Complexity Measures and Quantum Revivals

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Abstract: We investigate a newly introduced generalized statistical complexity measure as applied to wave packet revival phenomena in the one-dimensional infinite square-well potential.

Key–Words: complexity measures, quantum revivals, Rényi entropy, conjugate spaces, infinite square-well, fractional revivals

1 Introduction

The time evolution of bound wave packets reflects the complexity of quantum interference. Time evolving wave packets initially move as localized entities and oscillate with a classical period \( T_{cl} \) as predicted by classical mechanics, but eventually they deviate from the classical trajectories, spread out and collapse. At later times, however, collapsed wave packets may almost recover their initial shape and the classical motion revives temporarily afterward, in time windows that are separated by intervals \( T_{rev} \). At intermediate time scales \( p T_{rev} / q \), fractional revivals may take place when the wave packets split into a set of scaled and translated copies [1, 2, 3]. These different time scales are embodied in the first coefficients of the Taylor series of the system’s energy spectrum \( E_n \) around the energy \( E_{n0} \) corresponding to the peak of the wave packet,

\[
E_n \approx E_{n0} + E'_{n0}(n-n_0) + \frac{E''_{n0}}{2}(n-n_0)^2 + \cdots .
\]

The second- and third-order terms in this expansion provide the classical period of motion \( T_{cl} = 2\pi\hbar/|E''_{n0}| \) and the quantum revival time \( T_{rev} = 4\pi\hbar/|E''_{n0}| \), respectively [3]. Revivals and fractional revivals received a great deal of attention over the last decades. Both experimental and theoretical progress was made in atoms and molecules, Rydberg atoms [4], and Bose-Einstein condensates [5], to name just a few examples.

Revival behavior is usually analyzed in terms of the autocorrelation function, that is, by monitoring the overlapping between the initial wave packet and the time-evolved one [3]. When a revival takes place, the autocorrelation function reaches its initial value of unity whereas fractional revivals show up as relative maxima. However, recent entropy-based approaches have proved to be a very useful tool to study revival phenomena [6]. Within this approach, the occurrence of revivals and fractional revivals correspond to, respectively, the appearance of absolute and relative minima of suitable entropy functionals. Information entropies measure the spread of the probability density of the wave packet, and therefore can be used effectively to identify the collapse and the regenerating of initially well localized wave packets. Therefore, it seems natural to explore revival phenomena within the more general framework of complexity measures because many information entropies and statistical measures are defined as the product of two factors, one of which is the broadening of the distribution that defines the system and the other measures its narrowness. In particular, the Rényi entropy of order \( \alpha \) of a probability density \( f(r) \) is given by

\[
R_\rho^{(\alpha)} = \frac{1}{1-\alpha} \ln \int_{-\infty}^{\infty} [f(r)]^\alpha \, dr.
\]

From this definition, it is straightforward to obtain the following limiting behaviors:

\[
R_f^{(\alpha)} \underset{\alpha \to 1}{\longrightarrow} S_f \equiv - \int f(r) \ln f(r) \, dr,
R_f^{(\alpha)} \underset{\alpha \to \infty}{\longrightarrow} - \ln[\max_r f(r)].
\]
Consequently, in the limits $\alpha \to 1$ the Rényi entropy reduces to Shannon’s while when $\alpha \to \infty$ it gives the maximum of the probability density. Turning to wave packet propagation, the sum of Rényi entropies in position and momentum spaces, $\rho(p) = |\psi(p)|^2$ and $\gamma(\mathbf{p}) = |\phi(\mathbf{p})|^2$, reads

$$R_p^{(\alpha)} + R_\gamma^{(\beta)} = \frac{1}{1-\alpha} \ln \int_{-\infty}^{\infty} [\rho(r)]^\alpha dr$$

$$+ \frac{1}{1-\beta} \ln \int_{-\infty}^{\infty} [\gamma(r)]^\beta dr, \quad (4)$$

and the Rényi uncertainty relation is given by [7]

$$R_p^{(\alpha)} + R_\gamma^{(\beta)} \geq -\frac{1}{2(1-\alpha)} \ln \frac{\alpha}{\pi} - \frac{1}{2(1-\beta)} \ln \frac{\beta}{\pi}, \quad (5)$$

where $1/\alpha + 1/\beta = 2$. Due to the fact that the uncertainty relation (5) is saturated only for Gaussian wave packets, the temporary formation of fractional revivals corresponds to the relative minima of $R_p^{(\alpha)}(t) + R_\gamma^{(\beta)}(t)$.

A family of generalized statistical complexity measures can now be defined by [9, 10]

$$C_f^{(\alpha,\beta)} = e^{R_f^{(\alpha)} - R_f^{(\beta)}}, \quad 0 < \alpha, \beta < \infty. \quad (6)$$

Its mathematical properties have been thoroughly investigated in [10], where a calculation for different quantum systems was also carried out. Interestingly, for the special case $\beta \to \infty$, $C_f^{(\alpha,\beta)}$ factorizes into two terms that capture global and local information of the density distribution, respectively.

In what follows we investigate this newly introduced generalized complexity measure as applied to revival phenomena. The model system we take is the one-dimensional infinite square-well potential, which can be solved exactly for the bound states

$$\psi(x,0) = \frac{1}{\sqrt{\pi \sigma}} e^{-x^2/2\sigma^2} \mathrm{e}^{ip_0(x-x_0)/\hbar}. \quad (7)$$

Figure 1: Time dependence of $C_f^{(\alpha,\beta)}$, main fractional revivals, and collapse time for and initial Gaussian wave packet with $p_0 = 400\pi$ and $\sigma = \sqrt{2}/10$. Panel (a) corresponds to $(\alpha = 2/3, \beta = 2)$ and (b) to $(\alpha = 1/2, \beta = \infty)$.

The infinite square well has exact revivals because the energy levels are integral multiples of a common value (but not equally spaced). The classical and revival periods are $T_{cl} = 2mL^2/\hbar^2n_0$ and $T_{rev} = 4mL^2/\hbar\pi$, respectively [3]. It is easy to see by direct substitution in equation (7) that $\psi(L-x,t) = -\psi(x,0)$, so at a time $t = T_{rev}/2$ the initial state reforms exactly, reflected around the center of the well. This is the reason why the time span of the following analysis is $T_{rev}/2$ rather than $T_{rev}$.

We shall consider an initial Gaussian wave packet with a width $\sigma$, centered at a position $x_0$ and with a momentum $p_0$,

$$\psi(x,0) = \frac{1}{\sqrt{\sigma \pi \hbar}} e^{-i(x-x_0)^2/(2\sigma^2\hbar^2) + ip_0(x-x_0)/\hbar}. \quad (9)$$

Assuming that the integration region can be extended to the whole real axis, the expansion coefficients can be approximated with high accuracy by the analytic expression

$$a_n \approx \sqrt{\frac{4\sigma \pi}{L^2 \sqrt{\pi}}} e^{-ip_0x_0/\hbar} \frac{e^{i\pi n x_0/L} e^{-2(p_0+n\pi h/L)^2/2\hbar^2}}{2i} \left[ e^{i\pi x_0/L} e^{-2(p_0+n\pi h/L)^2/2\hbar^2} - e^{-i\pi x_0/L} e^{-2(p_0+n\pi h/L)^2/2\hbar^2} \right]. \quad (10)$$

2 Revival Behavior in the Infinite Square-Well through a Complexity Measure

Consider a particle of mass $m$ in 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

$$\psi(x,t) = \sum_n a_n u_n(x) e^{-iE_n t/\hbar}, \quad (7)$$
with p hereafter take momentum conjugate spaces. Figure 1 displays the location of the main fractional revivals for a wave packet with revivals, and collapse teme for an initial Gaussian values of α

Figure 2: Time dependence of $C^{(α,β)}$, main fractional revivals, and collapse teme for an initial Gaussian wave packet with $p_0 = 400\pi$ and $\sigma = \sqrt{2}/10$. Panel (a) corresponds to $(α = 2/3, β = 2)$ and (b) to $(α = 1/2, β = \infty)$.

To calculate the corresponding time dependent, momentum wave function we use the Fourier transform of the equation (7), that is,

$$\phi(p, t) = \sum_{n} a_n \phi_n(p) e^{-iE_n t/\hbar}, \tag{11}$$

where

$$\phi_n(p) = \sqrt{\frac{\hbar}{\pi L \sigma^2}} \frac{p_n}{p^2} \left[ (-1)^n e^{ipL/\hbar} - 1 \right], \tag{12}$$

with $p_n = \hbar \pi n / L$. Without loss of generality, we hereafter take $2m = \hbar = L = 1$, $\sigma = \sqrt{2}/10$, $p_0 = 400\pi$, and $x_0 = L/2 = 0.5$ for the initial wave packet. This implies that $ψ(x, 0)$ is sharply peaked around $n_0 = 400$.

We have computed the temporal evolution of the complexity measure $C^{(α,β)}_f$ both in position and momentum conjugate spaces. Figure 1 displays $C^{(α,β)}_f$ and the location of the main fractional revivals for $(α = 2/3, β = 2)$ (top panel) and $(α = 1/2, β = \infty)$ (bottom panel). Figure 2 shows $C^{(α,β)}_f$ for the same values of $α$ and $β$ as in figure 1. At early times, the Gaussian wave packet evolves quasiclassically with a period $T_{\text{cl}} = T_{\text{rev}}/2n_0 = T_{\text{rev}}/800$ (not shown), but in a few periods begins to delocalize and spreads almost uniformly across the entire well. This is the so-called collapse phase. The time-scale for this collapse has been estimated by means of an expectation value analysis to be $3, 11$,

$$T_{\text{coll}} = \frac{1}{\sqrt{6}} \frac{mL\sigma}{\hbar} \simeq 0.0144 \tag{13}$$

for the set of parameters defined above. We can see that the complexity measure in position space captures this collapse time-scale because it is close to the first maximum of $C^{(α,β)}_ρ$, but, by contrast, this is not the case in momentum space. Further, it can be appreciated that the two set of parameters $(α = 2/3, β = 2)$ and $(1/2, ∞)$ yield similar results, despite in this latter case the complexity measure $C^{(α,β)}_f$ factorizes as a product of global and local terms.

3 Conclusion

We have studied revivals and fractional revivals in an infinite square-well by means of a, newly derived family of generalized complexity measures $C^{(α,β)}_f$. We have shown that wave packet regeneration shows up as relative minima of $C^{(α,β)}_f$ both in position and momentum spaces, and that the collapse time-scale is also accounted for by the first maximum of $C^{(α,β)}_ρ$.

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