Identifying Wave-Packet Fractional Revivals by Means of Information Entropy

Elvira Romera and Francisco de los Santos

Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, Fuentenueva s/n, 18071 Granada, Spain

(Received 25 May 2007; published 28 December 2007)

Wave-packet fractional revivals is a relevant feature in the long time-scale evolution of a wide range of physical systems, including atoms, molecules, and nonlinear systems. We show that the sum of information entropies in both position and momentum conjugate spaces is an indicator of fractional revivals by analyzing three different model systems: (i) the infinite square well, (ii) a particle bouncing vertically against a wall in a gravitational field, and (iii) the vibrational dynamics of hydrogen iodide molecules. This description in terms of information entropies complements the usual one in terms of the autocorrelation function.

DOI: 10.1103/PhysRevLett.99.263601 PACS numbers: 42.50.Md, 03.65.Ge, 03.67.−a

The phenomenon of quantum wave-packet revivals has received wide attention over the last several years. It has been investigated theoretically in atomic and molecular quantum systems [1] and observed experimentally in, among others, Rydberg wave packets in atoms and molecules, molecular vibrational states, and Bose-Einstein condensates [2]. Revivals occur when a wave-packet solution of the Schrödinger equation evolves in time to a state that closely reproduces its initial waveform. Fractional revivals appear as the temporal formation of structures that are given by a superposition of shifted and rephased initial wave packets [3–5]. It has been shown [3,6] that the relevant time scales of wave function evolution are contained in the coefficients of the Taylor series of the energy spectrum, E_n, around the energy E_{n_0} corresponding to the peak of the initial wave packet. More precisely, the second-, third-, and fourth-order terms in this expansion are associated with, respectively, the classical period of motion $T_{\rm cl}$, the quantum revival time-scale $T_{\rm rev}$, and the so-called superrevival time. Fractional revival times can be given in terms of the quantum revival time-scale by $t = pT_{\rm rev}/q$, with p and q mutually prime [3], and are usually analyzed using the autocorrelation function $A(t)$, which is the overlap between the initial and the time-evolving wave packet [7]. At certain fractional revivals, however, the autocorrelation function may be of limited help since the wave packet reforms itself, possibly into a scaled copy of its original shape, in a location that does not generally coincide with its initial position. An expectation value analysis of wave-packet evolution has been recently proposed by some authors, but it misses to fully detect the fractional revivals [5,8,9].

In this Letter we study the wave-packet dynamics by means of the sum of the information entropies of the probability density of the wave packet, in both position and momentum spaces. We show that it provides a natural framework for fractional revival phenomena. The position-space information entropy measures the uncertainty in the localization of the particle in space, so the lower this entropy is, the more concentrated the wave function is, the smaller the uncertainty is, and the higher the accuracy is in predicting the localization of the particle. Momentum-space entropy measures the uncertainty in predicting the momentum of the particle. Thus, information entropy gives an account of the spreading (high entropy values) and the regenerating (low entropy values) of initially well localized wave packets during the time evolution. Moreover, if $\rho(x) = |\psi(x)|^2$ and $\gamma(p) = |\phi(p)|^2$ are, respectively, the probability densities in position and momentum spaces (where ψ and ϕ are the position and momentum wave packets), the uncertainty relation for the information entropy implies $S_\rho + S_\gamma \geq 1 + \ln\pi$, where $S_\rho = -\int \rho(x)\ln\rho(x)dx$ and, analogously, $S_\gamma = -\int \gamma(p) \times \ln\gamma(p)dp$. This inequality is a generalization of the standard variance-based Heisenberg uncertainty relation [10]. It is satisfied as a strict equality only for Gaussian wave packets and bounds from below the sum of the entropies to $1 + \ln\pi$. During the evolution of a Gaussian wave packet, the entropy sum decreases at the revival times to reach the above value, which plays a similar role to unity in the autocorrelation function. Furthermore, the formation of a number of "minipackets" of the original packet, i.e., fractional revivals of the wave function, will correspond to the relative minima of the total entropy. Notice that it is the sum of the entropies that is employed as an indicator of the fractional revivals, and not either of them separately, because only the sum embraces both the configurational and the motion aspects of the wave-packet dynamics. In this context, we point out that the sum of entropies for the phase and photon numbers has been used to study the formation of macroscopic quantum superposition states from an initially coherent state via interaction with a Kerr medium [11]. Additionally, we note that a finite difference eigenvalue method has been recently derived from which the various orders of revivals can be directly calculated rather than searching for them [12].

In what follows we investigate the time evolution of wave packets in three one-dimensional, model systems that exhibit fractional revival behavior, namely, the familiar infinite square well, the quantum "bouncer," that is, a quantum particle bouncing on a hard surface under the influence of gravity, and a superposition of molecular wave packets in a Morse potential describing the vibrations of hydrogen iodide molecules. The infinite square well is especially well suited for the understanding of fractional revival phenomena because of its amenability to analytical treatment and has been analyzed by several authors (see, for instance, [4,5,13]). On the other hand, the quantum bouncer is the quantum version of a familiar classical system and has also been studied in the context of wave-packet propagation and revival phenomena [5,14,15]. Recently, gravitational quantum bouncers have been realized using neutrons [16] and atomic clouds [17], hence endowing this system with great physical significance. Finally, molecular wave packets provide a realistic scenario for the assessment of the entropy approach. Revivals and fractional revivals have been observed experimentally in wave packets involving vibrational levels and can be probed by random-phase fluorescence interferometry [2,18].

Consider an infinite potential well defined as $V(x) = 0$ for $0 < x < L$ and $V(x) = +\infty$ otherwise. The time-dependent wave function for a localized quantum wave packet is expanded as a one-dimensional superposition of energy eigenstates as

$$\psi(x, t) = \sum_n a_n u_n(x) e^{-iE_n t/\hbar}, \tag{1}$$

where $u_n(x)$ represent the normalized eigenstates and E_n the corresponding eigenvalues, $u_n(x) = \sqrt{2/L}\sin(n\pi x/L)$, $E_n = n^2\hbar^2\pi^2/2mL^2$. Following the customary procedure, the classical period and the revival time can be computed as $T_{\rm cl} = 2mL^2/\hbar\pi n$ and $T_{\rm rev} = 4mL^2/\hbar\pi$, respectively. As an example, it is easy to see by direct substitution in (1) that $\psi(L - x, T_{\rm rev}/2) = -\psi(x, 0)$, so at time $t = T_{\rm rev}/2$ a copy of the initial state reforms itself, reflected around the center of the well [4].

We shall consider an initial Gaussian wave packet with a width σ, centered at a position x_0 and with a momentum p_0, $\psi(x, 0) = \exp[-(x - x_0)^2/2\alpha^2\hbar^2 + ip_0(x - x_0)/\hbar]/\sqrt{\alpha\hbar\sqrt{\pi}}$. Assuming that the integration region can be extended to the whole real axis, the expansion coefficients can be approximated with high accuracy by an analytic expression [5]. To calculate the corresponding time-dependent, momentum wave function we use the Fourier transform of the Eq. (1), and the momentum-space normalized eigenstates

$$\phi_n(p) = \sqrt{\frac{\hbar}{\pi L}}\frac{p_n}{p^2 - p_n^2}[(-1)^n e^{ipL/\hbar} - 1]. \tag{2}$$

Without loss of generality, we henceforth take $2m = \hbar = L = 1$, and $\sigma = 1/10$ for the initial wave packet.

In Fig. 1 the sum of entropies, $S_\rho(t) + S_\gamma(t)$, and the autocorrelation function, $|A(t)|$, are shown for an initial wave packet with $x_0 = 0.5$ and $p_0 = 400\pi$. At early times, the Gaussian wave packet evolves quasiclassically, but in a few periods the quantum and classical wave-packet trajectories start moving apart [Fig. 1(b)], the classical component of the wave function being defined as $\psi_{\rm cl}(x, t) = \sum_n a_n u_n(x) e^{-i2\pi nt/T_{\rm cl}}$ [5]. For longer time scales, a large amplitude modulation is superimposed on the quasiperiodic oscillations [Fig. 1(a)]. In this long-time regime, the wave packet initially spreads and delocalizes while undergoing a sequence of fractional revivals with the creation of subpackets, each of them similar to the initial one so that the sum of the entropies reaches a relative minimum and the modulus of the autocorrelation function a relative maximum. The most important fractional revivals are denoted by vertical dashed lines. It can be observed that the identification of some fractional revivals from the autocorrelation function is not so clear-cut as compared with the entropy approach (see, for example, the cases $t = pT_{\rm rev}/q$ with $q = 7$ or 9).

We have also investigated the interesting initial condition $x_0 = 0.8L$ and $p_0 = 0$, for which there is no classical periodic motion. Snapshots of the numerical simulation of the position-space probability density are given in Fig. 2 at several times. It is apparent from the bottom panel of Fig. 3 that the sum of entropies has a minimum at the main

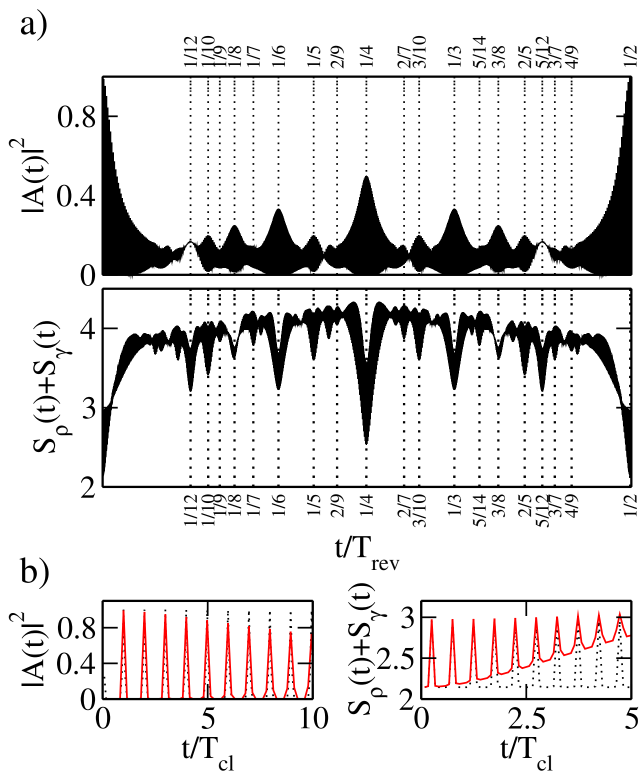

FIG. 1 (color online). Time dependence of $|A(t)|^2$ and $S_\rho(t) + S_\gamma(t)$ for an initial Gaussian wave packet with $x_0 = L/2$, $p_0 = 400\pi$, and $\sigma = 1/10$ in an infinite square well. (a) Long-time dependence. The main fractional revivals are indicated by vertical dotted lines. (b) First classical periods of motion. Quantum wave packets are represented by solid lines and their classical component by dashed lines.

fractional revivals, denoted by vertical dashed lines, except for the case $t = T_{\rm rev}/7$, where the position-space probability density has a shape compatible with a collapsed wave function (Fig. 2). The autocorrelation function, as plotted in the top panel of Fig. 3, fails to show the fractional revivals occurring at, for example, $t/T_{\rm rev} = 1/6$, $1/8$, and $3/10$. This discrepancy can be traced back to the fact that information entropies take into account individual mini-Gaussian packets independently of their relative positions, whereas the autocorrelation function depends on the relative position between the initial wave packet and the evolved one.

Next, we study the behavior of these same quantities in other physical situations. Consider a particle bouncing on a hard surface under the influence of gravity, that is, a particle in a potential $V(z) = mgz$, if $z > 0$ and $V(z) = +\infty$ otherwise. Upon introducing the characteristic gravitational length $l_g = (\hbar/2gm^2)^{1/3}$ and defining $z' = z/l_g$ and $E' = E/mgl_g$, as in [19], the eigenfunctions and eigenvalues are given by $E'_n = z_n$, $u_n(z') = \mathcal{N}_n \mathrm{Ai}(z' - z_n)$ with $n = 1, 2, 3, \ldots$, where $\mathrm{Ai}(z)$ is the Airy function, $-z_n$ denotes its zeros, and $\mathcal{N}_n$ is the $u_n(z')$ normalization factor. Very accurate analytic approximations to z_n and $\mathcal{N}_n$ can be found in [19]. Consider now an initial Gaussian wave packet localized at a height z_0 above the floor, with a width σ and an initial momentum $p_0 = 0$. The corresponding coefficients in Eq. (1) can be obtained analytically [19], and the classical period and the revival time are $T_{\rm cl} = 2\sqrt{z_0}$ and $T_{\rm rev} = 4z_0^2/\pi$, respectively.

The temporal evolution of the total entropy and of the autocorrelation function was computed numerically for the initial conditions $z_0 = 100$, $\sigma = 1$, and $p_0 = 0$ (see Fig. 4). For that, the corresponding wave packet in momentum space was obtained numerically by the fast Fourier transform method. One can see in the bottom panel of Fig. 4 that the reformation of subpackets at fractional revivals is captured by the successive relative minima of $S_\rho(t) + S_\gamma(t)$. Similar information is provided by the, somewhat less clear, sequence of relative maxima of $|A(t)|^2$ (top panel of Fig. 4).

Last, we address the case of a diatomic molecule, the vibrational dynamics of which is known to be well approximated by the Morse potential, $V(x) = D(e^{-2\beta x} - 2e^{-\beta x})$. Here, $x = r/r_0 - 1$, r is the internuclear distance, r_0 is the equilibrium bond distance, D is the dissociation energy, and β is a range parameter. Defining $\lambda = \sqrt{2\mu D} r_0/\beta\hbar$ and $s = 2\lambda\sqrt{-E/D}$, the associated eigenvalues and eigenfunctions for bounded states can be written as [20] $\psi_n^\lambda(\xi) = N e^{-\xi/2}\xi^{s/2} L_n^s(\xi)$, $E_n = -D(\lambda - n - 1/2)^2/\lambda^2$, with $\xi = 2\lambda e^{-\beta x}$, $0 < \xi < \infty$, and $n = 0, 1, \ldots, [\lambda - 1/2]$, $[x]$ being the integer part of x. $L_n^s(\xi)$ are the Laguerre polynomials and N is a normalization factor (see [20]).

We consider the HI molecule, for which $\beta = 2.07932$, $D = 0.1125$ a.u., $r_0 = 3.04159$ a.u., with the reduced mass $\mu = 1819.99$ a.u.. The number of bound states is $[\lambda - 1/2] + 1 = 30$, and the classical period and the revival time are given by $T_{\rm cl} = T_{\rm rev}/(2\lambda - 1)$ and $T_{\rm rev} = 2\pi\lambda^2/D$, respectively. Notice that in this case the autocorrelation function turns out to be symmetric about $T_{\rm rev}/2$ [21]. As an initial wave packet, we take a superposition of Morse eigenstates assuming a Gaussian population of vibrational levels $|c_n|^2 = \exp[(n - n_0)^2/\sigma]/(\pi\sigma)^{1/2}$, with $n_0 = 7$, $\sigma = 3$. As in the quantum bouncer case, the fast Fourier method is used to compute the entropy in the momentum space. These system parameters lead to the entropy and autocorrelation function depicted in Fig. 5, where the occurrence of fractional revivals at $t = 1/6$, $1/3$, $2/3$, and $5/6$ is transparent at first sight in the bottom panel, in contrast with the information provided by the autocorrelation function (top panel).

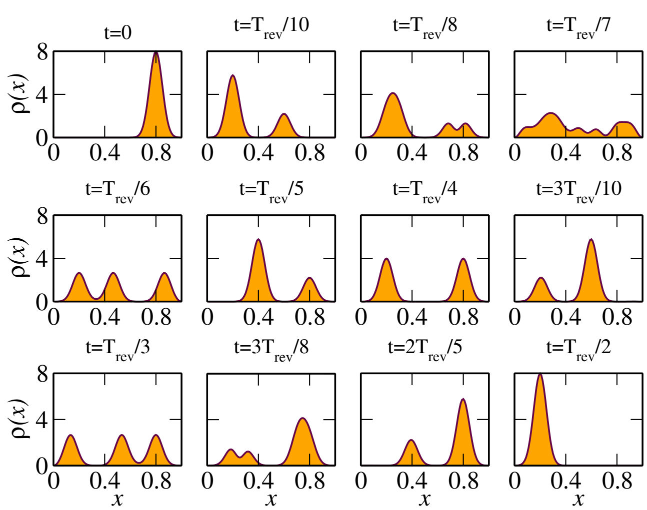

FIG. 2 (color online). Snapshots of the probability density in position space for an initial Gaussian wave packet with $x_0 = 0.8L$, $p_0 = 0$, and $\sigma = 1/10$ in an infinite square well and at different fractional revival times.

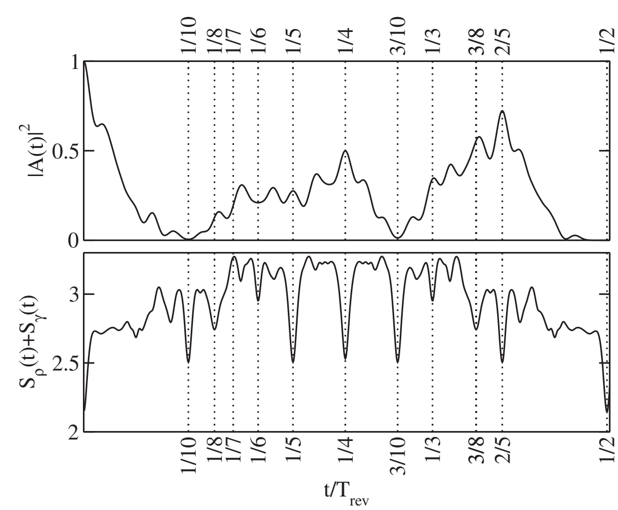

FIG. 3. Time dependence of (top panel) $|A(t)|^2$ and (bottom panel) $S_\rho(t) + S_\gamma(t)$ for an initial Gaussian wave packet in an infinite square well. Parameters as in Fig. 2.

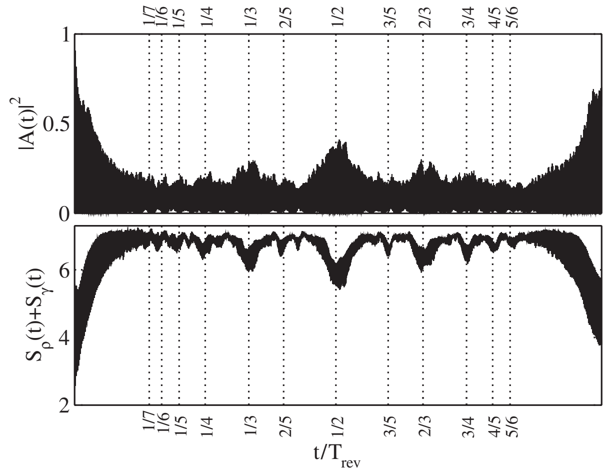

FIG. 4. Time dependence of (top panel) $|A(t)|^2$ and (bottom panel) $S_\rho(t) + S_\gamma(t)$ for an initial Gaussian wave packet with $z_0 = 100$, $p_0 = 0$, and $\sigma = 1$ in a quantum bouncer. The main fractional revivals are indicated by vertical dashed lines.

In conclusion, we have found that the manifestation of fractional revivals in the long time-scale evolution of quantum wave packets reflects in the sum of information entropies in conjugate spaces, which clearly shows relative minima at the fractional revival times, thus providing a useful tool to reckon with for visualizing fractional revivals, complementary to the conventional autocorrelation function. These minima appear independently of the relative position of the subpackets that configure the wave packet at the fractional revival time and are rigorously bounded from below. It would be very interesting to carry out a more systematic study extending this approach to systems with two or more quantum numbers.

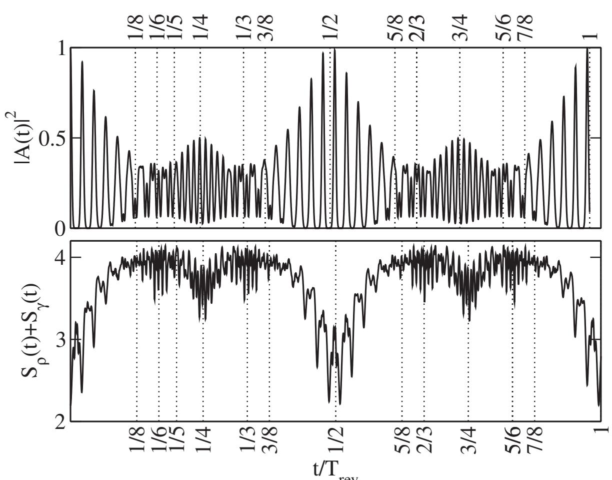

FIG. 5. Time dependence of (top panel) $|A(t)|^2$ and (bottom panel) $S_\rho(t) + S_\gamma(t)$ for an initial superposition of molecular wave packet with Gaussian weights in a Morse potential. The main fractional revivals are indicated by vertical dashed lines.

This work was supported by the Spanish projects FIS2005-00791/00973 and FQM-165/0207.

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