Comment on "Chaos in Axially Symmetric Potentials with Octupole Deformation"

In the Letter [1] Heiss *et al.* studied single-particle motion in a harmonic-oscillator potential which is characterized by a quadrupole deformation and an additional octupole deformation, and found that "The chaotic character of the motion is strongly dependent on the quadrupole deformation in that for a prolate deformation virtually no chaos is discernible while for the oblate case the motion shows strong chaos when the octupole term is turned on." In their left plot of Fig. 1 for an octupole deformation strength $\lambda = \frac{2}{3}\lambda_c$ for the prolate case, there is no chaos. We found, however, that there should be chaotic scatter of points in the central blank region of their Fig. 1 (left). Actually for $\lambda \leq 0.1\lambda_c$ there is no chaos, even for the oblate case ($b = 0.5$), and for $\lambda \geq 0.6\lambda_c$ there is chaos even for the prolate case ($b = 2$). We discovered that the chaos is connected with the curvature of the potential surfaces [2]. We define the curvature as

$$K(\rho, z) = \frac{\partial^2 V}{\partial \rho^2}\frac{\partial^2 V}{\partial z^2} - \left(\frac{\partial^2 V}{\partial \rho \partial z}\right)^2. \quad (1)$$

This function is closely related to and has the same sign as the Gaussian curvature [3] of a two-dimensional surface. Numerical calculations showed that there were negative-curvature regions in the potential surface for $\lambda > 0.1\lambda_c$ for the oblate case, and for $\lambda \geq 0.6\lambda_c$ for the prolate case.

Consider a fiducial trajectory $z = z(t)$ with

$$z = \begin{pmatrix} \vec{q} \\ \vec{p} \end{pmatrix}, \quad (2)$$

as well as a variation $z(t) + \delta z(t)$ of it. The Hamiltonian of the system shall be of the form $H(\vec{q}, \vec{p}) = p^2/2 + V(\vec{q})$. If one linearizes the Hamilton-Jacobi equations with respect to δz, one obtains the system of linear differential equations

$$\delta\dot{z} = M\delta z, \qquad M = \begin{pmatrix} 0 & 1_2 \\ S & 0 \end{pmatrix},$$
$$S = -\begin{pmatrix} \frac{\partial^2 V}{\partial q_1^2} & \frac{\partial^2 V}{\partial q_1 \partial q_2} \\ \frac{\partial^2 V}{\partial q_2 \partial q_1} & \frac{\partial^2 V}{\partial q_2^2} \end{pmatrix}, \quad (3)$$

where 2 degrees of freedom are considered. Via the time dependence of the fiducial trajectory, $S = S(z(t))$ is a function of time. In this sense M is a function of time. For any instant considered, M may be set constant in order to survey the character of the solution at that instant. Then the solution can be worked out explicitly with the result

$$\delta z(t) = \begin{pmatrix} \cosh(S^{1/2}t) & S^{-1/2}\sinh(S^{1/2}t) \\ S^{1/2}\sinh(S^{1/2}t) & \cosh(S^{1/2}t) \end{pmatrix}\delta z(0). \quad (4)$$

The eigenvalues of S are real because S is a real, symmetric matrix. Therefore the eigenvalues of $S^{1/2}$ are real or purely imaginary. This provides a qualitative understanding of the solution of Eq. (3). It is easy to see that

$$\lambda_{1,2} = \{\tfrac{1}{2}\,\mathrm{Tr}S \pm [\tfrac{1}{4}(\mathrm{Tr}S)^2 - K]^{1/2}\}^{1/2}, \quad (5)$$

where K is the determinant of S as defined in Eq. (1). When $K > 0$ both λ's are imaginary and the motion is stable. If $K < 0$, neighboring trajectories will typically diverge exponentially. This is a prerequisite for chaotic motion.

One gains some more insight from an inspection of the dynamics at points where $K = 0$. At such a point the determinant of the matrix M vanishes, and therefore Eq. (3) is not a useful approximation to the dynamics in any domain of δz. One has to carry the expansion of the Hamilton-Jacobi equations to second order in δz. This yields

$$\delta\dot{z} = (M + \tfrac{1}{2}\delta M)\delta z, \qquad \delta M = \begin{pmatrix} 0 & 0 \\ \delta T & 0 \end{pmatrix},$$
$$(\delta T)_{kk'} = \delta\vec{q}\cdot\vec{\nabla}\frac{\partial^2 V}{\partial q_k \partial q_{k'}}. \quad (6)$$

There is always an orthogonal transformation of the coordinate space which diagonalizes S, but there is, in general, none that diagonalizes δT. If S is diagonal, then M is blockwise diagonal, which means that as long as Eq. (3) is applicable, the motion locally separates with respect to the 2 degrees of freedom. Since δT depends on δz, the matrix $M + \frac{1}{2}\delta M$ in Eq. (6) generally cannot be diagonalized for all relevant δz. Hence, at the points with $K = 0$ it is generally impossible to even locally decouple the degrees of freedom.

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