Local Instabilities of Quantum Trajectories in Non-Linear Dynamical Systems

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Local instability of wave packets is related to an exponential increase of the second moments of the components ΔP_i^2 and ΔQ_i^2 of the momentum and position operator as a function of the expectation values $\langle P_i \rangle$ and $\langle Q_i \rangle$. Equations of motion for ΔP_i^2 and ΔQ_i^2 are derived. In the quasiclassical limit, the instability criterion approaches the Toda-Brumer criterion [1, 2] for classical trajectories.

Local instabilities for trajectories in classical n-dimensional dynamical systems can be related to the existence of an exponential time-dependence of the distance

$$\begin{aligned} \boldsymbol{d}(t) &= (d_1, d_2, \ldots, d_{2n}) \\ &= (q_1 - q_1', \ldots, q_n - q_n', p_1 - p_1', \ldots, p_n - p_n') \end{aligned}$$

of two initially adjacent trajectories $\boldsymbol{a} = (q_1, \ldots, p_n)$ and $\boldsymbol{a}' = (q_1', \ldots, p_n')$ in phase space $\{q_i, p_i\}$ [1, 2]. Following Toda [1] and Brumer [2] the onset of local instability as a function of the total energy E can be obtained from the requirement that the matrix $(V_{ij}) = (\partial^2 V / \partial q_i \partial q_j)$ has at least one negative eigenvalue $\lambda_j = \lambda_j(q_1, \ldots, q_n)$ in those phase space regions which can be reached by a trajectory on an energy shell $H(\boldsymbol{p}, \boldsymbol{q}) = H(\boldsymbol{a}) = E$. Here

$$H = \tfrac{1}{2} \sum_j p_j^2 + V(\boldsymbol{q})$$

is the Hamiltonian of the dynamical system in mass-weighted coordinates, and the potential energy is $V = V(q_1, \ldots, q_n)$, which may contain higher than second order terms. This condition for local instability is often cited as the Toda-Brumer criterion. If, for example, there is only one eigenvalue $\lambda_j < 0$ for a given energy, the time dependence of the difference $|\boldsymbol{d}(t)|$ of two adjacent trajectories is approximately $|\boldsymbol{d}(t)| \approx A\,|d(0)| \exp[(-\lambda_j)^{1/2} t]$ or, for the quadratic distance

$$d^2(t) \approx A^2 d^2(0) \exp[2(-\lambda_j)^{1/2} t]. \qquad (1)$$

The Toda-Brumer criterion is not a sufficient condition to predict global instabilities, i.e. to predict a transition from non-ergodic (regular) motion of trajectories to ergodic (non-regular) motion as a function of energy. This has recently been demonstrated by Benettin, Brambilla, and Galgani [3]. However, the criterion can be successfully used to study qualitative trends about ergodicity. The prediction of the onset energy for ergodic motion in a chain of a large number of particles with third-order anharmonicities is a good example of this application [4]. Moreover, the criterion was incorporated in theoretical concepts [3, 5] as a starting point toward a global criterion for the determination of the critical energy E_c for the onset of stochastical motion in classical non-linear systems.

In contrast to the situation with classical motion, the concept of trajectories is lacking in quantum mechanics [6]. Most of the work on quantum ergodicity has involved investigation of the transition from regular to irregular quantum states [8–12]. The concept of local and global states in quantum number space of Nordholm and Rice [11], which was generalized by Stratt, Handy, and Miller [12], represents a special formulation of a global criterion to obtain E_c in quantum vibrational systems.

In this paper the concept of trajectories is carried over into quantum mechanics in a straightforward manner. If we assume that the dynamical state of the system is described by some kind of time-dependent wave function $\psi(q, t)$, an obvious definition of a quantum trajectory is

$$\begin{aligned} a(t) &= (\langle \hat{q}_1 \rangle, \ldots, \langle \hat{q}_n \rangle, \langle \hat{p}_1 \rangle, \ldots \langle \hat{p}_n \rangle) \\ &= (x_1, \ldots, x_n, y_1, \ldots, y_n), \end{aligned} \qquad (2)$$

where the $\hat{q}_i$ and $\hat{p}_i = (-i\,\partial/\partial q_i)$ are the position and momentum operator respectively. The bracket

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$\langle \ldots \rangle$ denotes an expectation value $\langle \hat{0} \rangle = \langle \psi | \hat{0} | \psi \rangle$, and one has $\langle \hat{q}_i \rangle = x_i(t)$ and $\langle \hat{p}_i \rangle = y_i(t)$. How can one now obtain the difference d of adjacent quantum trajectories, and what is the form of the dynamic equation for that quantity? Instead of the classical square difference

$$d^2 = \sum_j \{(q_j - q_j')^2 + (p_j - p_j')^2\}$$

we introduce the operator

$$\hat{\Delta}^2 = \sum_j \{(\hat{q}_j - \langle \hat{q}_j \rangle)^2 + (\hat{p}_j - \langle \hat{p}_j \rangle)^2\} \tag{3}$$

as a natural generalization of the classical picture. As a conjecture we identified the classical square distance d^2 with the expectation value of $\hat{\Delta}^2$ in the quantum treatment.

$$\begin{aligned} d^2 &\stackrel{!}{=} \langle \hat{\Delta}^2 \rangle \\ &= \sum_j \{\langle \hat{q}_j^2 \rangle - \langle \hat{q}_j \rangle^2 + \langle \hat{p}_j^2 \rangle - \langle \hat{p}_j \rangle^2\} \\ &= \sum_j (\Delta \hat{q}_j^2 + \Delta \hat{p}_j^2) . \end{aligned} \tag{4}$$

Thus, d^2 is the sum of the mean square deviations of the position and momentum components. In this picture, local instability of the quantum trajectory $\boldsymbol{a}(t)$ is obtained if the spread of the wave packet $\psi(q, t)$ grows exponentially at least in one direction in coordinate space. The time dependence of d^2 can be evaluated using standard operator techniques [13]. We first expand the potential energy $V(q)$ in a Taylor series about $\boldsymbol{x} = (x_1, \ldots, x_n)$, giving

$$\begin{aligned} V(\hat{\boldsymbol{q}}) = V(\boldsymbol{x}) &+ (\hat{\boldsymbol{q}} - \boldsymbol{x})^{\mathrm{T}} \nabla V(\boldsymbol{x}) \\ &+ (\hat{\boldsymbol{q}} - \boldsymbol{x})^{\mathrm{T}} \mathbb{A} (\hat{\boldsymbol{q}} - \boldsymbol{x})/2 + \cdots . \end{aligned}$$

Here $\mathbb{A}$ is a symmetric real matrix with components $A_{jk} = A_{kj} = (\partial^2 V / \partial x_j \, \partial x_n)$ and $(\hat{\boldsymbol{q}} - \boldsymbol{x})^{\mathrm{T}}$ is a row vector with components of the column vector $(\hat{\boldsymbol{q}} - \boldsymbol{x})$. As in the corresponding classical case [1, 2, 5], one can always find a unitary transformation $\mathbb{U}$ which brings $\mathbb{A}$ into the diagonal form $\boldsymbol{\Lambda}$, with $\Lambda_{jk} = \lambda_j \delta_{jk}$ and real eigenvalues λ_j which indicate the curvature along local "normal" coordinates Q_j.

$$\boldsymbol{\Lambda} = \mathbb{U} \mathbb{A} \mathbb{U}^{-1} = \mathbb{U} \mathbb{A} \mathbb{U}^{\mathrm{T}} . \tag{5}$$

The local coordinates are defined as

$$\begin{aligned} &(\hat{\boldsymbol{Q}} - \boldsymbol{X}) = \mathbb{U} (\hat{\boldsymbol{q}} - \boldsymbol{x}) , \qquad \text{with} \\ &\boldsymbol{X} = (\langle \hat{Q}_1 \rangle, \ldots, \langle \hat{Q}_n \rangle) . \end{aligned}$$

The potential energy now has the form

$$\begin{aligned} V(\hat{\boldsymbol{Q}}) = V(\boldsymbol{X}) &+ \sum_j (\partial V / \partial X_j)(\hat{Q}_j - X_j) \\ &+ \tfrac{1}{2} \sum_j \lambda_j (\hat{Q}_j - X_j)^2 + \tfrac{1}{6} \sum_j \sum_k (\partial \lambda_j / \partial Q_k) \\ &\cdot (\hat{Q}_j - X_j)^2 (\hat{Q}_k - X_k) + \cdots . \end{aligned} \tag{6}$$

The general form of the kinetic energy is invariant under the transformation $\mathbb{U}$; i.e.

$$2\hat{T} = -\sum_j \partial^2 / \partial Q_j^2 = \sum_j \hat{P}_j^2$$

with $P_j = -\mathrm{i} \, \partial / \partial Q_j$.

The dynamical equations for ΔQ_j^2 and ΔP_j (the mean square deviations along the local normal coordinates) can now be evaluated. The equation of motion for ΔQ_j^2 is

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \Delta Q_j^2 &= -\mathrm{i} \langle [\hat{Q}_j^2, \hat{H}] \rangle - \frac{\partial}{\partial t} X_j^2 \\ &= \langle [\hat{Q}_j, \hat{P}_j]_+ \rangle - 2 \langle Q_j \rangle \langle P_j \rangle , \end{aligned} \tag{7}$$

where $[\hat{Q}_j, \hat{P}_j]_+$ is the anticommutator $\hat{Q}_j \hat{P}_j + \hat{P}_j \hat{Q}_j$, and standard operator and commutator relations apply for an operator $\hat{A}$ [13]

$$\begin{aligned} &[\hat{P}_j, \hat{A}] = -\mathrm{i} \, \partial \hat{A} / \partial \hat{Q}_j , \quad [\hat{Q}_j, \hat{A}] = \mathrm{i} \, \partial \hat{A} / \partial \hat{P}_j ; \\ &\mathrm{i} \, \mathrm{d} \langle \hat{A} \rangle / \mathrm{d}t = \langle [\hat{A}, \hat{H}] \rangle + \mathrm{i} \langle \partial \hat{A} / \partial t \rangle . \end{aligned}$$

For the second derivative one obtains, after some routine steps

$$\begin{aligned} \frac{\mathrm{d}^2}{\mathrm{d}t^2} \Delta Q_j^2 = 2 \langle \hat{P}_j^2 \rangle &- 2 \left\langle Q_j \frac{\partial \hat{V}}{\partial \hat{Q}_j} \right\rangle \\ &- 2 \langle \hat{P}_j \rangle^2 + 2 \langle \hat{Q}_j \rangle \left\langle \frac{\partial \hat{V}}{\partial \hat{Q}_j} \right\rangle . \end{aligned} \tag{8}$$

For ΔP_j^2 one has

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \Delta P_j^2 = &- \left\langle \left[\hat{P}_j, \frac{\partial \hat{V}}{\partial \hat{Q}_j} \right]_+ \right\rangle \\ &+ 2 \langle \hat{P}_j \rangle \left\langle \frac{\partial \hat{V}}{\partial \hat{Q}_j} \right\rangle \end{aligned} \tag{9}$$

which, after differentiation, yields

$$\begin{aligned} \frac{\mathrm{d}^2}{\mathrm{d}t^2} \Delta \hat{P}_j^2 = 2 &\left\{ \left\langle \left(\frac{\partial \hat{V}}{\partial \hat{Q}_j} \right)^2 \right\rangle - \left\langle \frac{\partial \hat{V}}{\partial \hat{Q}_j} \right\rangle^2 \right\} \\ &+ \tfrac{1}{2} \sum_k \left\{ \langle \hat{P}_j \rangle \left\langle \left[\hat{P}_k, \frac{\partial^2 \hat{V}}{\partial \hat{Q}_j \, \partial \hat{Q}_k} \right]_+ \right\rangle \right. \\ &\left. - 2 \left\langle \left[\hat{P}_j, \left[\hat{P}_k, \frac{\partial^2 \hat{V}}{\partial Q_j \, \partial Q_k} \right]_+ \right]_+ \right\rangle \right\} . \end{aligned} \tag{10}$$

One can now use the expansion of (6) to simplify the expressions (8) and (10). Retaining only terms up to the third order in the $\hat{Q}_i$ and $\hat{P}_k$, one finally obtains, from (8)

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\Delta Q_j^2 = 2\{\Delta P_j^2 - \lambda_j \Delta Q_j^2\} - \sum_k \frac{\partial \lambda_k}{\partial X_j}\langle(\hat{Q}_j - X_j)(\hat{Q}_k - X_k)^2\rangle + \cdots . \tag{11}$$

Equation (10) gives

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\Delta P_j^2 = &-2\lambda_j(\Delta P_j^2 - \lambda_j \Delta Q_j^2) \\ &+ 2\sum_k \frac{\partial \lambda_k}{\partial X_j}\{\langle \hat{P}_j\rangle\langle(\hat{Q}_k - X_k)\hat{P}_k\rangle \\ &- \langle \hat{P}_j(\hat{Q}_k - X_k)\hat{P}_k\rangle \\ &+ \lambda_j\langle(Q_j - X_j)(Q_k - X_k)^2\rangle\} + \cdots .\end{aligned} \tag{12}$$

These two equations provide the basis for a discussion of the possible onset of instability of the quantum trajectories in relation to the time-dependence of d^2 Eq. (4), or of the equivalent expression

$$D^2 = \sum_j (\Delta Q_j^2 + \Delta P_j^2) .$$

However, a complete solution of the system of Eqs. (11—12) is a more complicated problem than is the equivalent problem in classical mechanics. We will, therefore, discuss only some general properties of this system.

In the quasi-classical limit, one can assume that the potential energy is a smooth function of the coordinates over the extension of the wave packet; i.e., the potential can be well approximated as a piece-wise quadratic function. This approximation implies that the inhomogeneities in Eqs. (11—12) can be neglected to yield the quasi-classical equations

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\Delta P_j^2 &= -\lambda_j \frac{\mathrm{d}^2}{\mathrm{d}t^2}\Delta Q_j^2 \\ &= -2\lambda_j(\Delta P_j^2 - \lambda_j \Delta Q_j^2) .\end{aligned} \tag{13}$$

Since the eigenvalues λ_j are still functions of time as a consequence of the time-dependence of the $\langle Q_j\rangle = X_j(t)$, Eq. (13) represents a homogeneous system of two linear differential equations with non-constant coefficients which can be solved by standard techniques if the time-dependence of the λ_j is explicitly known. As in the corresponding classical treatment [1, 2], the solution of Eqs. (13) can be substantially simplified if the time dependence of the λ_j is smooth, i.e., if these quantities can be assumed to be constant in the time intervals of interest. In this case, there is a simple relation between ΔQ_j^2 and ΔP_j^2: $\Delta P_j^2 = -\lambda_j \Delta Q_j^2 + A + Bt$ with some constants A and B. One then obtains directly from Eq. (3)

$$\begin{aligned}\Delta Q_j^2 + \Delta P_j^2 = (1 - \lambda_j)\{&C_+ \exp[2i\lambda_j^{1/2}t] \\ &+ C_- \exp[-2i\lambda_j^{1/2}t]\} + L(\lambda_j, t)\end{aligned} \tag{14}$$

where $L(\lambda_j, t)$ is some linear function of time. If there is only one value $\lambda_j < 0$, the corresponding term $(1 + |\lambda_j|)C_- \exp[2|\lambda_j|^{1/2}t]$ may induce exponential instability of D^2. That is to say, the local stability criterion of a quantum trajectory in the quasi-classical limit is just the Toda-Brumer criterion [1, 2]. This result retrospectively justifies the conjecture made above.

If the quasi-classical description of the motion of quantum trajectory is only a very poor approximation, the inhomogeneities of Eqs. (13) can no longer be ignored. These terms explicitly contain the non-linear parts of the dynamical system which cause an exchange motion between the different degrees of freedom. For $k = j$, the terms $\partial\lambda_j/\partial X_k \cdot \langle(\hat{Q}_j - X_j)^3\rangle$, and

$$\begin{aligned}\partial\lambda_j/\partial X_j\{&\langle \hat{P}_j\rangle\langle(\hat{Q}_j - X_j)\hat{P}_j\rangle \\ &- \langle \hat{P}_j(\hat{Q}_j - X_j)\hat{P}_j\rangle\}\end{aligned}$$

represent some anharmonic forces for the widths of ΔQ_j^2 and ΔP_j^2 along the local "normal" coordinate Q_j, but they do not couple the quasi-classical Equations (13). For $k \neq j$, these inhomogeneities can be interpreted as forces for the motion of ΔP_j^2 and ΔQ_j^2 "towards stochasticity" since they cause other degrees of freedom to influence the motion along $\hat{Q}_j$. For separable systems, for which $\hat{Q}_j$ represent also global coordinates, these latter forces vanish, i.e., the spread independently in time and no "ergodic behaviour" (however this will be defined) is to be expected. One can conjecture that the inhomogeneities of Eqs. (11—12) are at least as important for the onset of instability as a function of energy as is the occurrence of eigenvalues $\lambda_j < 0$.

The onset of local instability of D can possibly be used to study the transition between ergodic and nonergodic behaviour of wave packets if one applies some kind of ensemble averaging in the energy shell

$\langle \hat{H} \rangle = E$ with suitable wave functions instead of time averaging. This has recently been demonstrated by Haensel [5] for the classical case.

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