Shape-invariant wave packets for three-dimensional harmonic oscillators

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It is shown that for a three-dimensional harmonic oscillator there exist families of Gaussian wave packets that retain their shape during the time evolution, i.e., the wave packet rotates around its center without spreading or deforming. This generalizes the concept of coherent vibrational motion to coherent rotational motion.

I. INTRODUCTION

The time propagation of wave packets has been a favorite topic ever since the early days of quantum mechanics when the relation to classical mechanics was an obvious concern.[1] In the 1960s, after Glauber's contribution to quantum optics,[2] wave packets as coherent states became an important subject. Again recently, quantum wave packets in the wider context of generalized coherent states have attracted much attention.[3] This may be due to the imminence of time resolved experiments in various fields of physics. Already today, a number of experiments in atomic physics have shown that wave packets can be experimentally prepared and various aspects of their evolution in time can be studied.[4]

It is well known in quantum mechanics that wave packets propagating in free space disperse completely. When bounded by potential walls, wave packets tend to become "flexible": the dispersion and the collision with the walls counteract each other and the result is a wave packet whose shape changes, increasing and decreasing in size, as it moves about. This is true even for Gaussian wave packets in harmonic oscillator potentials. In one dimension the width of such a wave packet oscillates periodically unless the initial width is matched exactly to the harmonic oscillator potential. In the latter case the shape (here the width) of the wave packet remains rigid while its center moves along a classical trajectory (Glauber state). In three dimensions, the shape of the wave packet is defined as the spatial form of the probability density distribution, and in general it will deform in a complicated way when the wave packet evolves in time.

In this paper we are interested in finding the generalization of conditions for a wave packet to have rigid shape for three dimensions. This is motivated by the fact that if the shape of the wave packet is fixed, the motion can only consist of a translation and a change of orientation, i.e., rotation. It is well known that rotations occur in a great variety of physical systems. Molecular rotations are the best established examples.[5] In nuclear physics, many rotational spectra are observed[6] and recently also in atomic physics collective electron motion is found to exhibit rotations.[7] In actual fact such rotation will never be perfect because of the coupling with other forms of motion. However, as a first approximation, the idealization of a perfectly rotating wave packet may be useful. As the study of a single particle in a mean field is the basis of all microscopic models of many-body systems, we investigate in this paper the possibility of wave packets with a rigid shape for one particle in an oscillator potential in three dimensions.

In a previous paper[8] we have considered the two-dimensional case. It was found that there exists a one-parameter family of Gaussian wave packets whose shape remains rigid during propagation in a harmonic oscillator potential. The shape of these wave packets, as determined from the equidensity lines of their density distribution, is an ellipse. The parameter can be taken to define the deformation or elongation of that ellipse. Then if the wave packet is started with the appropriate angular momentum, the density distribution will at all times retain the same deformation. Its orientation, however, will change and the wave packet will rotate uniformly around its center. Our family of rigid wave packets contains the two-dimensional analogs of the Glauber state as the special case with no deformation, i.e., the ellipse is a circle. Unlike these Glauber states, a generic member of the one-parameter family is not a minimum uncertainty wave packet. However, its uncertainty products, taken along the principal axes of the density distribution, are equal and constant in time.

In this paper we investigate the existence of rigid Gaussian wave packets in a three-dimensional harmonic oscillator potential. In Sec. II we present the equations of motion for a general Gaussian wave packet. In Sec. III we establish the necessary and sufficient conditions for constant shape. It turns out that the conditions are much more difficult to analyze than in the two-dimensional case. In Sec. IV we present the solutions in the form of two families of rotating wave packets. In Sec. V we look into the properties particular to the wave packets in these two families.

II. GAUSSIAN WAVE-PACKET DYNAMICS

The most general Gaussian wave packet describing a particle in three dimensions can be written, up to a phase and normalization factor,

$$\Psi(\mathbf{x})=\exp-\tfrac{1}{2}[(\mathbf{x}-\mathbf{q})\underline{U}^{-1}(\mathbf{x}-\mathbf{q}) -i(\mathbf{x}-\mathbf{q})\underline{V}(\mathbf{x}-\mathbf{q})-2i\mathbf{p}\cdot\mathbf{x}] \ . \quad (1)$$

We shall assume all lengths to be expressed in units of b, the oscillator length, and all momenta in units of $\hbar/b$. The particle coordinate is $\mathbf{x}$ whereas $\mathbf{q}$, $\mathbf{p}$, $\underline{U}$, and $\underline{V}$ are parameters. The position and momentum of the center of the wave packet are given by $\mathbf{q}$ and $\mathbf{p}$; the probability density $\rho=\Psi^*\Psi$ is determined by the symmetric, positive matrix $\underline{U}$. Up to normalization we have

$$\rho(\mathbf{x})=\exp[-(\mathbf{x}-\mathbf{q})\underline{U}^{-1}(\mathbf{x}-\mathbf{q})] \ . \quad (2)$$

The surfaces of constant probability density are ellipsoids. The lengths of their axes (squared) and their orientation are determined by the eigenvalues and eigenvectors of the matrix $\underline{U}$. The probability current density (in units $\hbar/mb$) is given by

$$\mathbf{j}(\mathbf{x})=\rho(\mathbf{x})[\mathbf{p}+\underline{V}(\mathbf{x}-\mathbf{q})] \ . \quad (3)$$

The symmetric matrix $\underline{V}$ is the "rate of strain" tensor[9] ($V_{ij}=\partial v_i/\partial x_j$) pertaining to the velocity field $\mathbf{v}=\mathbf{j}/\rho$.

When the wave packet (1) is considered as the initial state and the particle is moving in an isotropic harmonic oscillator potential $\frac{1}{2}\omega\mathbf{x}^2$, then it is well known that the time-dependent wave function will remain of the form (1) at all times. The time dependence of the parameters $\mathbf{q}$ and $\mathbf{p}$ is determined by Ehrenfest's equations and hence by the formulas of a classical oscillator. This indicates that the center of the wave packet follows a classical trajectory. The shape dynamics of the wave packet is governed by the equations of motion of the matrices $\underline{U}$ and $\underline{V}$:

$$\frac{d\underline{U}}{dt}=\omega(\underline{U}\,\underline{V}+\underline{V}\,\underline{U}) \ , \quad (4)$$

$$\frac{d\underline{V}}{dt}=\omega(\underline{U}^{-2}-\underline{V}^2-\underline{1}) \ . \quad (5)$$

These can be obtained as generalized Ehrenfest's equations bearing in mind that the elements of the matrices $\underline{U}$ and $\underline{V}$ are expectation values of bilinear expressions in the particle coordinates and momenta. The derivation is rather straightforward and is outlined in the Appendix.

Obviously, the rigid shape conditions are most easily expressed when the equations of motion are referred to the body-fixed frame, i.e., the frame with coordinate axes along the principal axes of $\underline{U}$. If we introduce the instantaneous angular velocity $\underline{\Omega}$ of the body-fixed frame with respect to the space-fixed frame,

$$\Omega_{ij}=e_{ijk}\Omega_k \ , \quad (6)$$

Eqs. (4) and (5), in the body-fixed frame, read

$$\frac{d\underline{U}}{dt}=\omega(\underline{U}\,\underline{V}+\underline{V}\,\underline{U})+[\underline{\Omega},\underline{U}] \ , \quad (7)$$

$$\frac{d\underline{V}}{dt}=\omega(\underline{U}^{-2}-\underline{V}^2-\underline{1})+[\underline{\Omega},\underline{V}] \ . \quad (8)$$

Here, and henceforth, the symbol d/dt stands for the *rate of change with respect to the body-fixed axes*. These equations are the matrix analogs for the traditional vectorial equations in the classical mechanics of rotating frames. Equations (7) and (8) constitute the dynamical system that we need to investigate.

The $\underline{U}$- and $\underline{V}$-dependent parts of the angular momentum and energy are conserved quantities with respect to the equations of motion above. The internal angular momentum (cf. Appendix) is connected with the matrix $\underline{V}$ by

$$\underline{L}=\tfrac{1}{2}(\underline{U}\,\underline{V}-\underline{V}\,\underline{U}) \quad (9)$$

or, using *components with respect to the body frame* in which $\underline{U}$ is diagonal $U_{ij}=U_i\delta_{ij}$, we obtain

$$L_{ij}=e_{ijk}L_k=\tfrac{1}{2}(U_i-U_j)V_{ij} \ . \quad (10)$$

The energy E separates (cf. Appendix) in U-dependent terms and a V-dependent kinetic term that can be written as

$$T=(\omega/4)\mathrm{Tr}(\underline{V}\,\underline{U}\,\underline{V}) \quad (11)$$

or expressed in components referring to the body frame:

$$T=\omega\left[\frac{1}{4}\sum_{i=1}^{3}U_iV_{ii}^2+\sum_{k=1}^{3}L_k^2/2I_k\right] \ . \quad (12)$$

We distinguish a vibrational and rotational part. The first term is called vibrational because the equation of motion (7) reveals that V_{ii} is proportional to dU_i/dt, i.e., the rate of change of the length of the ellipsoid. Thus V_{ii} controls the shape vibration along the i axis. The second term is proportional to angular momentum squared and clearly rotational. It contains the "dynamical moments of inertia"

$$I_1=\frac{(U_2-U_3)^2}{2(U_2+U_3)} \ , \quad I_2=\frac{(U_3-U_1)^2}{2(U_3+U_1)} \ , \quad I_3=\frac{(U_1-U_2)^2}{2(U_1+U_2)} \ . \quad (13)$$

In general these moments of inertia depend on time via the shape parameters of the wave packet. From the nondiagonal elements of (7), we deduce the relation between Ω_i, L_i and I_i, namely,

$$L_i=I_i\Omega_i \ . \quad (14)$$

The conservation of angular momentum can be expressed as

$$\frac{d\underline{L}}{dt}=[\underline{\Omega},\underline{L}] \ . \quad (15)$$

By using (14), we can obtain the relations

$$\frac{d(I_1\Omega_1)}{dt}=(I_2-I_3)\Omega_2\Omega_3 \ , \quad \frac{d(I_2\Omega_2)}{dt}=(I_3-I_1)\Omega_3\Omega_1 \ , \quad \frac{d(I_3\Omega_3)}{dt}=(I_1-I_2)\Omega_1\Omega_2 \ , \quad (16)$$

which extend Euler's equations to a deformable body.

III. MOTION WITH CONSTANT SHAPE

The equations of motion of the preceding section describe how the shape of the wave packet will evolve. In general the orientation and the size and deformation of the density ellipsoids will change as nonharmonic periodic functions.

A numerical solution of the equations of motion [Eqs. (4) and (8)] can be obtained straightforwardly by solving the system of simultaneous first-order differential equations by one of the standard methods, starting from given initial conditions. This solution yields in particular the time evolution of the matrix $\underline{U}$ (i.e., of its matrix elements) which characterizes the shape and orientation of the density ellipsoids. By diagonalizing the matrix $\underline{U}$ one obtains eigenvalues and eigenvectors. The former define the size and deformation (or shape), the latter the orientation of the density ellipsoid as the eigenvectors indeed define the rotation matrix diagonalizing $\underline{U}$. By considering the general form for a rotation matrix[10]

$$\underline{R}=\underline{1}+\underline{N}\sin\alpha+\underline{N}^2(1-\cos\alpha) \tag{17}$$

where

$$\begin{aligned} &\mathbf{n}\cdot\mathbf{n}=1 ,\\ &N_{ij}=-\epsilon_{ijk}n_k ,\\ &N^2_{ij}=n_in_j-\delta_{ij} ,\\ &\underline{N}^3=-\underline{N} , \end{aligned} \tag{18}$$

and using $\mathbf{n}=(n_1,n_2,n_3)$ with

$$\begin{aligned} &n_1=\sin\theta\cos\phi ,\\ &n_2=\sin\theta\sin\phi ,\\ &n_3=\cos\theta , \end{aligned} \tag{19}$$

one easily deduces expressions for the orientation angles θ, ϕ, and α; θ (measured with respect to the 3-axis in the laboratory frame) and ϕ (measured with respect to the 1-axis in the laboratory frame) fix the rotation axis, whereas α yields the rotation angle.

We have calculated the time evolution with initial conditions for the $\underline{U}$ matrix equal to $U_{11}=1.2$, $U_{12}=0.1$, $U_{22}=0.6$, $U_{13}=0.18$, $U_{23}=0$, and $U_{33}=1.8$ and for the $\underline{V}$ matrix equal to $V_{11}=0.04$, $V_{12}=1.0$, $V_{22}=0.06$, $V_{13}=0.4$, $V_{23}=0.01$, and $V_{33}=0.04$, the results of which are shown in Fig. 1. From this figure one notices the nonharmonic behavior in time of the deformation of the wave packet, as well as a rather wild rotational motion. A closer look at the lower panel shows, however, that with these initial conditions the rotation is not too far from a uniform one, around an axis that is reasonably stable. The discontinuities in θ and ϕ defining the axis of rotation, as well as the change of slope in the rotation angle α only indicate that the direction of the axis and the angle of rotation are not uniquely defined.

We have also restricted the initial conditions to planar dynamics by the choice $U_{11}=1.0$, $U_{12}=0$, $U_{22}=0.7$, $U_{13}=0$, $U_{23}=0.2$, and $U_{33}=1.8$ for the $\underline{U}$ matrix and $V_{11}=0$, $V_{12}=0$, $V_{22}=0.06$, $V_{13}=0$, $V_{23}=0.5$, and $V_{33}=0.04$, for the $\underline{V}$ matrix with the time evolution of $\underline{U}$ shown in Fig. 2. Again we notice the nonharmonic behavior of the deformation and the near uniformity of the rotation for this set of initial conditions, now of course around a fixed axis (all couplings between direction 1 and the other two are zero in the initial condition matrices).

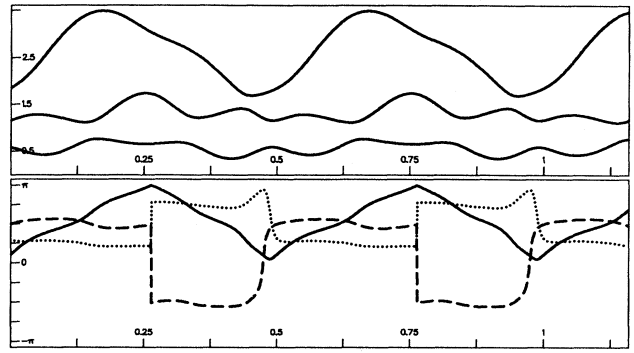

FIG. 1. Time evolution of the shape and orientation parameters of the $\underline{U}$ matrix in a general case (for initial conditions see text). Eigenvalues are shown in the upper panel, orientation angles in the lower panel (solid line, α; dotted line θ; dashed line, ϕ). Time in units $2\pi/\omega$.

We now wish to look for special initial conditions for which the shape of the wave packet remains constant and hence the probability density evolves as if it were a rigid body. The necessary and sufficient conditions for rigidity of the wave packet are

$$\frac{dU_1}{dt}=\frac{dU_2}{dt}=\frac{dU_3}{dt}=0 \tag{20}$$

at all times. These conditions must be substituted in Eqs. (7) and (8) in order to ascertain that such special orbits can exist. Let us first look at Eq. (7). Its diagonal elements reduce to

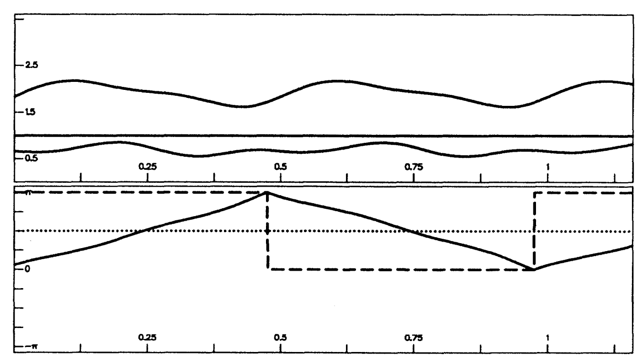

FIG. 2. Time evolution of the shape and orientation parameters of the $\underline{U}$ matrix in an axial case (for initial conditions see text). Same caption as for Fig. 1.

$$2U_iV_{ii}=0 \quad (21)$$

while the off-diagonal elements yield

$$(U_1-U_2)\Omega_3=\omega(U_1+U_2)V_{12} ,$$
$$(U_2-U_3)\Omega_1=\omega(U_2+U_3)V_{23} , \quad (22)$$
$$(U_3-U_1)\Omega_2=\omega(U_3+U_1)V_{13} .$$

From the former it follows immediately that

$$V_{11}=V_{22}=V_{33}=0 . \quad (23)$$

This was to be expected for we had noticed that the V_{ii} define the rate of change of the U_i and we have required these to be constant. Let us now rewrite (8), taking into account that the dV_{ii}/dt must be zero and substituting for the elements V_{ij} their expression in terms of Ω_k from (22). We obtain from the diagonal elements of (8) that

$$\xi_{13}(\xi_{13}-2)\Omega_2^2+\xi_{12}(\xi_{12}-2)\Omega_3^2=\omega^2(U_1^{-2}-1) ,$$
$$\xi_{23}(\xi_{23}-2)\Omega_1^2+\xi_{12}(\xi_{12}+2)\Omega_3^2=\omega^2(U_2^{-2}-1) , \quad (24)$$
$$\xi_{23}(\xi_{23}+2)\Omega_1^2+\xi_{13}(\xi_{13}+2)\Omega_2^2=\omega^2(U_3^{-2}-1) ,$$

where we have set

$$\xi_{ij}=\frac{U_i-U_j}{U_i+U_j} . \quad (25)$$

The set of Eq. (24) expresses the components Ω_k in terms of the shape parameters U_i. Therefore if U_i are constant in time, the Ω_k also are and hence also the V_{ij}. This result already tells us that the instantaneous angular velocity is constant, so the wave packet will rotate uniformly about a fixed axis. Furthermore due to $d\underline{V}/dt$ being zero, the off-diagonal elements of (8) simplify to

$$(\xi_{13}\xi_{23}-\xi_{13}-\xi_{23})\Omega_1\Omega_2=0 ,$$
$$(\xi_{12}\xi_{23}+\xi_{12}-\xi_{23})\Omega_1\Omega_3=0 , \quad (26)$$
$$(\xi_{12}\xi_{13}+\xi_{12}+\xi_{13})\Omega_2\Omega_3=0 .$$

Conditions (24) and (26) constitute six equations for the six unknowns U_i and Ω_k, while Eqs. (23) and (22) define the corresponding V_{ij}. The equations are highly nonlinear. In the next section we shall attempt to find and classify their solutions.

IV. RIGID WAVE PACKETS

Let us analyze systematically the conditions (26) and (24). Equations (26) can be satisfied by setting respectively, all, two, one, or none of the $\underline{\Omega}$ components equal to zero. This produces four different situations that we will investigate separately.

A. Case 1

Let us suppose

$$\Omega_1=\Omega_2=\Omega_3=0 \quad (27)$$

then (24) immediately requires

$$U_1=U_2=U_3=1 . \quad (28)$$

The solution is nothing but the three-dimensional Glauber state with matched width. It has a spherically symmetric shape and no rotational dynamics.

B. Case 2

Let us suppose

$$\Omega_1\neq 0;\quad \Omega_2=\Omega_3=0 . \quad (29)$$

Equations (26) are automatically satisfied. From the first equation in (24) we see that $U_1=1$. Now either $\xi_{23}=0$ or $\xi_{23}\neq 0$. In the former case the other two equations (24) again imply $U_2=U_3=1$ and we are back in case 1. In the latter case the equations (24) can be transformed by straightforward substitution to the conditions

$$\Omega_1^2=\omega^2 \quad \text{and} \quad U_2^{-1}+U_3^{-1}=2 . \quad (30)$$

Since $\xi_{23}\neq 0$ we know that $U_2\neq U_3$ and the above relation tells us that U_2 and U_3 both are different from 1 and hence from U_1. In this case the wave packet has a triaxial deformation. This type of solution constitutes a one-parameter family of wave packets, rotating uniformly with angular velocity ω around a fixed axis along the principal 1-axis. In fact we have here six different families corresponding to the three different choices of nonzero $\underline{\Omega}$ component and its sign ($\pm\omega$).

C. Case 3

Let us suppose

$$\Omega_1=0,\quad \Omega_2\neq 0,\quad \Omega_3\neq 0 . \quad (31)$$

Equations (26) are satisfied if (and only if)

$$\xi_{12}\xi_{13}+\xi_{12}+\xi_{13}=0 . \quad (32)$$

If now ξ_{12} or ξ_{13} were to be zero, relation (32) would impose that they be both zero and again we would be reduced to case 1. So we take both ξ_{12} and ξ_{13} to be nonzero and because of (32) they must also be different from one another. Again we have triaxial wave packets. Equations (24) can be viewed as three linear equations for two unknowns (Ω_2^2 and Ω_3^2). The existence of a solution implies a compatibility relation between the parameters ξ_{ij}. Together with (32) these relations can be put in a simple form in terms of the parameters U_i:

$$U_1^{-1}+U_2^{-1}+U_3^{-1}=3 , \quad (33)$$
$$U_1=U_2U_3 . \quad (34)$$

These operations of nonlinear equations are almost intractable but can easily be performed using a symbolic manipulation package such as MATHEMATICA.

The solutions of (24) can be written in the form

$$\Omega_2^2=(4\omega^2)\frac{U_2-U_1}{U_2-U_3},\quad \Omega_3^2=(4\omega^2)\frac{U_1-U_3}{U_2-U_3} , \quad (35)$$

from which it follows that $\Omega=\pm 2\omega$. Notice that the right-hand side in the above equations is always positive because (33) and (34) tell us that either $U_2 > U_1 > U_3$ or $U_3 > U_1 > U_2$. In fact here we have 12 different families corresponding to the three possible choices of nonzero Ω components and to the four different sign combinations for Ω_2 and Ω_3 obtained from (35).

D. Case 4

Let us finally suppose all Ω_i to be different from zero. Then (26) immediately requires all ξ_{ij} to be zero and we are back to case 1.

In this section we have shown that the conditions for shape conservation of the Gaussian wave packet can be solved and that the solutions, apart from the trivial spherical Glauber state, come in two classes. One family of solutions has angular velocity ω and another 2ω. This is not surprising. Indeed, the shape parameters, being expectation values of bilinear products of coordinates and momenta, will contain time-dependent terms with frequency at most equal to 2ω.

V. RESULTS AN DISCUSSION

Aside from the trivial "spherical" Glauber states, we have found two distinct classes of rigid wave packets. The first is defined by the relations

$$\begin{aligned} &U_1=1, \quad U_2^{-1}+U_3^{-1}=2 , \\ &\Omega_1=\pm\omega, \quad \Omega_2=\Omega_3=0 . \end{aligned} \tag{36}$$

The wave packet has a triaxial shape because either $U_2 < U_1 < U_3$ or $U_3 < U_1 < U_2$. The angular momentum is given by

$$L_1=\pm I_1\omega, \quad L_2=L_3=0 . \tag{37}$$

It is parallel to the rotation axis, which is the 1-axis, i.e., the middle axis of the density ellipsoid. Thus we have a rigid wave packet that rotates uniformly with angular velocity ω around a fixed axis.

The second family of solutions is defined by the relations

$$\begin{aligned} &U_1^{-1}+U_2^{-1}+U_3^{-1}=3, \quad U_1=U_2U_3 , \\ &\Omega_1=0, \quad \Omega_2=\pm 2\omega \left[\frac{U_2-U_1}{U_2-U_3} \right]^{1/2} , \\ &\Omega_3=\pm 2\omega \left[\frac{U_1-U_3}{U_2-U_3} \right]^{1/2} . \end{aligned} \tag{38}$$

Again the wave packet has a triaxial shape because either $U_2 < U_1 < U_3$ or $U_3 < U_1 < U_2$. However, one can also easily derive that the dynamical moments of inertia I_2 and I_3 are equal. Although the probability distribution of the wave packet is triaxial the ellipsoid defined by the dynamical moments of inertia is axially symmetric and the usual relations

$$\underline{L}=I\underline{\Omega}, \quad T=\tfrac{1}{2}I\underline{\Omega}^2 \tag{39}$$

for the axial rotor apply. We conclude that in this case also we obtain a one-parameter family of rigid wave packets rotating uniformly with angular velocity 2ω around a fixed axis in the (2,3)-principal plane, i.e., the plane that is orthogonal to the middle axis of the density ellipsoid.

The two sets of wave packets described above are the only possible geometries, in oscillator dynamics, for rotational motion with a rigid shape. It is noteworthy that none of these geometries corresponds to an axial shape. This may be traced back to the fact that the wave packet is indeed not a rigid body. To have a rigid shape, the force of the oscillator field must counteract the centrifugal forces due to the rotation. At an axially symmetric configuration, the former forces also act symmetrically while the latter do not. Hence axial symmetry cannot be an equilibrium configuration in the shape dynamics.

Whereas the traditional spherical Glauber states are minimum uncertainty wave packets, our more general shape-conserving states are not. However, their uncertainty relations are simple. If we consider the matrices $\underline{\Delta}x_{ij}^2=\langle x_i x_j \rangle$ and $\underline{\Delta}p_{ij}^2=\langle \hat{p}_i\hat{p}_j \rangle$ then we can introduce the "uncertainty determinant" Δ by the relation

$$\Delta^2=\det\underline{\Delta}x^2\det\underline{\Delta}p^2 . \tag{40}$$

From the arguments exposed in the Appendix it can easily be derived that Δ is constant in time and has the value

$$\Delta=\tfrac{1}{2}U_1U_2U_3 . \tag{41}$$

In order to illustrate the dynamics of shape-conserving wave packets we have performed numerical calculations using initial conditions constrained by the conditions (36), respectively (38). In Fig. 3 we show an example of the former (case 2) and in Fig. 4 an example of the latter (case 3). All the features described above are clearly displayed in these figures: the fixed rotation axis, the constant angular velocity either equal to ω or to 2ω.

In this paper we have been concerned with the propagation of three-dimensional Gaussian wave packets under the action of a harmonic force field. It is well known that the center of the wave packet moves along a classical trajectory and in the special case where the wave packet has spherical shape we can speak of "coherent vibrational

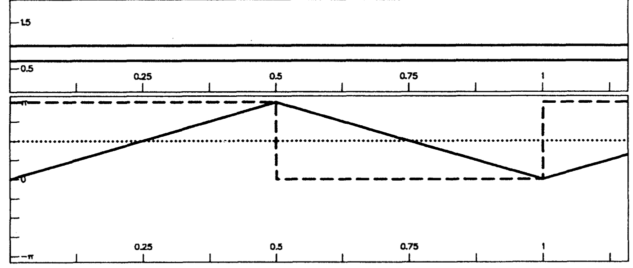

FIG. 3. Time evolution for the $\underline{U}$ matrix for initial conditions corresponding to "case 2" ($U_{33}=2$). Same caption as for Fig. 1.

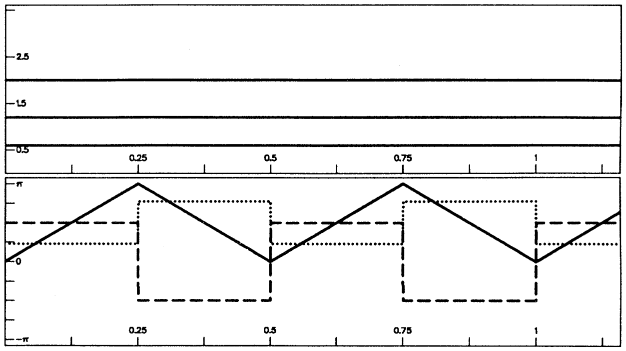

FIG. 4. Time evolution for the U matrix for initial conditions corresponding to "case 3" ($U_{33}=2$). Same caption as for Fig. 1.

motion." Here, on the contrary, we have been mainly interested in the evolution of a deformed wave packet relative to its center. In general this deformation changes incoherently and erratically. It is shown in this paper how one can prepare the wave packet in a state such that its relative motion is a "coherent rotation." We have obtained two rotational modes, one for which the angular velocity is equal to the basic oscillator frequency and another for which it is double the basic frequency. We conclude that the analogy between classical pictures of motion and quantal behavior of wave packets can be generalized from translational to rotational degrees of freedom.

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APPENDIX

The structure of Gaussian wave packets and their parametrization is intimately connected to the set of operators (i,j stand for x,y,z directions)

$$x_i,\ \ p_i,\ \ 1\ , \tag{A1}$$

$$x_ix_j,\ \ x_ip_j,\ \ p_ix_j,\ \ p_ip_j\ . \tag{A2}$$

Together they constitute the so-called inhomogeneous symplectic algebra ISp(6,$\mathbb{R}$) that is a semidirect sum of the Weyl algebra and the symplectic algebra. The parameters of the Gaussian wave packet Ψ may be identified through expectation values with respect to these operators:

$$\langle\Psi|x_i|\Psi\rangle=q_i\ , \tag{A3}$$

$$\langle\Psi|p_i|\Psi\rangle=p_i\ , \tag{A4}$$

$$\langle\Psi|x_ix_j|\Psi\rangle=q_iq_j'+\tfrac{1}{2}U_{ij}\ , \tag{A5}$$

$$\langle\Psi|x_ip_j|\Psi\rangle=q_ip_j+\tfrac{1}{2}(\underline{U}\,\underline{V})_{ij}+\frac{i}{2}\delta_{ij}\ , \tag{A6}$$

$$\langle\Psi|p_ix_j|\Psi\rangle=p_iq_j+\tfrac{1}{2}(\underline{U}\,\underline{V})_{ji}-\frac{i}{2}\delta_{ij}\ , \tag{A7}$$

$$\langle\Psi|p_ip_j|\Psi\rangle=p_ip_j+\tfrac{1}{2}(\underline{V}\,\underline{U}\,\underline{V})_{ij}+\tfrac{1}{2}U_{ij}^{-1}\ . \tag{A8}$$

From these formulas one can immediately derive the expressions for energy and angular momentum referred to in the main text. They each separate into a $(\mathbf{q},\mathbf{p})$-dependent or orbital contribution and a $(\underline{U},\underline{V})$-dependent or internal contribution. Equations of motion for the $\mathbf{q}$ and $\mathbf{p}$ parameters in the Gaussian wave packet are determined through Ehrenfest's theorem. A similar approach can be used for $\underline{U}$ and $\underline{V}$. Let us therefore refer the coordinates to the center of the wave packet. Then we can set $q_i=0$ and $p_i=0$ in formulas (A5)–(A8). We wish to derive equations of motion for $\underline{U}$ and $\underline{V}$, i.e., expressions for $\dot{\underline{U}}$ and $\dot{\underline{V}}$. From (A6) we immediately obtain

$$\frac{1}{2}\frac{dU_{ij}}{dt}=i\langle\Psi|[H,x_ix_j]|\Psi\rangle\ . \tag{A9}$$

For the oscillator Hamiltonian $H=(\omega/2)(p^2+x^2)$ we get immediately [using (A6) and (A7)]

$$\frac{d\underline{U}}{dt}=\omega(\underline{U}\,\underline{V}+\underline{V}\,\underline{U})\ . \tag{A10}$$

From (A6) we obtain

$$\frac{1}{2}\frac{d(\underline{U}\,\underline{V})_{ij}}{dt}=i\langle\Psi|[H,x_i\hat{p}_j]|\Psi\rangle\ . \tag{A11}$$

Working out the commutator and using (A8) we obtain easily

$$\frac{d(\underline{U}\,\underline{V})}{dt}=\omega(\underline{U}^{-1}+\underline{V}\,\underline{U}\,\underline{V}-\underline{U})\ . \tag{A12}$$

Using (A10) to eliminate $\dot{\underline{U}}$ (A12) becomes

$$\underline{U}\frac{d\underline{V}}{dt}=\omega(\underline{U}^{-1}-\underline{UV}^2-\underline{U})\ . \tag{A13}$$

Multiplying by $\underline{U}^{-1}$ from the left we get (5), the equation of motion for $\underline{V}$. Finally, it may be remarked that Eqs. (A5) and (A8) show that the matrices $\underline{U}$ and $\underline{W}=(\underline{U}^{-1}+\underline{V}\,\underline{U}\,\underline{V})$ can be transformed into each other by interchanging x and p. In the oscillator dynamics this interchange corresponds to a time translation over $\pi/2\omega$, therefore we can conclude

$$\underline{W}(t)=\underline{U}\left[t+\frac{\pi}{2\omega}\right]\ . \tag{A14}$$

For shape-conserving wave packets we know that

$$\underline{U}(t)=\underline{R}(t)\underline{U}(0)\underline{R}^{-1}(t) \tag{A15}$$

(where $\underline{R}$ is the rotation operator) and hence

$$\underline{W}(t)=\underline{R}\left[t+\frac{\pi}{2\omega}\right]\underline{U}(0)\underline{R}^{-1}\left[t+\frac{\pi}{2\omega}\right]\ . \tag{A16}$$

Thus, in particular, $\underline{U}$ and $\underline{W}$ have the same eigenvalues.

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