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# Transient phase-space localization

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We show that dynamics can, in general, be used to enhance the coherence of a Hamiltonian ensemble and we analyze the transient coherence using the coarse-grained entropy. We illustrate this concept using a Rydberg atom subject to an impulsive momentum transfer or ''kick.'' Classical simulations predict that the wave packet generated by the kick undergoes strong transient phase-space localization, which forms an excellent starting point for its further control and manipulation. Moreover, we show that such localized states can be ''trapped'' for extended periods using a train of subsequent kicks.

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In recent years there has been increasing interest in the control and manipulation of atomic wave functions to generate wave packets that, for example, mimic classical behavior or that are tailored for specific applications such as data storage [1]. Such control can be achieved by use of carefully engineered ultrashort laser pulses or by application of one or more ultrashort unidirectional electric-field pulses, termed half-cycle pulses (HCPs) [2]. The ease with which some specific targeted final states can be produced is governed by the initial position and momentum distributions of the electron. In essence, the more tightly the initial state is localized in phase space, the more straightforward it is to access some selected final state [3]. In this paper, we demonstrate that the dynamics of the atom after application of a single HCP can lead to strong transient localization of the wave packet in phase space. Since the coherence of a statistical ensemble corresponds to the degree to which all the elements of the ensemble behave in a similar fashion, such phase-space localization corresponds to a transient increase in the coherence of the ensemble. We analyze this coherence by considering the time development of the coarse-grained entropy of the ensemble.

The present scheme can be described most conveniently with the aid of a one-dimensional (1D) atom and model Hamiltonian,

$$H_{at}=\frac{p^2}{2}-\frac{1}{q}+\frac{\Lambda^2}{2q^2}, \tag{1}$$

where $q$ and $p$ denote the position and momentum of the electron, respectively, and $\Lambda\rightarrow 0$ is a quasiangular momentum. Earlier work has shown that the behavior of an atom subject to one or more HCPs can be discussed using this 1D model Hamiltonian [4,5]. Consider now such a stationary Rydberg 1D ''atom'' in a given $n$ level with a binding energy $E_n=-1/(2n^2)$, which is represented classically by a microcanonical phase-space distribution $\rho_i(q,p)=c\,\delta(H_{at}(q,p)-E_n)$, where $c$ is a normalization constant, $\delta$ is the Dirac delta function, and atomic units are used throughout. Figure 1(a) displays this initial microcanonical distribution. This was constructed by considering a large number of initial phase-space points chosen according to this distribution, and the displayed value of $\rho(q,p,t)$ is the fraction of this ensemble in each of a rectangular grid of cells (bins) of area $\delta p_o \delta q_o$ described in more detail below. (The results are scaling invariant and are displayed in scaled units $p_o \equiv np, q_o \equiv q/n^2$ for scaled bin sizes $\delta p_o=0.1, \delta q_o=0.1$.) Every member of this ensemble traces the same periodic orbit, with a period $T_n=2\pi n^3$. The ensemble is distributed in phase space in inverse proportion to the time this orbit spends in a given region (leading to the characteristic peak at the outer classical turning point) and the expectation values of all observables (including $p,q$) remain stationary in time.

Suppose that at $t=0$ a short HCP of duration $T_p$ is applied to the atom. In the limit that $T_p \ll T_n$, the HCP $F_{HCP}(t)$ simply delivers an impulsive momentum transfer or ''kick'' $\Delta p=-\int F_{HCP}(t)\ dt$ to the electron. This translates the entire distribution in momentum by an amount $\Delta p_o \equiv n\Delta p$ ($=-0.1$ for the results in Fig. 1) and also causes an energy change $\Delta E=\Delta p^2/2+p_i\Delta p$ (where $p_i$ is the momentum of the electron immediately before the kick), resulting in the population of a range of final energy levels. Different elements of the phase-space distribution now evolve at different rates and the probability density $\rho(q,p,t)$ becomes time dependent and evolves according to the classical Liouville equation. The effects of these dynamics are seen in Figs. 1(b)–1(d) that show the distribution at successively later times following the kick.

As evident from Fig. 1(b), at a scaled time $t_o \equiv t/T_n \approx 1.1$, the distribution becomes strongly localized. Since $\Delta p$ is very small, the average period of the orbits after the kick remains very close to $T_n$. At somewhat later times the distribution broadens, reaching a maximum at $t_o \approx 1.5$ [see Fig. 1(c)]. It then begins to narrow and periodic variations in localization continue for several cycles before finally damping out due to the continuous spectrum of frequencies in the classical ensemble. At very long times the system relaxes to its (new) equilibrium phase-space distribution shown in Fig. 1(d).

 

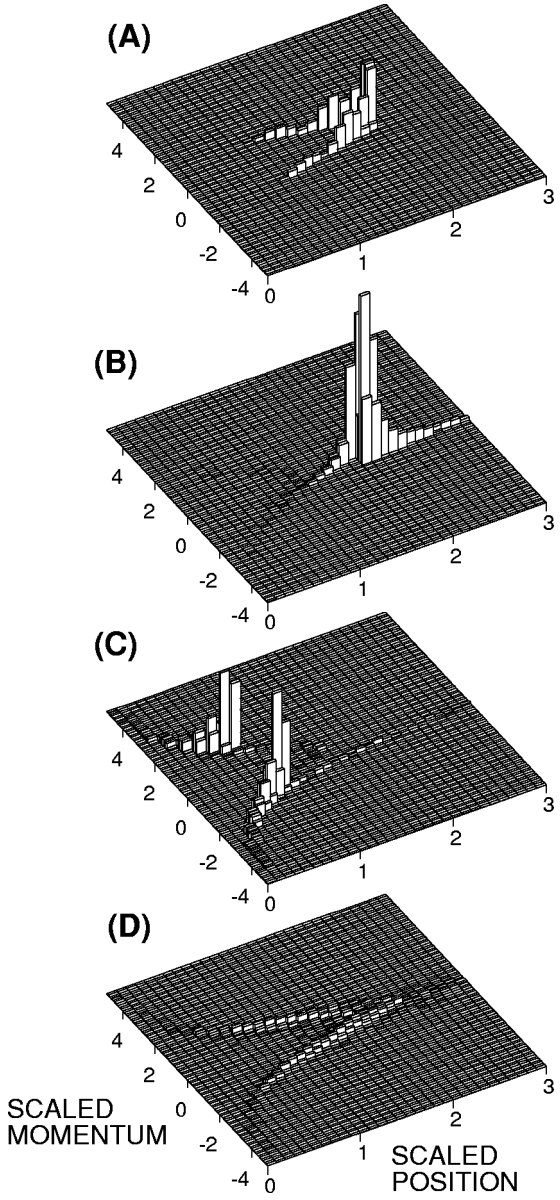


FIG. 1. Phase-space distributions $\rho(p,q,t)$ for (a) the initial or parent Rydberg state and (b)–(d) for $t_o$ of 1.10, 1.45, and 15, respectively, following an impulsive scaled momentum transfer $\Delta p_o = n\Delta p = -0.1$.

The time development of $\rho(q,p,t)$ leads to beats in the mean values $\langle A\rangle \equiv \mathrm{Tr}(\rho A)$ of many observables, where Tr denotes the trace or integral over all phase-space variables. Previous studies [6] have extensively analyzed the time development of $\langle q\rangle, \langle p\rangle$. Here we are concerned with the possibility of transient phase-space localization of the wave packet and, therefore, consider the time development of the widths of the momentum and coordinate distributions $\sigma_q^2 = \langle q^2\rangle - \langle q\rangle^2$ and $\sigma_p^2 = \langle p^2\rangle - \langle p\rangle^2$, shown in Figs. 2(a) and 2(b). Remarkably, both $\sigma_q$ and $\sigma_p$ minimize simultaneously after a time $t_o \approx 1$. Thus, the localization of the phase-space distribution can be significantly improved by application of a single kick.

Such oscillatory behavior of phase-space localization and

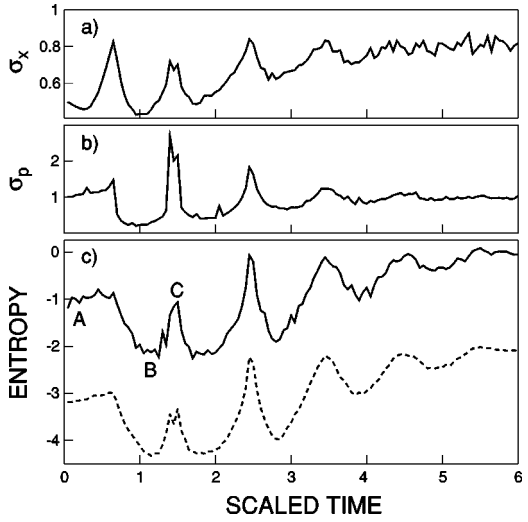


FIG. 2. Time development of the widths of (a) the coordinate and (b) the momentum distributions following an impulsive scaled momentum transfer $\Delta p_o = -0.1$. The corresponding evolution of the coarse-grained entropy $S_c(t)$ is shown in (c) for the bin sizes $\delta p_o = 0.1, \delta q_o = 0.1$ (——) and $\delta p_o = 0.0125, \delta q_o = 0.125$ (– – –).

coherence is to be expected on general grounds for integrable Hamiltonian systems. A reasonable measure of the coherence of $\rho(q,p,t)$ is provided by the negative of the entropy of the distribution, either the Gibbs entropy $-\mathrm{Tr}[\rho \ln(\rho)]$ or the analytically more useful Renyi entropy [7] $-\ln[\mathrm{Tr}(\rho^2)]$. The Liouville equation, $d\rho(q(t),p(t),t)/dt = 0$, requires that all functions of $\rho$, including the entropy, be constant in time. Thus, to measure the coherence through the entropy a small but finite coarse graining must be used to distinguish a sharply localized distribution from one that is more spread out. We, therefore, divide phase-space into equally spaced rectangular cells of area $\delta q\, \delta p$ centered at phase-space points $(q_i, p_j) i,j = 1,2,\ldots$. The entropy is then defined in the usual way [8] as

$$S_c(t) = -\ln\left[\delta q\, \delta p \sum_{i,j=1}^{\infty} \rho_{i,j}^2(t)\right], \tag{2}$$

where $\rho_{i,j}(t)$ is the average value of $\rho(q,p,t)$ in the cell centered at $(q_i, p_j)$ and is easily approximated within the classical trajectory Monte Carlo approach. In particular, if one follows the Hamiltonian dynamics of a large ensemble of $N_{traj}$ trajectories and a subset $N_{i,j}$ of these lie within the intervals $(q_i - \delta q/2, q_i + \delta q/2)$ and $(p_j - \delta p/2, p_j + \delta p/2)$ then

$$\rho_{i,j}(t) = \lim_{N_{traj}\to\infty} \frac{1}{\delta q\, \delta p} \frac{N_{i,j}}{N_{traj}}. \tag{3}$$

Figure 1 displays the behavior of precisely this quantity. In Fig. 2 we compare the time evolutions of $S_c(t), \sigma_q(t), \sigma_p(t)$. Remarkably, $S_c(t)$ oscillates as a function of time and the positions of its minima coincide with the minima for $\sigma_q(t)$ and $\sigma_p(t)$. This oscillatory behavior of $S_c(t)$ can be understood analytically using an alternate representation of

coarse graining where we locally smooth $\rho(\vec{x},t)$ [where $\vec{x}\equiv(q,p)$] by a Gaussian of width $\delta=\delta_p=\delta_q$. The coarse-grained Renyi entropy can then be written as $S_c = -\ln \mathrm{Tr}(\exp[-\delta\Sigma_i(\partial^2/\partial x_i^2)\rho(\vec{x})]^2)$. In terms of the Fourier transform $\tilde{\rho}(\vec{k})$ of $\rho$, this becomes

$$S_c = -\ln(\mathrm{Tr}[\exp(-2\delta k^2)|\tilde{\rho}(\vec{k})|^2]), \tag{4}$$

where hereafter the trace runs over $k$ values. In the limit $\delta \to 0$, $S_c$ can be written, neglecting terms $O(\delta^2)$, as

$$S_c = -\ln(\mathrm{Tr}[\tilde{\rho}^2] - 2\delta \mathrm{Tr}[k^2|\tilde{\rho}|^2]) = -\ln\{(1-2\delta\chi^2)\mathrm{Tr}[\tilde{\rho}^2]\}, \tag{5}$$

where $\chi^2 \equiv \mathrm{Tr}(k^2|\tilde{\rho}|^2)/\mathrm{Tr}(|\tilde{\rho}|^2)$ is approximately the mean-square Fourier radius of $\rho$ and is a measure of the structure in $\rho$. It has been shown [9] that if the dynamics of the system is regular (nonchaotic), $\chi^2$ executes bounded oscillations for short times, with a slow increase for longer times. If $\chi$ remains small, the time dependence of $S_c$ is well approximated by

$$S_c(t) = C + 2\delta\chi^2(t), \tag{6}$$

where $C$ is some constant dependent upon the initial distribution. Since $S_c$ is oscillating, it is to be expected that it can be less than its initial value at certain times following the perturbation, pointing to transient increases in coherence as evident in Fig. 2. The minimum in $S_c$, labeled B, corresponds to the localized distribution shown in Fig. 1(b) and the maximum labeled C corresponds to the broad distribution evident in Fig. 1(c). Figure 2 includes results for two different bin sizes: $\delta p_o = 0.1, \delta q_o = 0.1$ and $\delta p_o = 0.0125, \delta q_o = 0.0125$. Similar structure is observed in both data sets, independent of bin size [10]. Two time scales are apparent in Fig. 2. The shorter time scale associated with the individual oscillations corresponds to an average over the classical periods of the product states. The longer time scale over which the oscillations damp is governed by the spread in energy of the product states. These time scales and oscillations have been previously recognized in the expectation values of position and momentum [6]. However, their crucial role in the transient coherence of the system has not been considered.

The transient coherence that results from application of the kick can be investigated experimentally by the application of a short half-cycle probe pulse after a variable time delay, where this probe leads to ionization if it is sufficiently large. The inset in Fig. 3 shows the calculated survival probability as a function of the size of the probe impulse for conditions where it is applied to the initial "parent" state, and at times $t_o = 1.0$ and 1.5 corresponding to the phase-space distributions shown in Figs. 1(b) and 1(c), respectively. Phase space localization leads to a sharp onset in ionization, which is a clear signature of the enhanced coherence.

Although the enhanced localization obtained is transient, it can be maintained to later times by exploiting the mixed phase space associated with the kicked Rydberg atom, i.e., a Rydberg atom subject to a train of identical equispaced $\delta$-function impulses. As discussed elsewhere [5], the phase

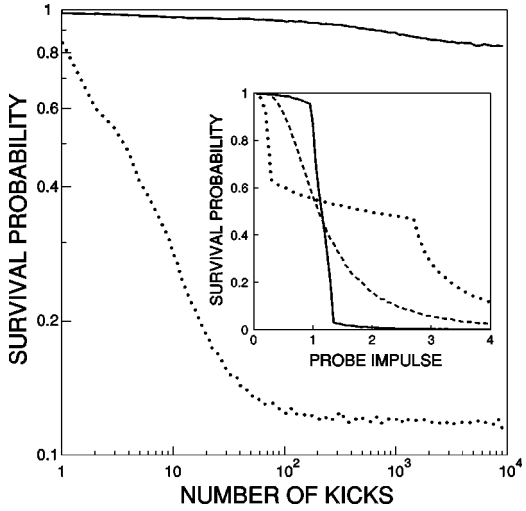


FIG. 3. Calculated survival probability vs the number of kicks $N$ for a scaled kick repetition frequency $\nu_o = \nu_k/\nu_n = 0.94$ and scaled momentum transfer $\Delta P_o = -0.5$ (see text for details). Data are included for the initial phase-space distributions in Figs. 1(b) (——), and 1(c) (– – –). The inset shows the calcuated survival probability vs kick strength following the application of a single half-cycle "probe" pulse to atoms with the initial phase-space distributions shown in Figs. 1(a) (——), 1(b) (– – –), and 1(c) (· · ·), respectively.

space for the kicked 1D (and 3D) atom contains a number of stable islands (associated with dynamical stabilization) that are embedded in a chaotic sea. If the system is strongly localized within one of these islands, it will remain strongly localized over a very large number $N$ of kicks, i.e., over an

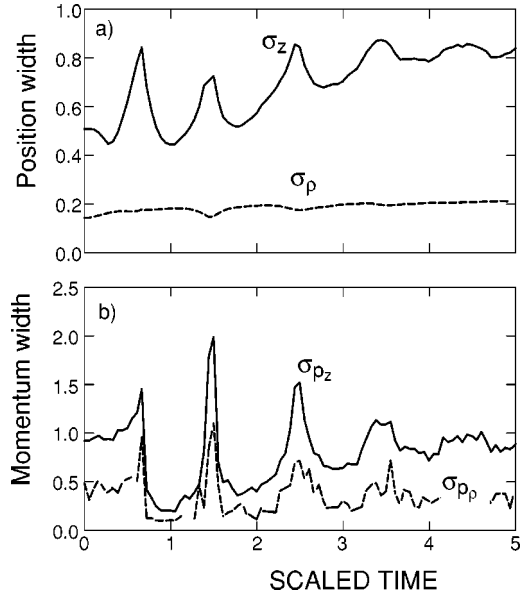


FIG. 4. Time development of the widths of (a) the coordinates and (b) the momentum distributions for 3D Rydberg atoms initially in an incoherent statistical distribution of extreme Stark states with $n=390$, $|m|<2$, $369 \leqslant k \leqslant 389$, following the application of an impulsive scaled momentum transfer $\Delta p_o = -0.1$ along the $z$ axis. Cylindrical coordinates $z$ and $\rho = \sqrt{x^2+y^2}$ are used.

extended time interval. For each of the principal (period-1) stable islands, the momentum of the electron prior to each kick is $\approx \Delta P/2$, where $-\Delta P$ is the impulse delivered by a single kick. Each kick then simply reverses the electron momentum, $\Delta P/2 \rightarrow -\Delta P/2$, with little change in its energy. The subsequent electron orbital motion is such that its momentum has the value $\Delta P/2$ immediately prior to the next kick. The dominant stable island is associated with a kick repetition frequency in the train $\nu_k \approx \nu_n$, where $\nu_n (\equiv 1/T_n)$ is the classical electron orbital frequency. A localized phase-space distribution such as that shown in Fig. 1(b) with its momentum centered about $p \approx 0$ can be positioned within a stable island by applying a kick $\pm \Delta P/2$ immediately prior to the train of kicks. The subsequent behavior of this distribution is illustrated in Fig. 3 showing the calculated survival probability as a function of the number $N$ of kicks for a scaled-kick repetition frequency $\nu_o \equiv \nu_k/\nu_n = 0.94$ and a scaled momentum transfer $\Delta P_o = -0.5$. The overall survival probability is very large, even after $N \geqslant 10^4$ kicks, indicating that the great majority of the initial states are trapped within the stable island and maintain their phase-space localization and coherence. For comparison, Fig. 3 also includes results obtained under the same conditions using the broad initial phase-space distribution shown in Fig. 1(c). The reduced survival probability indicates that only a small fraction of the initial states overlap a stable island. Those that do survive, however, will be localized in phase-space.

The present paper demonstrates that a single kick can be used to localize, at least transiently, the phase-space distribution of a system. Although the results presented were derived using a simple 1D model, quasi-one-dimensional atoms can be created by exciting the extreme members of individual Stark manifolds and these display similar behavior. This is illustrated in Fig. 4, which shows the results of 3D simulations for a band of extreme Stark states created parallel to the kick, i.e., the $z$ axis. The widths of the momentum distributions and the distribution of position along the $z$ axis mimic the 1D simulation closely. Note that the wave packet is effectively localized in 3D because the transverse width of the initial Stark state is very narrow. The present approach thus provides a practical means of generating wave packets that display strong transient phase-space localization. Furthermore, this coherence can be maintained by exploiting the phase-space structure of the kicked system. Such methods have recently been used to select those atoms in an initial ensemble that lie within specific localized regions of phase space [11]. This approach has the disadvantage that it is not unitary (i.e., a large number of initial Rydberg atoms are discarded). In contrast, the present scheme is nearly unitary. Finally, the present paper illustrates that dynamics can, in general, be used to control the coherence of any Hamiltonian ensemble. Such dynamics can be induced, as here, by application of a short-lived external perturbation or through a sudden change in the Hamiltonian.

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