Quantum dispersion and its exponential growth of a wave packet in chaotic systems

Li Junqing,[1,2,3] Liu Fang,[4] Xing YongZhong,[3] Zuo Wei,[1,2,3] and W. D. Heiss[5]
[1]Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator, 730000 Lanzhou, China
[2]CCAST (World Laboratory), P.O. Box 8730, Beijing, 100080 China
[3]Institute of Modern Physics, Chinese Academy of Sciences, 730000 Lanzhou, China
[4]Institute of Modern Physics, Department of Physics, North-West University, 710069 Xian, China
[5]Department of Physics, University of Witwatersrand, P.O. Wits 2050, Witwatersrand, South Africa
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The quantum correspondence of one particular signature of classical chaos—the exponential instability of motion—can be characterized by the initial exponential growth rate of the spreading of the propagating quantum wave packet. The growth rate is approximately twice the classical maximum Lyapunov exponent of the system. In the regular case, the dispersion of the wave packet is only due to the usual quantum effect that should vanish in the classical limit. In contrast, in the chaotic case, the evolution behavior of the wave packet is due to the dynamical effect associated with the nonlinearity and persists as long as the spatial extension of the initial wave packet is kept finite.

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The propagation of quantum wave packets under the action of a Hamiltonian that shows classically soft chaotic behavior, meaning that the classical phase space has regular and chaotic regions, is of interest as it sheds light on the quantum-classical correspondence of one characteristic phenomenon in chaotic systems—the exponential instability of motion [1–7]. In a former study [7] a one to one correspondence has been found between the initial growth rate of the spreading width of the quantum wave packet (SWWP) and the corresponding classical trajectories. In the present paper we further substantiate these studies using a coherent wave packet in the harmonic oscillator as initial state. We find that the SWWP initially increases with time exponentially if the mean values of coordinate and momentum of the wave packet start from a point where the corresponding classical trajectory is chaotic. Otherwise the increase with time is linear. By construction, without perturbation the SWWP is constant. It does spread when perturbed, no matter how small the perturbation so that it always attains its steady state if given sufficient time.

Toda and Ikeda [8] proposed a quantal Lyapunov exponent, which tends asymptotically towards the maximal Lyapunov exponent in the classical limit. In a different approach Gu [9] starts from nonequilibrium ensembles and associates the phase space distributional heterogeneity of nonequilibrium ensembles with the maximal Lyapunov exponent. Both attribute a quantitative measure to the spreading character of the wave packet that is briefly recapitulated next.

We begin with the entropy for the density $\rho=|\psi|^2$ for a wave function ψ, viz.,

$$S(\rho)=-\ln(\mathrm{Tr}|\rho|^2). \tag{1}$$

Note that the trace is taken over all variables implying an integration over space. Thus the entropy S is rather a functional of ρ. Using a suitable coarse graining function $\delta_\epsilon(x)$ which, for $\epsilon\to 0$, yields the Dirac δ function we smear out the density by

$$\rho_\epsilon(x)=\int \delta_\epsilon(y)\rho(y-x)\mathrm{d}y \tag{2}$$

to obtain $S(\rho_\epsilon)$. In Ref. [9] it is shown that

$$\Delta S=S(\rho_\epsilon)-S(\rho)\geqslant 0. \tag{3}$$

The heterogeneity of phase space is defined by

$$h(\rho)=\lim_{\epsilon\to 0}\frac{\Delta S}{\epsilon}. \tag{4}$$

This quantity has an exponential growth rate related to the maximal Lyapunov exponent. In fact, from Eq. (12) and Eq. (13) of Ref. [9] it can be concluded that

$$\lim_{t\to\infty}\frac{1}{2t}\ln h(\rho(t))=\Lambda, \tag{5}$$

where Λ is the maximum Lyapunov exponent with the maximum taken over the domain of phase space of the corresponding classical system that is associated with $\rho(t)$.

For a single particle wave function with N degrees of freedom the heterogeneity turns out to be [9]

$$h(\rho(t))=\frac{2}{\hbar^2}\sum_{j=1}^{N}[(\Delta q_j)^2+(\Delta p_j)^2], \tag{6}$$

where, with $\langle\psi|\psi\rangle=1$,

$$(\Delta q)^2=\langle\psi|q^2|\psi\rangle-\langle\psi|q|\psi\rangle^2$$

and similar for p. It is argued in Ref. [9] that this quantity has an upper bound determined by the uncertainty relation, i.e., $|h(\rho)|\leqslant 4L^2/\hbar^2$ where $L=\max(\Delta q,\Delta p)$, the maximum of the spreading in position and momentum. This implies that the exponential growth stated in Eq. (5) can apply only for some initial time until the saturation $4L^2/\hbar^2$ has been attained. Equations (4)–(6) establish a remarkable connection between classical and quantum mechanical behavior of chaotic systems. The very notion of the Lyapunov exponent being a classical quantity has been related to the growth in time of the quantum mechanical uncertainty. To elucidate this point further we investigate in the following the dynamical problem, i.e., $h(\rho(t))$, in a particular single particle two degrees of freedom system that has been dealt with classically and quantum mechanically as a stationary problem before [10]. Particular emphasis is put upon the analogy between classical and quantum mechanical behavior for systems with soft chaos, where depending on the initial conditions in phase space a classical orbit can be regular ($\Lambda=0$) or chaotic ($\Lambda>0$).

We consider the Hamiltonian

$$H=H_0+\lambda V,$$

$$H_0=-\frac{\hbar^2}{2m}(\Delta_x+\Delta_z)+\frac{1}{2}m\omega^2\left(x^2+\frac{z^2}{b^2}\right),$$

$$V(x,z)=\frac{1}{2}m\omega^2\frac{2z^3-3zx^2}{\sqrt{x^2+z^2}}. \tag{7}$$

The two-dimensional harmonic oscillator H_0 is perturbed by $V(x,z)$, an octupole deformation with the deformation strength λ. Note that both, H_0 and H_1, are invariant under rotations about the z axis. For any given b, there exists a critical value λ_c, such that for $\lambda>\lambda_c$ the potential no longer binds. For $b=0.5$, $\lambda_c=1.64$. In this paper we always take $b=0.5$. Varying λ from zero to λ_c, the motion of the classical particle changes from regular to fully chaotic where no regular region is left in phase space (see [10,11]). The eigenfunctions of H_0 are used as a basis, we denote them by $|n_x n_z\rangle$. We assume the system to be initially in a coherent state of the axial symmetric harmonic oscillator. Fixing the mean values of position and momentum in four-dimensional phase space and denoting them by x_0, p_{x0}, z_0, p_{z0}, respectively, this state is given by

$$|\alpha_0\rangle=\exp\left[-\frac{1}{2}(|\alpha_x|^2+|\alpha_z|^2)\right]\times\sum_{n_x=0}^{\infty}\sum_{n_z=0}^{\infty}\frac{(\alpha_x)^{n_x}(\alpha_z)^{n_z}}{\sqrt{n_x!n_z!}}|n_x n_z\rangle, \tag{8}$$

where $\alpha_x=x_0+ip_{x0}$, $\alpha_z=z_0+ip_{z0}$ thus determining the initial wave packet in four-dimensional phase space. The initial coherent state evolves under the action of H. The wave packet becomes at later times

$$|\alpha(\lambda,t)\rangle=\exp\left[-\frac{i}{\hbar}H(\lambda)t\right]|\alpha_0\rangle, \tag{9}$$

where

$$\exp\left[-\frac{i}{\hbar}H(\lambda)t\right]=\sum_m |\psi_m(\lambda)\rangle\exp\left[-\frac{i}{\hbar}E_m(\lambda)t\right]\langle\psi_m(\lambda)|.$$

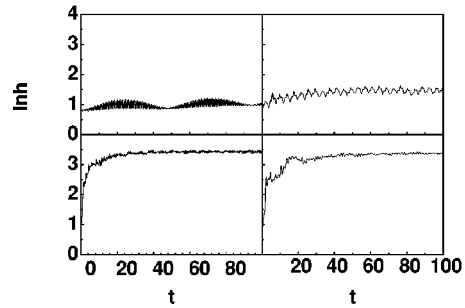

FIG. 1. The evolution of the logarithm of the total uncertainty measure of the propagating wave packet. Here and in the following figures the time units are determined by the inverse frequency used for the harmonic oscillator. For the choice of parameters see main text.

Here the exact energies $E_m(\lambda)$ and eigenfunctions $|\psi_m(\lambda)\rangle$ are obtained numerically by diagonalization in the unperturbed basis $|n_x n_z\rangle$. The diagonalization yields the matrix elements

$$C_{m,n_x n_z}=\langle\psi_m(\lambda)|n_x n_z\rangle. \tag{10}$$

Note that the octupole term breaks the reflection symmetry $z\rightarrow -z$ of the unperturbed Hamiltonian while the corresponding symmetry in x still prevails. Consequently, the problem of diagonalization reduces into two orthogonal settings, one with even and one with odd n_x. However, in Eq. (8) even and odd values of n_x occur. As an example of the time dependent matrix elements needed in the following we give the expression for $\langle x^2\rangle_t$ which reads

$$\langle\alpha(t)|x^2|\alpha(t)\rangle=\sum_{m,m'}D_m^* X_{m,m'}D_{m'}\exp[-i(E_m-E_{m'})t/\hbar], \tag{11}$$

$$X_{m,m'}=\sum_{n_x n_z n_x' n_z'}C_{m,n_x n_z}\langle n_x n_z|x^2|n_x' n_z'\rangle C^*_{n_x' n_z',m'},$$

$$D_m=\sum_{n_x n_z}C_{m,n_x n_z}\langle n_x n_z|\alpha_0\rangle.$$

The quantity of interest

$$h(\alpha(t))=\frac{2}{\hbar}[(\Delta x)^2+(\Delta z)^2+(\Delta p_x)^2+(\Delta p_z)^2] \tag{12}$$

can now easily be calculated.

The time evolution of the logarithm of this quantum heterogeneity is shown in Fig. 1 using the coherent state Eq. (8) as initial state. Note that for this state $h(\alpha(t))$ remains constant in time for $\lambda=0$. The left column of the figure displays purely regular (top) and purely chaotic (bottom) behavior irrespective of the initial condition as the respective values for $\lambda=0.1$ and $\lambda=0.95$ give rise to pure regular and pure chaotic phase space, respectively. The initial coherent state in the left column is $|\alpha_3\rangle=\{x,p_x;z,p_z\}=\{0.0,3.78,2.0,0.0\}$. In contrast, the right hand column represents results for an in-

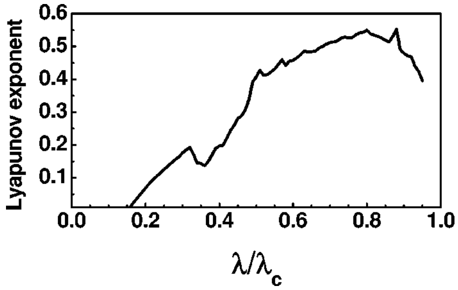

FIG. 2. The maximum Lyapunov exponent as a function of the deformation strength λ/λ_c.

termediate value of $\lambda=0.5$ where the phase space is mixed. Here, similar to classical trajectories, the qualitative behavior of the wave packet depends critically on the initial condition. The initial coherent state in the upper right column is $|\alpha_1\rangle=\{x,p_x;z,p_z\}=\{0.0,3.78,0.0,0.0\}$, classically the motion is regular. The initial coherent state in the lower right column is $|\alpha_2\rangle=\{x,p_x;z,p_z\}=\{2.83,1.89,0.0,-4.62\}$, classically the motion is chaotic. When starting in a regular region the spreading of the wave packet (top right) is virtually as one of the plain regular case for a smaller λ (top left). The apparent striking difference, i.e., the beat observed for $\lambda=0.1$ is in this context of secondary importance; it is due to the very small deviations from the harmonic spectrum occurring for small perturbation and giving rise to very small frequency contributions in Eq. (11).

In Fig. 2 the maximum Lyapunov exponent is shown as a function of the octupole deformation strength λ/λ_c for the corresponding classical system; for $\lambda/\lambda_c=0.95$ it is about 0.42. The exponential growth rate of $h(t)$ during expansion time [12] is shown in Fig. 3 for $\lambda/\lambda_c=0.95$ and indicated by the curved line. The straight line is a best fit to the curve. The exponential growth rate is about 0.9, which is about twice the classical maximum Lyapunov exponent of the system and thus agrees with the above theory.

Next we address the question about the classical limit that is of interest since spreading of the wave function is a pure quantum mechanical phenomenon while chaos is strictly defined only in classical terms. The classical limit is associated

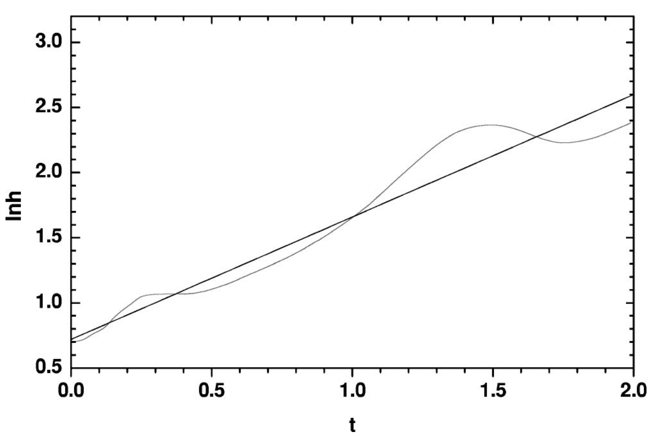

FIG. 3. The evolution of the logarithm of the total uncertainty measurement of the propagating wave packet and a linear best fit.

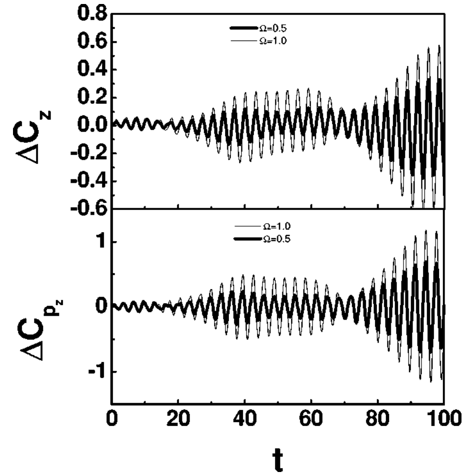

FIG. 4. ΔC_z and ΔC_{p_z} for a regular case ($\lambda/\lambda_c=0.1$) and for different effective Planck's constant.

with $\hbar\rightarrow 0$. As this is a quantity with dimensions we rather prefer to rewrite the Hamiltonian in dimensionless quantities [13,14]. Therefore the unperturbed Hamiltonian

$$H_0=\frac{1}{2m}\sum_{j=1,2}p_j^2+\frac{1}{2}m\omega^2\sum_{j=1,2}q_j^2$$

with $[q_j,p_j]=i\hbar$ is transformed into

$$H_0=\frac{1}{2}\sum_{j=1,2}(p_j^2+q_j^2) \tag{13}$$

by dividing p_j, q_j, and t by $\sqrt{m\omega_0\hbar}$, $(\omega_0/\omega)\sqrt{(\hbar/m\omega_0)}$ and $(\omega_0/\omega)(1/\omega_0)$, respectively. A reference frequency ω_0 is used for dimensional reasons. In these new units it is $[q_j,p_j]=i(\omega/\omega_0)=i\Omega$. Here Ω plays the role of an effective Planck constant. Its variation corresponds to a change of the size of the system as the spatial extension of the oscillator is determined by ω. Thus when $\Omega\rightarrow 0$, the system tends towards the classical limit. The limit is associated with either the large time limit or a large sized system or a combination of both. The total Hamiltonian reads

$$H=\frac{1}{2}\left(p_x^2+p_z^2+x^2+\frac{z^2}{b^2}+\lambda\frac{2z^3-3zx^2}{\sqrt{x^2+z^2}}\right). \tag{14}$$

We define the difference

$$\Delta C_Q=\langle Q\rangle_{\mathrm{coh}}-\langle Q\rangle_{\mathrm{clas}}, \tag{15}$$

where $\langle Q\rangle_{\mathrm{coh}}$ denotes the expectation value of an arbitrary phase space coordinate while $\langle Q\rangle_{\mathrm{clas}}$ is the corresponding classical trajectory value for the same initial condition. In Figs. 4 and 5 the time evolution of this difference is shown for $Q=z$ and $Q=p_z$ for different effective Planck constant. The fine line represents the quantum mechanical case ($\Omega=1$) while the thick line ($\Omega=0.5$) is closer to the classical limit and gives an indication about the trend towards the classical limit; we note that the limit itself cannot be attained by numerical means, in fact it is a nonuniform limit.

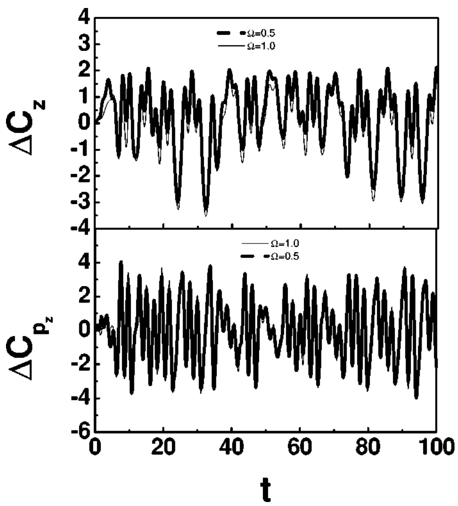

FIG. 5. Same as Fig. 4, but for a chaotic case ($\lambda/\lambda_c=0.8$).

We recall that, for $\lambda=0$, (i) the coherent state does not spread and (ii) the expectation values for position and momentum follow strictly the classical trajectories. In Fig. 4 we display the differences ΔC_z and ΔC_{p_z} for $\lambda=0.1$. As expected, now the differences are finite, and they decrease with decreasing effective Planck constant; if the classical limit is attained, the differences would vanish (not shown in figures). In a regular system the classical limit is attained smoothly in that the corresponding expectation values follow the classical trajectories the more closely the smaller the effective Planck constant. Also in this case, the spreading of the wave function is linear in time and is a typical and pure quantum (or rather wave) mechanical phenomenon irrespective of the dynamics as long as the system evolves under a regular regime. In contrast, the differences do not vanish in this limit as illustrated in Fig. 5 where the motion of the chaotic system ($\lambda=0.8$) is depicted. For chaotic dynamics, not only is the spreading of the wave function exponential but also the quantum mechanical mean values do not approach the values of the classical trajectories. Here we see a demonstration of the nonuniform nature of the classical limit. In fact, the classical limit of the evolution operator $\exp(-iHt/\hbar)$ is ill defined for a chaotic Hamiltonian: the limit attained depends on the specific way in which it is taken. The limit taken in the present paper corresponds to the limit of large time and/or large spatial extension before the limit $\hbar\rightarrow 0$ is taken. As a consequence, quantum mechanical behavior prevails eventually as long as the effective $\hbar$ is finite. To phrase it in different words: as long as we keep the spatial extension of the initial wave packet finite, it will spread exponentially under the regime of a chaotic Hamiltonian and the mean values do not uniformly approach the classical values.

In summary, the propagation of the quantum wave packet in the perturbed Hamiltonian system manifests the correspondence of the specific signature of classical chaos—the exponential instability of motion. Furthermore, the exponential growth rate of the SWWP, from which the growth rate of the total uncertainty is calculated ($\ln h$), has been established to be approximately twice the classical maximum Lyapunov exponent of the system. The very notion "quantum chaos" receives from the study of the time behavior of wave functions a much clearer defined concept than in stationary problems. The exponential behavior, unknown in stationary quantum problems, is retrieved in time dependent quantum mechanics and unequivocally related to the nonlinear character of the motion. In the regular case, the dispersion of the wave packet is only due to the usual quantum effect that should vanish in the classical limit. In contrast, in the chaotic case, the evolution behavior of the wave packet is due to the dynamical effect associated with the nonlinearity and persists as long as the spatial extension of the initial wave packet is kept finite.

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