_{-}^{2}) + 1)} \tag{54}$$

while

$$\vec{J}_{+}^{2} - \vec{J}_{-}^{2} = \frac{1}{4}(\vec{L}\vec{M} + \vec{M}\vec{L}) = 0. \tag{55}$$

Hence the Coulomb eigenstates can be constructed as a linear superposition of product eigenstates of $\vec{J}_{+}^{2}, J_{+z}$ and $\vec{J}_{-}^{2}, J_{-z}$ respectively with the same maximum eigenvalue of $\vec{J}_{\pm}^{2} = j(j+1)$, and the corresponding Coulomb energy

$$E = -\frac{1}{(2j+1)^{2}} \tag{56}$$

$$\Psi >= exp(i\theta_{+} J_{+x} + \theta_{-} J_{-x} |j, j+ > |j, j- > \tag{57}$$

A numerical example of a coherent Kepler state Ψ_K, Eq. (40) which is localized on a Keplerian ellipse is shown in Fig. 1 ref. [9] which demonstrates that the probability function $\Psi^{\dagger}\Psi$ is localized on an elliptical orbit. This distribution is nearly the same as the corresponding classical distribution satisfying a stationary solution of the Liouville equation for an ensemble of classical orbits with energy E and the same distribution in angular momentum and eccentricity. The observed peak in the distribution is due to the slowing down of the particles when reaching the apogee of the orbit while the minimum occurs, as expected, at perigee where the particle reach maximum velocity.

To obtain a solution which represents an ensemble of classical particles initially localized in angular coordinates on an elliptic orbit, we must consider a linear superposition of these coherent Kepler energy eigenstates. Such a superposition is a time-dependent solution of the Schrödinger equation which generally takes the form

$$\Psi_K(t) = \sum a_n \psi_n \exp(-iE_n t), \tag{58}$$

where the coefficient a_n are constants. We assume that these coefficients have a Gaussian form with a maximum value at $n = \bar{n}$ and a width σ which is determined by experimental conditions,

$$a_n = (2\pi\sigma^2)^{-1/4} exp[-(n-\bar{n})^2]/4\sigma^2]. \tag{59}$$

To show analytically that this superposition gives rise to an angular localized wave packet we consider the special case of a circular orbit in d=2. In this case the coherent state

$$\Psi_{n,l_n}(r,\phi) \propto r^{l_n} exp(-r/(l_n+1)) exp(il_n\phi) \tag{60}$$

where $n = l_n + 1/2$. Expanding the energy eingenvalue E_n up to first order in the difference $n - \bar{n}$ we have

$$E_n \approx E_{\bar{n}} + \frac{2\pi}{\tau}(n-\bar{n}) \tag{61}$$

were $\tau = 2\pi\bar{n}^3$ corresponds to the Kepler period for the orbit. Substituting this expression in Eq. 58, neglecting the dependence on radial coordinates, and approximating the sum over l_n by an integral we obtain

$$\Psi_K \propto exp(il_n\phi - iE_{\bar{n}}t)\ exp[-(\phi - 2\pi t/\tau)^2\sigma^2]. \tag{62}$$

Hence the maximum of this wave packet is at $\phi = 2\pi t/\tau$ representing a classical ensemble of particles moving in circular uniform motion with the Kepler period τ. Substituting $t \to t - t_0$ in Eqs 58 shifts the location of this maximum to $\phi = 2\pi(t-t_0)/\tau$, and corresponds to multiplying the coefficients a_n, Eq. 59 by the complex phase factor $exp(iE_n t_0)$.

Fig. 2 shows a numerical evaluation of the probability distribution $\Psi_K^*\Psi_K$ for a corresponding coherent wave packet in the case of a superposition of elliptic states with mean eccentricity $< A_x >= e$ and angular momentum $< L_z >= l_{\bar{n}}\sqrt{1-e^2}$ where $e = .6$ and $l_{\bar{n}} = 40$ at intervals of one tenth of a Kepler period $T_K = 2\pi n^3$. This wave packet has been launched at perigee at $t = 0$, and it slows down, contracts and becomes steeper as it reaches apogee at $t = \tau/2$. As the wave packet returns to perigee it speeds up again, but it also spreads as can be seen from the figure, and althought it returns to perigee at the end of a Kepler period, $t = \tau$, it has a somewhat more spread out shape. This overall spreading is of classical origin due to the spread in the position and momentum demanded by Heisenberg's uncertainty principle in the corresponding initial ensemble of classical orbits represented by this state. It is this spreading which concerned Lorentz in his correspondence with Schrödinger and lead him to question the validity of Schrödinger's theory which he assumed would represent the behavior of a single electron in the case of the hydrogen atom, rather than that of a classical ensemble of such electrons, as we now properly interpret quantum mechanics. The spreading of the wave packet can be taken into account by including the second order terms in the expansion of the energy eigenvalues E_n in powers of $n - \bar{n}$.

$$E_n = E_{\bar{n}} + E'_{\bar{n}}(n - \bar{n}) + \frac{1}{2}E''_{\bar{n}}(n - n_{\bar{n}})^2 \tag{63}$$

where $E'_{\bar{n}} = 1/\bar{n}^3$ and $E''_{\bar{n}} = -3/\bar{n}^4$. In the approximation that the summation over n is replaced by an integral we then obtain for the the circular wave packet Eq. 62, with $1/\sigma^2$ replaced by $1/\sigma^2 + 2iE''_{\bar{n}}t$

Wave packet Revivals

Evidently this spreading must continue in time, and therefore we expect quantum mechanical interference effects to occur when the head of the wave packet catches up with its tail. Indeed, as we pointed out earlier, the onset of this interference marks the breakdown of the quantum-classical correspondence. However, further surprises are in store. After a certain number of Kepler periods I found that unexpectedly the original wave packet reappeared. This revival had been predicted from numerical calculations of radial wave packets in [11] [12], and it is now well understood analytically [13], [14]. The essential point is that the previous approximation of replacing the sum over

n by and integral is not valid for times t longer than approximately $1/E''_{\bar{n}}$. According to Eq. 63, the phase which appear in Eq. 58 takes the form

$$\theta = 2\pi \frac{t}{\tau}(n - \bar{n})(1 - \frac{3}{2\bar{n}}(n - \bar{n})) \tag{64}$$

Setting

$$t = t_{rev} = ([\bar{n}/3] + \mu)\tau \tag{65}$$

where $[\bar{n}/3]$ is the closest integer to $\bar{n}/3$, we obtain

$$\theta \approx 2\pi(n - \bar{n})([\frac{\bar{n}}{3}] + \mu + \frac{1}{2}(n - \bar{n})) \tag{66}$$

Hence for $\mu = \pm 1/2$, θ is approximately an integer multiple of 2π and consequently the initial wave packet reappears at the revival time t_{rev}, Eq. 65.

This behavior is demonstrated numerically in Fig. 3 which shows the time dependence of the autocorrelation function

$$C(t) =< \Psi_K(t), \Psi_K(0) >= \sum |a_n|^2 exp(iE_n t) \tag{67}$$

in units of the Kepler period for the case that $\bar{n} = 80$ at $\sigma = 6.$. The autocorrelation function measures the overlap of the initial wave packet with the wave packet at a later time t. In this case $\bar{n} = 80$ and therefore $[\bar{n}/3] = 26$. The results during the first few Kepler periods are those expected from the quantum-classical correspondence principle for an ensemble of classical particles moving on nearby elliptic trajectories. Initially after each Kepler period the increased spreading of the wave packet **decrease the overlap with the initial wave packet, and consequently the peak of the autocorrelation decreases while the width broadens until the head of the wave packet catches up with its tail. The onset of interference is seen in the figure after 4 1/2 Kepler periods. As expected at $[\bar{n}/3] = 26$ the initial overlap reappears displaced by 1/2 a Kepler period as predicted by Eq. 65. In addition to this revival, Fig. 3 show that there are more complex revivals of the wave packet which occur near $t = t_{rev}/2$ and other fractional multiples of t_{rev}. These have been discussed in detail by Averbukh and Perelman [13] For example the revival at $t_{rev}/2$ re-occurs at half the Kepler period and correspond to the splitting of the original wave packet into two copies which appear half a Kepler period apart.

Recently Klauder [15] has discussed a specific choice of coefficients a_n in Eq. 58 for time dependent wave packets which form a non-orthogonal but overcomplete set, and provide a representation for the identity operator. However, for a mean principal quantum number n which is typical of current experiments ($n = 50 - 100$) these generalized coherent states spread too rapidly, usually within a Kepler period, and therefore do not exhibit classical behavior or the interesting revival behavior which we have discuss here.

Dynamics of Coulomb Wave Packets in weak time- dependent Electromagnetic Fields

During the past years the laser excitation of electronic wave packets in Rydberg atoms and the manipulation of these states in external electromagnetic fields has become a very active field . In this section our discussion of the dynamics of coherent quantum wave packets in a Coulomb potential is extended to include the effects of time-dependent weak electromagnetic fields, when the energy associated with these fields is small compared to the Coulomb field [20]-[21]. In particular, we consider periodic fields such as microwaves and radio fields with slowly varying amplitudes relevant to experiments. In this case there are at least five important time scales which must be taken into account associated with the following frequencies: the unperturbed Kepler frequency of the electron in the atom $\omega_K = (-2E)^{3/2}$ where $E = -1/(2n^2)$ is the Kepler energy for a principal quantum number n, the frequency ω of the microwave or radio field, the Stark frequency $\omega_s = (3/2)F/\sqrt{(}-2E)$, where F is the Electric field, the Larmour frequency $\Omega = B$, where B is the magnetic field, and the characteristic time T_s to switch-on the fields. I consider the regime where all the applied frequencies are small compared to the unperturbed Kepler frequency, i.e., $\omega << \omega_K$, $\omega_s << \omega_K$ and $\Omega << \omega_K$ in which case a good approximation is to restrict the quantum dynamics to the set of unperturbed degenerate states of a fixed principal quantum number n . It can be readily shown that the reduced Hamiltonian in this approximation is the same as the corresponding classical Hamiltonian obtained by taking a time average over a Kepler period [16].

For the case of crossed electric and magnetic fields, let the x-y plane be the polarization plane of the electric field F, and the z-axis the direction of the magnetic field B. Then the reduced Hamiltonian takes the form

$$H = H_K + \omega_x(t)M_x + \omega_y(t)M_y + \omega_z(t)L_z, \tag{68}$$

where H_K is the unperturbed Coulomb Hamiltonian for the electron in the hydrogen atom, $w_x(t)$ and $w_y(t)$ are the x and y components of the Stark frequency. and Ω_z is the Larmour frequency. The time dependent Schrödinger equation for the state $|\Psi(t)>$ is

$$i\frac{\partial}{\partial t}|\Psi(t)>= H|\Psi(t)> . \tag{69}$$

which we now solve in the adiabatic approximation. S We first find an eigenstate of the time dependent Hamiltonian

$$H|\psi(t)) = E(t)|\psi(t)> \tag{70}$$

where

$$|\psi(t)) = U(t)|\psi(0)> \tag{71}$$

and $U(t)$ is a unitary operator in an SO(3) subgroup of SO(4), Eq. 48.

$$U(t) = exp(iL_z\alpha_t)exp(iM_x\beta_t). \tag{72}$$

Setting

$$w_x = \Delta_t sin(\theta_t)sin(\phi_t), \tag{73}$$

$$w_y = \Delta_t sin(\theta_t)cos(\phi_t), \tag{74}$$

and

$$w_z = \Delta_t cos(\theta_t), \tag{75}$$

we require that $U(t)$ have the property

$$U(t)L_zU(t)^\dagger = sin(\theta_t)(cos(\phi_t)M_x + sin(\phi_t)M_y) + cos(\theta_t)L_z. \tag{76}$$

This relation implies that $\alpha_t = \phi_t$ and $\beta_t = \theta_t$. Assuming that the initial state $|\Psi(0)>$ is the maximal circular eigenstate of L_z with eigenvalue $n-1$ then $\Psi(t)>$ is an eigenstate of H, Eq. 71 corresponding to an eigenvalue $E = E_K + (n-1)\Delta(t)$. Then the adiabatic solution of the time dependent Schrödinger equation, Eq.69 has the form

$$|Psi(t)>= |psi(t)> exp(-iE_K - i(n-1)\int dt\Delta(t) + i\nu_B) \tag{77}$$

where ν_B is the Berry phase [29], [30]. Substitutin Eq. 80 in Eq. 69 we obtain

$$\dot{\nu}_B = -i < \psi(t)|\frac{\partial U(t)}{\partial t}U(t)^\dagger|\psi(t) > \tag{78}$$

where

$$i\frac{\partial U(t)}{\partial t}U(t)^\dagger = -\dot{\phi}L_z - \dot{\theta}_t(cos(\phi_t)M_x - sin(\phi_t)M_y) \tag{79}$$

It is straightforward to evaluate the expectation values of these operators in terms of the the initial condition and we obtain

$$\nu_B = (n-1)\int dt\dot{\phi}_t cos(\theta_t) \tag{80}$$

The above adiabatic solution is valid only for the special initial condition that the state correspond to a maximum circular state, and the condition $U(0) = 1$ imply that that the external fields must also vanish $t = 0$ To obtain a more general solution we introduce a similar unitary transformation

$$U(t) = \exp(i\alpha_t L_z)\exp(i\beta_t M_x)\exp(i\gamma_t L_z), \tag{81}$$

which corresponds to a rotation parametrized by the time dependent Euler angles α_t, β_t and γ_t we set

$$|\Psi(t) >= U(t)U(0)^\dagger \exp(-iH_K t)|\Psi(0) > . \tag{82}$$

Substituting this expression in Eq. (69) we obtain the relations

$$\omega_z = -(\dot{\alpha}_t + \dot{\gamma}_t cos(\beta_t), \tag{83}$$

$$\omega_x = -(\dot{\beta}_t cos(\alpha_t) + \dot{\gamma}_t sin(\beta_t)sin(\alpha_t)), \tag{84}$$

and

$$\omega_y = (\dot{\beta}_t sin(\alpha_t) - \dot{\gamma}_t sin(\beta_t)cos(\alpha_t)). \tag{85}$$

which lead to first order differential equations for these parameters,

$$\dot{\alpha}_t = cot(\beta_t)[\omega_x(t)sin(\alpha_t) + \omega_y(t)cos(\alpha_t)] - \omega_z(t), \tag{86}$$

$$\dot{\beta}_t = -\omega_x(t)cos(\alpha_t) + \omega_y(t)sin(\alpha_t), \tag{87}$$

$$\dot{\gamma}_t = -\frac{1}{sin(\beta_t)}[\omega_x(t)sin(\alpha_t) + \omega_y(t)cos(\alpha_t)]. \tag{88}$$

The initial conditions α_0 , β_0 and γ_0 can now be chosen arbitrarily In general these nonlinear equations are solved numerically , but for special cases analytical solutions can also be obtained. For external fields that change adiabatically we find an approximate solution for these equations. Setting $\omega_x(t) = \omega_s(t) sin(\phi_t)$, $\omega_y(t) = \omega_s(t) cos(\phi_t)$, and Eqs (86)-(88) simplify to

$$\dot{\alpha}_t = \omega_s(t) cot(\beta_t) cos(\alpha - \phi_t) - \omega_z(t), \tag{89}$$

$$\dot{\beta}_t = -\omega_s(t) sin(\alpha - \phi_t), \tag{90}$$

$$\dot{\gamma}_t = -\frac{\omega_s(t)}{sin(\beta_t)} cos(\alpha_t - \phi_t). \tag{91}$$

In the adiabatic approximation when the amplitude of the electric and magnetic fields are varying slowly in time an approximate special solution of these equations is obtained by setting

$$\alpha_t = \phi_t + \delta\alpha \tag{92}$$

Then $\delta\alpha$ must satisfy the equation

$$\delta\alpha \cong \dot{\beta}/\omega_s(t), \tag{93}$$

where to first order in $\delta\alpha$

$$tan(\beta_t) = \omega_s(t)/(\dot{\phi}_t + \omega_z(t)). \tag{94}$$

Hence $sin(\beta_t) = \omega_s/\Delta_t$, where where $\Delta_t = \sqrt{(\omega_s(t)^2 + (\dot{\phi}_t + \omega_z(t))^2)}$, and

$$\gamma_t = -\int_0^t dt' \Delta_{t'}. \tag{95}$$

For $\dot{\phi}_t << \omega_z(t)$ we have

$$\Delta_t \approx \sqrt{\omega_s(t)^2 + \omega_z(t)^2} + \dot{\phi}_t \frac{\omega_z(t)}{\sqrt{\omega_s(t)^2 + \omega_z(t)^2}} \tag{96}$$

where the second term corresponds to the previously calculated Berry phase Eq. 80.

While L_z, M_x and M_y are the generators of an $SO(3)$ subgroup of $SO(4)$, this is not the case for the remaining operators M_z, L_x and L_y. However,

$Lz^2 + M_x^2 + M_y^2$ and $M_z^2 + L_z^2 + L_y^2$ are separately constants of the motion, while $L^2 + M^2 = -1/2E - 1$ is fixed by the Kepler energy $E = -1/(2n^2)$.

The time dependence of the Heisenberg operators L and M can also be obtained from the evolution operator U(t), eg. $L_z(t) = U(0)U(t)^\dagger L_z U(t)U(0)^\dagger$, where $U(t)^\dagger$is the hermitian adjoint of U(t). These operators satisfy the equation

$$\dot{L}_z(t) = i[H, L_z(t)] = \omega_x(t)M_y(t) - \omega_y(t)M_x(t), \tag{97}$$

$$\dot{M}_x(t) = i[H, M_x(t)] = \omega_y(t)L_z(t) - \omega_z(t)M_y(t), \tag{98}$$

$$\dot{M}_y(t) = i[H, M_y(t)] = \omega_z(t)M_x(t) - \omega_x(t)L_z(t). \tag{99}$$

which are exactly the same as the corresponding classical equation. The general solution of these equations can be written explicitly in terms of the Euler angles $\alpha_t, \beta_t, \gamma_t$, and the initial operators, $L_z(0), M_x(0)$ and $M_y(0)$. We have,

$$\begin{aligned} L_z(t) &= [cos(\beta_t)cos(\beta_0) + sin(\beta_t)sin(\beta_0)cos(\gamma_t)]Lz(0) \\ &+[sin(\beta_t)sin(\gamma_t)]M_x(0) \\ &+[cos(\gamma_t)sin(\beta_0) - cos(\beta_0)sin(\beta_t)cos(\gamma_t)]M_y(0), && (100) \\ M_x(t) &= cos(\alpha_t)\bar{M}_x(t) + sin(\alpha_t)\bar{M}_y(t), && (101) \\ M_y(t) &= -sin(\alpha_t)\bar{M}_x(t) + cos(\alpha_t)\bar{M}_y(t), && (102) \end{aligned}$$

where $\bar{M}_x(t)$ and $\bar{M}_y(t)$ are the operators $M_x(t)$ and $M_y(t)$ in a frame of reference rotated by and angle α_t about the $z - axis$,

$$\begin{aligned} \bar{M}_x(t) &= -sin(\gamma_t)sin(\beta_0)L_(0) + cos(\gamma_t)M_x(0) \\ &+sin(\gamma_t)cos(\beta_0)M_y(0), && (103) \\ \bar{M}_y(t) &= [-cos(\beta_t)sin(\beta_0)cos(\gamma_t) + sin(\beta_t)cos(\beta_0)]L_z(0) \\ &-cos(\beta_t)sin(\gamma_t)M_x(0) \\ &+[cos(\beta_t)cos(\beta_0)cos(\gamma_t) + sin(\beta_0)sin(\beta_t)]M_y(0), && (104) \end{aligned}$$

It can be verified that $< L_z >^2 + < M_y >^2 + < M_x >^2$ and $< L_z^2 > + < M_y^2 > + < M_x^2 >$ are both conserved but have different values. The difference corresponding to quantum fluctuations and the classical states are those for which these quantum fluctuations are a minimum. For example, for an orbit in the plane of polarization, we have $< L_z >^2 + < M_y >^2 + < M_x >^2 = (n-1)^2$ and $\Delta L_z^2 + \Delta M_y^2 + \Delta M_x^2 = (n-1)$.

For the case of a circular polarized electric field we can simplify the equations by going to a frame of reference rotating with frequency ω. Setting

$$< L_z(0) >= (n-1)cos(\eta), \tag{105}$$

$$< M_x(0) >= (n-1)sin(\eta)cos(\delta), \tag{106}$$

and

$$< M_y(0) >= (n-1)sin(\eta)sin(\delta), \tag{107}$$

we obtain from Eqs. (100)-(103)

$$< L_z(t) >= (n-1)[cos(\eta)cos(\beta_t) + sin(\eta)sin(\beta_t)sin(\gamma_t - \delta)], \tag{108}$$

$$< \bar{M}_x(t) >= (n-1)sin(\eta))cos(\gamma_t - \delta), \tag{109}$$

and

$$< \bar{M}_y(t) >= (n-1)[cos(\eta)sin(\beta_t) - sin(\eta)cos(\beta_t)sin(\gamma_t - \delta)], \tag{110}$$

An interesting application of Eqs. (108)-(109) is the case that the electric field amplitude F is increased slowly to a value such that $\omega_s/\omega >> 1$. As $\beta_t \to \pi/2$,

$$< L_z(t) >\to (n-1)sin(\eta)sin(\gamma_t - \delta), \tag{111}$$

$$< M_x(t) >\to (n-1)sin(\eta)cos(\gamma_t - \delta), \tag{112}$$

and

$$< M_y(t) >\to (n-1)cos(\eta) \tag{113}$$

For $\eta = 0$, corresponding to initial motion in a circular state, the orbit approaches asymptotically maximum eccentricity along the y-axis. In particular when $\omega_s/\omega >> 1$

$$< M_y(t) >\to (n-1) \tag{114}$$

which implies that asymptotically the component of the Laplace vector along the field in the rotating frame is determined by the mean value of the initial angular momentum [16]. Alternatively, if $\eta = \pi/2$, corresponding initially to zero angular momentum, the orbit approaches a circular state when $\gamma_t - \delta = \pi/2$.

$$< L_z(t) > \rightarrow (n-1) \tag{115}$$

Another interesting solution is obtained for the case that β_t is a constant and $\delta = \pi/2$, [22] in which case Eqs. 92 - 95 are exact.

$$< L_z(t) >= (n-1)[cos(\eta) + (1 - cos(\gamma_t)sin(\beta_0)(sin(\eta - \beta_0))] \tag{116}$$

$$< \bar{M}_x(t) >= (n-1)[sin(\eta - \beta_0))sin(\gamma_t)] \tag{117}$$

$$< \bar{M}_y(t) >= (n-1)[sin(\eta) + (cos(\gamma_t) - 1)cos(\beta_0)sin(\eta - \beta_0)] \tag{118}$$

Then for $\eta = \pi/2$, $\beta_0 = \pi/4$, if γ_t increases from 0 to π an initial state of zero angular momentum is transformed into a circular state. For the case $\eta = \beta_0$ the evolution is time independent in the rotating frame of reference.

Time dependent Semiclassical Approximation for Coulomb Wave Packets

We will now discuss a new semiclassical theory which gives some further insight in the correspondence between quantum and classical mechanics, and provides a useful approximation method for time dependent calculations in quantum mechanics in the correspondence limit. This method was developed originally by Heller, Tomsovic and their collaborators [31] to evaluate correlation functions by the use of multiple periodic classical trajectories, and it is based on a semiclassical approximation to the time dependent Green's function developed by van Vleck. We will describe here a simpler but equivalent form of this technique [33] by solving approximately the time dependent Schrödinger equation for the propagation of a Gaussian wave packet [34], [35] in the Coulomb potential.

The Schrödinger equation in one degree of freedom is

$$i\frac{\partial\psi(q,t)}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi(q,t)}{\partial q^2} + V(q)\psi(q,t), \tag{119}$$

where $V(q) = -1/q$ for the Coulomb potential. A *local* solution of Eq. (119) near a time dependent trajectory q_t is obtained by expanding the potential $V(q)$ up to quadratic terms in the neigborhood of this trajectory,

$$V(q) \approx V(q_t) + V'(q_t)(q - q_t) + \frac{1}{2}V''(q_t)(q - q_t)^2. \tag{120}$$

In this approximation the solution of the Schrödinger equation is a Gaussian wave packet

$$\psi_\beta(q, t) = A \exp[i(\xi_t(q - q_t) + \alpha_t(q - q_t)^2 + \gamma_t)]. \tag{121}$$

where the trajectory q_t is determined by a suitably chosen solution of the classical equations of motion for the Hamiltonian $H = p^2/2 + V(q)$, and the variables ξ_t, α_t, and γ_t are *complex* functions of time which satisfy ordinary nonlinear differential equations [33] obtained by substituting Eq. (121) in the Schrödinger equation (119) with V(q) approximated by Eq. (120). Their initial conditions are determined by the parameters of the initial Gaussian wave packet, and the specific reference trajectory. For example, a normalized initial Gaussian wave packet of variance σ_β^2, centered at q_β and with mean momentum p_β has the form

$$\psi_\beta(q, 0) = (\pi\sigma_\beta^2)^{-1/4} \exp\left(ip_\beta(q - q_\beta) - \frac{(q - q_\beta)^2}{2\sigma_\beta^2}\right). \tag{122}$$

Comparing with Eq. (121) at $t = 0$, one obtains

$$\begin{aligned}
\alpha_0 &= i/2\sigma_\beta^2, \\
\xi_0 &= p^\beta + 2\alpha_0(q_0 - q^\beta), \\
\gamma_0 &= (q_0 - q^\beta)[\alpha_0(q_0 - q^\beta) + p^\beta],
\end{aligned} \tag{123}$$

where q_0 denotes the reference trajectory's initial position and $A = (\pi\sigma_\beta^2)^{-1/4}$.

We now evaluate the autocorrelation function $C_\beta(t)$, where

$$C_\beta(t) = \int dq \psi_\beta^*(q, 0)\psi_\beta(q, t), \tag{124}$$

by constructing the time dependent state as a superposition of wavefunctions, Eq. (121) , corresponding to different reference trajectories, with relative phase equal to unity [33]. For the special case that $q_t = q_0$ we obtain for $t > \tau_\beta$,

$$C_\beta(t) = \sum_j \left\{ \sqrt{\frac{1}{(1 - i\nu_\beta j^2/t)}} \exp\left[3i\frac{\tau_\beta}{q_\beta} j^{2/3} t^{1/3} - \frac{q_\beta^2}{\sigma_\beta} \frac{[(t/j)^{2/3} - 1]^2}{[1 + it/\nu_\beta j^2]}\right] \right\} \tag{125}$$

where the subscript j refers to a given trajectory, t is the time in units of the mean Kepler period $\tau_\beta = 2\pi q_\beta$, and $\nu_\beta = (3/4)\tau_\beta \sigma_\beta^2 / q_\beta^3$. This result is in excellent agreement with exact numerical evaluation of the autocorrelation function [33], see Fig. 4. It can be readily shown that by expanding the phase factors in each term of Eq. (125) to second order in $(j - N)$ at $t = N + \delta$, where N is an integer, these terms add constructively when $N = [n_\beta/3]$ and $\delta = \pm 1/2$, where $q^\beta = 2n_\beta^2$. This implies that the original Gaussian wave packet reappears approximately after a period $t = [n_\beta/3] \pm 1/2$. While the reference trajectories depend generally on time, at the recurrence time these trajectories correspond precisely to the quantized Bohr orbits [14].

Concluding remarks

We have shown that wave packets elucidate the correspondence between quantum and classical mechanics, and give valuable insights in the behaviour of Rydberg atoms in weak electromagnetic fields. The formation of such wave packets has been made possible by the development of tunable short pulsed lasers which has ushered a fruitful series of experiments in atomic, molecular and condensed matter physics and chemistry. Unexpected phenomena like wave packet revivals, which had not been anticipated by the founders of quantum mechanics, have now been confirmed experimentally and may turn out to have valuable applications. Although wave packets emerged early in the development of quantum mechanics, they have occupied center stage only recently with the increasing role of the time domain in experiments. In the presence of strong external fields where chaotic dynamics emerges in the classical regime, a wave packet analysis helps clarify the behavior in quantum mechanics, and surprisingly some recent evidence has shown that revivals can occur even in this domain [38].

The importance of wave packets extends also to other branches of physics. For example, neutrino oscillations which have been observed recently [36] can be understood properly only by a wave packet analysis [37]. Although these oscillations are due to interference effects between different mass eigenstates of the neutrino, and therefore appear to be a pure wave phenomena, it turns out that the neutrino must also travel along nearly classical trajectories. Wave packets are essential in dealing with such wave-particle duality which has marked the physics of this century.

Figure Captions

Fig. 1 The probability distribution for a coherent Coulomb wave packet, Eq. 40, with principal angular momentum $l_n = 40$ and $\delta = 0.8$ which corresponds to eccentricity $e = 0.6$ and mean angular momentum $< L_z >= 32$

Fig. 2 A wave packet moving in an elliptic orbit under the action of a Coulomb potential. The probability distribution is shown here each tenth of a Kepler period.

Fig. 3 The absolute square for the autocorrelation function for a wave packet moving in a Coulomb potential as a function of time in units of the Kepler period. For a mean principal quantum number of $n = 80$, the first full recurrence of the wave packet occurs at $t_r = 26.5$ as predicted by the theory. The figure also shows partial recurrences at $t \approx (1/2)t_r$ with half the Kepler period, and at $t \approx (1/3)t_r$ and $t \approx (2/3)t_r$ with a third of the Kepler period.

Fig. 4 A comparison between the Fourier transform of our semiclassical autocorrelation function, Eq. 125 (solid line), and the corresponding quantum spectra (circles) for the case of $q^\beta = 7200$ and $\sigma_\beta = 600$.

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