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On the evolution of wave packets for particles in central potentials

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Abstract. The manner in which the extension of a small wave packet moving in a circular orbit in a central potential $V(r)$ changes with time is examined. It is shown that in general, the extension in the orbital plane increases indefinitely at large times unless $rV'' - V' = 0$ at the radius of the orbit. The question whether there exist any special 'coherent' wave packets which retain a finite size for arbitrary times in a Coulomb potential is investigated, and the answer is shown to be in the negative.

1. Introduction

One of the strange features of quantum mechanics is the spreading of wave packets representing particle states (Darwin 1927, Kennard 1927). The indefinite spreading of free wave packets, though at an extremely small rate in the case of macroscopic objects, has appeared disturbing enough to induce attempts to suppress it through modification of the theory. de Broglie (1960), notably, has suggested that the Schrödinger equation should be replaced by some nonlinear equation which would preserve the main quantum-mechanical structure but inhibit the spread of wave packets‡. As an alternative possibility, the use of singular solutions§ of the Schrödinger equation has been advocated, for describing point particles (Petiau 1954a,b, 1955, de Broglie 1960). There has also been an attempt (Karolhazy 1966) to link the problem of the spread of wave packets with the curvature of space-time in the general theory of relativity in the hope that this curvature would enable particle wave packets to move along definite trajectories without unlimited spreading. None of these attempts can be said to have really made much headway, and the standard form of quantum mechanics has the allegiance of practically all physicists¶.

It is surprising however that not much attention has been paid to the study of the motion of wave packets in simple realistic systems within the ambit of orthodox theory. Besides the free particle, the harmonic oscillator (in one or more dimensions) seems to

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‡ For a discussion of the spreading of a 'classical wave packet' (ie the group of samples of a statistical ensemble around some point in phase space) see Born and Hooton (1955, 1956), and Born (1958).

§ Such solutions have been called 'the double solutions'. For a discussion of these see de Broglie (1960).

¶ Another aspect of quantum mechanics which has troubled many is the probabilistic nature of its predictions. The possibility of accounting for this in terms of deterministic theories with 'hidden' variables has been subjected to experimental test recently (Freedman and Clauser 1972). The results seem to rule out local hidden variable theories (see for example Bell 1964).

be the only system to have been extensively investigated. It has long been recognized that the latter, unlike the free particle, has wave-packet states such that the size of the packet remains time independent. These are the so-called coherent states which are well known in the literature (Schrödinger 1926, Glauber 1963, Sudarshan 1963, Carruthers and Nieto 1965) and are characterized by a minimum value for the product of the extensions in coordinate and momentum spaces. But even in the case of such an important system as a particle in a Coulomb potential, not much seems to be known about the behaviour of a small three-dimensional wave packet as time progresses, and in particular, as to whether there exist coherent (in the limited sense of non-spreading) wave packets in such a potential.

In view of this situation it seems interesting to investigate the behaviour of wave packets bound in spherically symmetric potentials in three dimensions. Our aim is to check whether there exist wave-packet states in which the uncertainties in the various components of position, momentum etc are time independent. We shall refer to such states as coherent states, for brevity, but it must be noted that the standard usage of this term in the context of the harmonic oscillator implies much more than the mere consistency of the uncertainties. We have pointed out in an earlier paper (Mathews and Eswaran 1973) that in the case of the harmonic oscillator there exists a large class of states representing wave packets whose mean positions move simple harmonically and whose sizes remain time independent but which are not necessarily coherent states in the usual sense; we had termed such states as semi-coherent states. It is conceivable that such states might exist in more general cases too and might show up if one demands coherence only in the loose sense of constancy in position and momentum uncertainties.

The investigation of this question in three-dimensional problems is rendered rather complicated by the interlinking of different degrees of freedom through the potential. However, when the trajectory of the centre of the packet (ie of the mean position of the particle) is circular, the resulting symmetry can be exploited to make the problem tractable. Considering the components of position and momentum in the direction perpendicular to the plane of the orbit and in the radial and tangential directions, we define, in § 2, the uncertainties in these quantities as well as certain correlations among different components. A closed set of coupled equations which determine the temporal variation of these uncertainties and correlations is then obtained under the assumption that the wave packet has a small size. The general solution of this system of equations is presented in § 3. In § 4 we consider the important case of the Coulomb potential and investigate whether there is any choice of the initial form of the wave packet which would ensure that the packet remains coherent (without indefinite spreading) for all times. It turns out that no such possibility exists.

2. Behaviour of a three-dimensional wave packet bound in a spherically symmetric potential

Let us consider a wave packet representing a particle in a central potential and determine how various parameters representing the extension of the wave packet (in the configuration and momentum spaces) change with time. To avoid non-essential complications we shall assume that the mean position moves in a circular orbit of radius R . Defining

$$X = \langle x \rangle, \quad P = \langle p \rangle, \quad (1)$$

we observe that for a circular orbit (of radius $|X| = R = \text{constant}$) in which the particle

moves with angular velocity ω ,

$$\mathbf{X} \cdot \mathbf{P} = 0, \tag{2}$$

$$\mathbf{P}^2 = m^2 \omega^2 R^2, \quad m\omega^2 = \frac{1}{R} \frac{dV}{dR}. \tag{3}$$

To take advantage of the symmetry of the orbit we shall consider uncertainties in the position and momentum components parallel to \mathbf{X} , \mathbf{P} and $\mathbf{X} \times \mathbf{P}$. In the following, these directions will be indicated by subscripts R, T, z respectively (for radial, tangential and z directions, the last being chosen perpendicular to the plane of the orbit). With the notation

$$\delta \mathbf{x} = \mathbf{x} - \mathbf{X}, \quad \delta \mathbf{p} = \mathbf{p} - \mathbf{P}, \tag{4}$$

we define

$$\chi_R = R^{-2} \langle (\delta \mathbf{x} \cdot \mathbf{X})^2 \rangle \tag{5a}$$

$$\chi_T = (m\omega R)^{-2} \langle (\delta \mathbf{x} \cdot \mathbf{P})^2 \rangle \tag{5b}$$

$$\chi_z = \langle (\delta z)^2 \rangle \tag{5c}$$

$$\pi_R = (m\omega R)^{-2} \langle (\delta \mathbf{p} \cdot \mathbf{X})^2 \rangle \tag{5d}$$

$$\pi_T = (m^2 \omega^2 R)^{-2} \langle (\delta \mathbf{p} \cdot \mathbf{P})^2 \rangle \tag{5e}$$

$$\pi_z = (m\omega)^{-2} \langle (\delta p_z)^2 \rangle. \tag{5f}$$

The factors of $m\omega$ and R in the above definitions serve to reduce the dimensions of all the quantities to (length)².

The rates of change of the quantities (5) can be calculated using the quantum equation of motion (Messiah 1966). We present here the resulting equations relegating to the appendix the details of derivation in a couple of typical cases. For χ_z and π_z we obtain the following coupled equations which do not involve any of the quantities referring to uncertainties in the orbital plane:

$$\dot{\chi}_z = 2\pi_z - 2(m\omega^2)^{-1} V_{33} \chi_z \tag{6a}$$

$$\dot{\pi}_z = -(m\omega^2)^{-1} V_{33} \dot{\chi}_z. \tag{6b}$$

Here and elsewhere in this paper, dots indicate differentiation with respect to the non-dimensional parameter

$$\tau = \omega t. \tag{7}$$

The value of $V_{33} \equiv (\partial^2 V / \partial z^2)_{\mathbf{x}=\mathbf{X}}$ is $m\omega^2$, by equations (A.5c) and (3). Equations of the same form as (6), with V_{33} replaced by $m\omega^2$, hold also for a one-dimensional harmonic oscillator†.

As regards χ_R , χ_T , π_R , π_T , which measure the extension in the orbital plane, their first derivatives involve also the following cross correlations among the position and

† Murakhver (1966) obtains the same set of equations for an arbitrary potential in one dimension. Except in the case of the harmonic oscillator, the derivation of these equations involves the neglect of third and higher order terms in the Taylor expansion of $V(\mathbf{x})$ about $\langle \mathbf{x} \rangle$, assuming the smallness of the wave packet.

momentum components:

$$\chi_{RT} = (m\omega R^2)^{-1} \langle (\delta x \cdot X)(\delta p \cdot P) \rangle \tag{8a}$$

$$\pi_{RT} = (m^3 \omega^3 R^2)^{-1} \langle (\delta p \cdot X)(\delta p \cdot P) \rangle \tag{8b}$$

$$\mu_{RR} = (m\omega R^2)^{-1} \langle (\delta x \cdot X)(\delta p \cdot X) + (\delta p \cdot X)(\delta x \cdot X) \rangle \tag{8c}$$

$$\mu_{RT} = (m^2 \omega^2 R^2)^{-1} \langle (\delta x \cdot X)(\delta p \cdot P) \rangle \tag{8d}$$

$$\mu_{TR} = (m^2 \omega^2 R^2)^{-1} \langle (\delta x \cdot P)(\delta p \cdot X) \rangle \tag{8e}$$

$$\mu_{TT} = (m^3 \omega^3 R^2)^{-1} \langle (\delta x \cdot P)(\delta p \cdot P) + (\delta p \cdot P)(\delta x \cdot P) \rangle. \tag{8f}$$

The notation here is as follows: χ stands for a correlation between two components of δx ; π involves two components of δp ; and μ is a cross correlation between one component of δx and one of δp . The first of the subscripts on μ indicates which component of δx is involved, while the second subscript identifies the component of δp . The operators involved in (8d) and (8e) are not explicitly symmetrized with respect to δx and δp but do not differ from the symmetrized forms in the case of circular orbits, in view of equation (2).

The equations for the ten coupled quantities, written in matrix form, appear as follows:

$$\begin{bmatrix} \dot{\chi}_R \\ \dot{\chi}_T \\ \dot{\chi}_{RT} \\ \dot{\pi}_R \\ \dot{\pi}_T \\ \dot{\pi}_{RT} \\ \dot{\mu}_{RR} \\ \dot{\mu}_{RT} \\ \dot{\mu}_{TR} \\ \dot{\mu}_{TT} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 2 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ -1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & \eta & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 1 & 0 & 0 & \eta & -1 & 0 \\ 2\eta & 0 & 0 & 2 & 0 & 0 & 0 & 2 & 2 & 0 \\ 0 & 0 & -1 & 0 & 0 & 1 & -\frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \eta & 0 & 0 & 1 & -\frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & -2 & 0 & 0 & 2 & 0 & 0 & -2 & -2 & 0 \end{bmatrix} \begin{bmatrix} \chi_R \\ \chi_T \\ \chi_{RT} \\ \pi_R \\ \pi_T \\ \pi_{RT} \\ \mu_{RR} \\ \mu_{RT} \\ \mu_{TR} \\ \mu_{TT} \end{bmatrix} \tag{9a}$$

or

$$\dot{u} = Mu \tag{9b}$$

where M is the matrix and u the column vector appearing on the right of equation (9a). The parameter η which appears in M is defined by

$$\eta = - \left(1 + \frac{R}{\omega^2} \frac{\partial \omega^2}{\partial R} \right) = - \left(\frac{rV''}{V'} \right)_{r=R}, \tag{10}$$

the equality of the two forms being a consequence of equation (3).

3. Time dependence of the extension of the wave packet

The manner in which the extension of the wave packet perpendicular to the orbital plane varies with time can be seen from equations (6). Their general solution may be readily verified to be

$$\chi_z(\tau) = \frac{1}{2}(\chi_z(0) + \pi_z(0)) + \frac{1}{2}(\chi_z(0) - \pi_z(0)) \cos 2\tau + \frac{1}{2}\dot{\chi}_z(0) \sin 2\tau \tag{11a}$$

$$\pi_z(\tau) = (\chi_z(0) + \pi_z(0)) - \chi_z(\tau). \tag{11b}$$

Both χ_z and π_z have at most a simple harmonic variation, at twice the orbital frequency. Initial conditions can in fact be so chosen that $\chi_z(0) = \pi_z(0)$ and $\dot{\chi}_z(0) = 0$ making χ_z and π_z time independent.

Consider now equation (9) for the quantities describing extension in the orbital plane. The solution of equations of this form can usually be expressed (Gantmacher 1960) in terms of the eigenvectors $u^{(i)}$ and eigenvalues λ_i of the matrix M as $u = \sum u^{(i)} e^{\lambda_i \tau}$. However the general solution is of this simple type only if M is diagonalizable. In the present case it so happens that M is not a diagonalizable matrix (except for $\eta = -1$). The eigenvalues of M are

$$0 \text{ (4 times), } \quad \pm(\eta - 3)^{1/2} \text{ (twice), } \quad \pm 2(\eta - 3)^{1/2}. \tag{12}$$

If M were diagonalizable, the product $\prod_i (M - \lambda_i)$, wherein the distinct eigenvalues are taken just once each, should vanish. Actual evaluation shows that this product, $M[M^2 - (\eta - 3)][M^2 - 4(\eta - 3)]$, is $(\eta + 1)$ times a nonzero matrix. So M is diagonalizable if $\eta = -1$ (corresponding to a harmonic oscillator potential) but not for any other value of η . The minimal equation of M for general η turns out to be

$$M^3[M^2 - (\eta - 3)]^2[M^2 - 4(\eta - 3)] = 0, \tag{13}$$

showing that M has only two independent eigenvectors belonging to the eigenvalue 0, and only one each belonging to $\pm(\eta - 3)^{1/2}$. This means that the Jordan canonical form of M is

$$M_c = SMS^{-1} =$$

$$\left(\begin{array}{cccccccccccc} 0 & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 0 & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & (\eta - 3)^{1/2} & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & (\eta - 3)^{1/2} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -(\eta - 3)^{1/2} & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -(\eta - 3)^{1/2} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 2(\eta - 3)^{1/2} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -2(\eta - 3)^{1/2} & \cdot & \cdot \end{array} \right) \tag{14}$$

(all zero elements, except on the main diagonal, are indicated by dots). In this canonical representation, our equation (9b) becomes

$$\dot{v} = M_c v, \quad v = Su. \tag{15}$$

The solution of this equation is obtained trivially. By expressing this solution in terms of the elementary vectors $v^{(i)}$ defined by

$$v_j^{(i)} = \delta_{ij}, \tag{16}$$

and then replacing the $v^{(i)}$ by $u^{(i)} \equiv S^{-1}v^{(i)}$, we obtain the general solution of (9) as

$$\begin{aligned} u(\tau) = & (c_1 + c_2\tau + \frac{1}{2}c_3\tau^2)u^{(1)} + (c_2 + c_3\tau)u^{(2)} + c_3u^{(3)} + c_4u^{(4)} + (c_5 + c_6\tau) e^{i\alpha\tau}u^{(5)} \\ & + c_6 e^{i\alpha\tau}u^{(6)} + (c_7 + c_8\tau) e^{-i\alpha\tau}u^{(7)} + c_8 e^{-i\alpha\tau}u^{(8)} \\ & + c_9 e^{2i\alpha\tau}u^{(9)} + c_{10} e^{-2i\alpha\tau}u^{(10)}. \end{aligned} \tag{17}$$

Here we have written

$$(\eta - 3)^{1/2} = i\alpha \quad \text{and} \quad u^{(i)} = S^{-1}v^{(i)}. \tag{18}$$

Potentials for which $\eta > 3$ are of no interest in the present context since they lead to exponentially increasing terms in (17). The constants c_j are determined by the initial values of the components of $u(\tau)$ as

$$c_j = v_j(0) = [Su(0)]_j. \tag{19}$$

It may be noted that

$$\begin{aligned} Mu^{(1)} &= 0, & Mu^{(2)} &= u^{(1)}, & Mu^{(3)} &= u^{(2)} \\ Mu^{(4)} &= 0 \\ Mu^{(5)} &= i\alpha u^{(5)}, & Mu^{(6)} &= i\alpha u^{(6)} + u^{(7)} \\ Mu^{(7)} &= -i\alpha u^{(7)}, & Mu^{(8)} &= -i\alpha u^{(8)} + u^{(7)} \\ Mu^{(9)} &= 2i\alpha u^{(9)} \\ Mu^{(10)} &= -2i\alpha u^{(10)}. \end{aligned} \tag{20}$$

These equations are deduced by similarity transformations from the canonical representation where equations of identical form evidently hold (with M_c and $v^{(i)}$ in the place of M and $u^{(i)}$). As already noted, M has only six independent eigenvectors, namely $u^{(1)}, u^{(4)}$ (both belonging to the eigenvalue zero), $u^{(5)}, u^{(7)}, u^{(9)}$ and $u^{(10)}$. Since M is a real matrix, the eigenvectors belonging to complex conjugate eigenvalues are complex conjugates of each other. It may thus be seen that

$$u^{(5)*} = u^{(7)}, \quad u^{(6)*} = u^{(8)}, \quad u^{(9)*} = u^{(10)}. \tag{21}$$

The components of $u(\tau)$ have to be real, in view of their physical significance, and so

$$c_5^* = c_7, \quad c_6^* = c_8, \quad c_9^* = c_{10}. \tag{22}$$

Explicit expressions for the $u^{(i)}$ are needed for the discussion of the question whether the wave packet can retain a small size for all time. It is not difficult to show that in the case of greatest interest, namely the Coulomb potential ($\eta = 2, \alpha = 1$), the $u^{(i)}$

defined by (18) and (16) are (up to arbitrary normalization factors)

$$\begin{matrix}
 u^{(1)} & u^{(2)} & u^{(3)} & u^{(4)} & u^{(5)} & u^{(6)} & u^{(9)} \\
 \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ -1 \\ 0 \end{bmatrix} & \begin{bmatrix} 0 \\ 0 \\ -\frac{1}{3} \\ 0 \\ 0 \\ -\frac{1}{6} \\ \frac{2}{3} \\ 0 \\ 0 \\ \frac{1}{3} \end{bmatrix} & \begin{bmatrix} \frac{2}{9} \\ 0 \\ 0 \\ 0 \\ \frac{1}{18} \\ 0 \\ 0 \\ -\frac{1}{9} \\ 0 \\ 0 \end{bmatrix} & \begin{bmatrix} 1 \\ 3 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ -1 \\ -1 \\ 0 \end{bmatrix} & \begin{bmatrix} 0 \\ 2 \\ -\frac{1}{2}i \\ 1 \\ 0 \\ -\frac{1}{2}i \\ i \\ 0 \\ -\frac{3}{2} \\ i \end{bmatrix} & \begin{bmatrix} \frac{2}{3}i \\ \frac{2}{3}i \\ -\frac{1}{2} \\ \frac{1}{3}i \\ \frac{1}{3}i \\ 0 \\ \frac{1}{3} \\ -\frac{1}{2}i \\ -\frac{1}{2}i \\ \frac{1}{3} \end{bmatrix} & \begin{bmatrix} 1 \\ -4 \\ 2i \\ -1 \\ 1 \\ i \\ -2i \\ -1 \\ 2 \\ -4i \end{bmatrix}
 \end{matrix} \tag{23}$$

The vectors $u^{(7)}, u^{(8)}, u^{(10)}$ are not shown above, since they are given by (21).

4. Do non-spreading wave packets exist?

We are now in a position to address the question whether it is possible to choose initial conditions in such a way that the wave packet is initially small and remains small for all time. If the size is to remain constant, it is clear that all the coefficients in (17) except c_1 and c_4 must vanish. If this is not possible we may still ask whether it is possible to arrange at least that $c_2 = c_3 = c_6 = c_8 = 0$. (If this can be done, the size will not increase indefinitely though it will have an oscillatory behaviour.) The answer to these questions turns out to be in the negative, however. To see this, let us just consider the constant c_3 which appears as the coefficient of t^2 . It can be expressed in terms of the initial values of the components of u . In the case of the Coulomb potential ($\eta = 2$), for instance, we have

$$c_3 = 18[\chi_R(0) + \pi_T(0) + 2\mu_{RT}(0)], \tag{24}$$

as may be verified by evaluating the right-hand side using (17) and (23). In view of the definitions (5) and (8), the quantity in square brackets can be expressed as

$$\langle [\delta \mathbf{x} \cdot \mathbf{X} R^{-1} + (m^2 \omega^2 R)^{-1} \delta \mathbf{p} \cdot \mathbf{P}]^2 \rangle_{t=0}. \tag{25}$$

This is seen to be the expectation value of the square of a hermitian operator. So it can vanish (making $c_3 = 0$) only in states ψ such that

$$[R^{-1} \delta \mathbf{x} \cdot \mathbf{X} + (m^2 \omega^2 R)^{-1} \delta \mathbf{p} \cdot \mathbf{P}] \psi = 0. \tag{26}$$

However, no such ψ can represent a *small* wave packet, as we shall now see.

Let us choose the x axis so as to pass through the mean position at the initial instant, so that

$$\mathbf{X} = (R, 0, 0), \quad \mathbf{P} = (0, m\omega R, 0) \quad \text{at } t = 0. \tag{27}$$

Then equation (26) reduces to

$$\left[(x - R) + \left(\frac{-i\hbar}{m\omega} \frac{\partial}{\partial y} - R \right) \right] \psi = 0, \quad (28)$$

with the general solution

$$\psi(x, y, z) = \exp\left(\frac{im\omega}{\hbar}(2R - x)y\right) f(x, z), \quad (29)$$

where f is an arbitrary function of x and z . It is evident that ψ merely oscillates, and does not fall off in the y direction. Thus there exists no compact wave packet for which the term proportional to t^2 in (17) is absent.

It is to be noted however that the uncertainties in the radial component of position and the tangential component of momentum (χ_R and π_T) do remain constant or vary at most periodically. This is because the columns $u^{(1)}$, $u^{(2)}$, $u^{(5)}$, which are the only ones appearing with factors of t or t^2 in (17), do not contribute to χ_R and π_T . On the other hand $u^{(1)}$ and $u^{(5)}$ do contribute to χ_T , and this quantity increases indefinitely, ie, the wave packet, even if it is well defined initially, spreads gradually in the tangential direction.

The case of central potentials other than the Coulomb potential can be analysed similarly, using the vectors $u^{(i)}$ for arbitrary η instead of the special forms (23) valid for $\eta = 2$. The results in general are similar to those obtained above, except when $\eta = -1$. Apart from the isotropic harmonic oscillator potential for which $\eta = -1$ identically, other potentials too may have particular values of the radius R at which η has this special value; a wave packet in orbit at such a radius would then keep a constant size indefinitely (within the approximations based on the smallness of size). In all other cases the wave packet must necessarily spread, and the spreading is in the direction tangential to the orbit.

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Appendix

We indicate here briefly the derivation of equations (9) governing the spreading of a wave packet moving in a circular orbit in a central potential $V(r)$. The derivation is somewhat simplified if expressions for the χ , π etc which take into account equations (2) and (3) are used from the beginning. For example

$$\begin{aligned} \chi_R &= R^{-2} X_i X_j \langle x_i x_j \rangle - R^2, \\ \pi_R &= (m\omega^2 R)^{-2} X_i X_j \langle p_i p_j \rangle, \\ \mu_{RR} &= (m\omega R^2)^{-1} X_i X_j \langle p_i x_j + x_i p_j \rangle, \end{aligned} \quad (A.1)$$

etc where the convention of summation over repeated indices is assumed. We also use the fact that for a small wave packet in a circular orbit

$$dX/dt = \mathbf{P}/m \quad \text{and} \quad d\mathbf{P}/dt = - (dV/dR)(\mathbf{X}/R).$$

The rates of change of $x_i x_j$, $p_i p_j$ etc, and hence of their expectation values are obtained from the Heisenberg equation of motion

$$\frac{dA}{dt} = \frac{1}{i\hbar}[A, H] + \frac{\partial A}{\partial t}. \tag{A.2}$$

In the case of χ_R one obtains then

$$m\omega R^2 \dot{\chi}_R = X_i X_j \langle x_i p_j + p_i x_j \rangle + \langle x_i x_j \rangle (X_i P_j + P_i X_j).$$

In view of (A.1), this reduces to

$$\dot{\chi}_R = \mu_{RR} + 2\chi_{RT}, \tag{A.3}$$

which is just the first row of the matrix equation (9). This is exact.

In the case of π_R we obtain, with the aid of (A.2),

$$\dot{\pi}_R = \frac{1}{m^2 \omega^3} \left[-\frac{X_i X_j}{R^2} \left(\left\langle \frac{\partial V}{\partial x_i} p_j \right\rangle + \left\langle p_i \frac{\partial V}{\partial x_j} \right\rangle \right) + \frac{1}{mR^2} \langle p_i p_j \rangle (X_i P_j + P_i X_j) \right]. \tag{A.4}$$

Now we expand V in Taylor series about $X(t)$, and neglect terms of order higher than the second in δx (assuming that the size of the packet is much less than R).

$$V(r) \simeq V(R) + V_i \delta x_i + \frac{1}{2!} V_{ij} \delta x_i \delta x_j \tag{A.5a}$$

where

$$V_i = \left(\frac{\partial V}{\partial x_i} \right)_{\mathbf{x}=\mathbf{x}} = X_i \frac{1}{R} \frac{dV}{dR} \tag{A.5b}$$

$$V_{ij} = \left(\frac{\partial^2 V}{\partial x_i \partial x_j} \right)_{\mathbf{x}=\mathbf{x}} = \delta_{ij} \frac{1}{R} \frac{dV}{dR} + X_i X_j \frac{1}{R} \frac{d}{dR} \left(\frac{1}{R} \frac{dV}{dR} \right). \tag{A.5c}$$

We then have, for instance,

$$\left\langle \frac{\partial V}{\partial x_i} p_j \right\rangle = V_i P_j + V_{ik} \langle x_k p_j \rangle - X_k P_j. \tag{A.6}$$

This quantity appears contracted with $X_i X_j$ in equation (A.4), and in this process, the terms proportional to P_j in (A.6) drop out in view of equation (2). So we are left with

$$\begin{aligned} X_i X_j \left\langle \frac{\partial V}{\partial x_i} p_j \right\rangle &= R^{-2} X_i X_j \langle x_i p_j \rangle V_{it} = X_i X_j \langle x_i p_j \rangle \left[\frac{1}{R} \frac{dV}{dR} + R \frac{d}{dR} \left(\frac{1}{R} \frac{dV}{dR} \right) \right] \\ &= -X_i X_j \langle x_i p_j \rangle m\omega^2 \eta. \end{aligned} \tag{A.7}$$

Introducing this in (A.4), we obtain

$$\dot{\pi}_R = 2\pi_{RT} + \eta \mu_{RR}, \tag{A.8}$$

which is the fourth row of equation (9). The remaining rows of the equation may be obtained in a similar fashion, the approximation (A.5) being used where necessary to obtain a closed set of equations.

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