Wigner function for discrete phase space: exorcising ghost images

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Abstract

We construct, using simple geometrical arguments, a Wigner function defined on a discrete phase space of arbitrary integer Hilbert-space dimension that is free of redundancies. "Ghost images" plaguing other Wigner functions for discrete phase spaces are thus revealed as artifacts. It allows to devise a corresponding phase-space propagator in an unambiguous manner. We apply our definitions to eigenstates and propagator of the quantum baker map. Scars on unstable periodic points of the corresponding classical map become visible with unprecedented resolution.

Key words: Wigner function, finite Hilbert-space dimension, toroidal phase space, propagator, scars, quantum baker map PACS: 03.65.Wi, 05.30.-d, 05.45.Mt

1 Introduction

Since the conception of the Wigner function in 1932 [1], phase-space representations of quantum mechanics have found a wide range of applications. Notably in complex quantum dynamics, they have become popular as they allow to compare classical and quantum dynamics on the same footing. The Wigner function in particular has become the standard tool whenever the full information contained in the density matrix, including coherences, has to be represented.

In many cases the "quantum phase space" underlying the Wigner function is fundamentally different from the corresponding classical one in that it is discrete. This occurs, for example, if both classical phase-space variables are

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cyclic, i.e., if the classical phase space has the topology of a torus so that the periodicity of either variable implies quantization of the other. Likewise, it is inevitable once, e.g., in numerical implementations of wave-packet scattering, the spatial variable is reduced to a discrete lattice and at the same time restricted to some finite total length, with periodic boundary conditions. Finally, discrete phase spaces allow to define a perfectly self-consistent quantum mechanics living on a finite-dimensional Hilbert space [2].

A straightforward generalization of the original definition to the discrete case leads to a Wigner function that contains the information of the density operator in several replicas. This redundancy is reflected in so-called ghost images of features standing out in the quantum state [3,4]. Modified definitions that avoid these redundancies have been proposed in [5,6]. We here start from the version in Ref. [6], giving a transparent derivation in simple geometric terms that readily generalizes to arbitrary (not necessarily odd or even prime) integer Hilbert-space dimensions. It allows to construct a propagator on the discrete phase space, which can be defined unambiguously only for a Wigner function free of redundancy. As an illustrative example, we apply it to the quantum baker map [7]. A more detailed account of our findings will be published elsewhere [8].

2 Non-redundant Wigner function and propagator

The original definition of the Wigner function [1], $W(p,q) = h^{-1} \int_{\infty}^{\infty} dq' e^{-ipq'/\hbar}$ $\rho(q+q'/2,q-q'/2)$ for a density operator $\hat{\rho}$ consists of two steps, a transformation to sum-and-difference coordinates $q = (q_1 + q_2)/2$, $q' = q_1 - q_2$ of the density matrix $\rho(q_1, q_2) = \langle q_1 | \hat{\rho} | q_2 \rangle$, followed by a Fourier transform along q'. The difficulty in applying this to a discrete spatial basis $|n\rangle$, $n=0,\ldots,N-1$ arises from the fact that in (q, q')-space the original square lattice appears as "base-centered cubic", with even and odd points in terms of $n_1 \pm n_2$. Augmenting it to become "simple cubic" again by introducing fictitious extra lattice points where $\rho(n, n') = 0$ lead, upon Fourier transformation (of size 2N), to a fourfold redundancy of the resultant Wigner function [3,4], call it $W_{\text{double}}(\mathbf{m})$, abbreviating the discrete phase-space vector $\mathbf{m} = (\lambda, n)$. We remove the redundancy as follows: By an additional Fourier transform (size 2N), now in the q-direction, the redundancy takes the explicit form of an identical repetition, up to sign changes, of the coefficients in four $N \times N$ -blocks within the total $2N \times 2N$ "Brillouin zone". We cut out a single $N \times N$ -block, chosen centered around the origin so as to preserve twofold symmetries that reflect the reality of the Wigner function, by multiplying with a two-dimensional discrete box function. Upon undoing the additional second Fourier transform (now of size N only), the Wigner function is recovered, free of redundancies.

Cutting out the $N \times N$ -block from the Fourier-transformed Wigner function $\widetilde{W}_{\text{double}}$ is equivalent to a convolution of W_{double} with a Fourier-transformed box function \widetilde{S}

$$W(\mathbf{m}) = \sum_{\lambda', n' = -N}^{N-1} W_{\text{double}}(2\mathbf{m} - \mathbf{m}') \tilde{S}(\mathbf{m}'), \tag{1}$$

$$\tilde{S}(\mathbf{m}) = \tilde{s}_{\lambda} \tilde{s}_{n}, \quad \tilde{s}_{k} = \begin{cases}
\delta_{k \mod 2N} & k \text{ even,} \\
\frac{\sin(\pi k/2)}{N \sin(\pi k/2N)} e^{-i\pi k/2N} & k \text{ odd.}
\end{cases}$$
(2)

Apart from revealing "ghost images" as artifacts and removing them, this procedure becomes indispensable once a propagator of the Wigner function is to be defined in an unambiguous manner. The reason is that with a redundant Wigner function, there is no unique way of relating the coefficients of the final Wigner function to those of the initial one. Denoting the transformation outlined above symbolically as $T_{\rm W}$, so that $W(\mathbf{m}) = T_{\rm W} \rho(\mathbf{n})$, with $\mathbf{n} = (n_1, n_2)$, we find for the discrete Wigner function propagator

$$K_{W}(\mathbf{m}'', t''; \mathbf{m}', t') = T_{W}K(\mathbf{n}'', t''; \mathbf{n}', t')T_{W}^{-1},$$
 (3)

where $K(\mathbf{n''}, t''; \mathbf{n'}, t')$ propagates the density matrix from time t' to t'', i.e., $\rho(\mathbf{n''}, t'') = \sum_{\mathbf{n}}' K(\mathbf{n''}, t''; \mathbf{n'}, t') \rho(\mathbf{n'}, t')$.

If the time evolution is unitary, generated by a Hamiltonian \hat{H} , the propagator can be expressed in terms of energy eigenstates $\hat{H}|\alpha\rangle = E_{\alpha}|\alpha\rangle$ as $K(\mathbf{n''}, t''; \mathbf{n'}, t') = \sum_{\alpha,\beta} e^{-i(E_{\alpha} - E_{\beta})(t'' - t')/\hbar} \rho_{\alpha,\beta}^*(\mathbf{n''}) \rho_{\alpha,\beta}(\mathbf{n'})$, denoting $\rho_{\alpha,\beta}(\mathbf{n}) = \langle \alpha | n_1 \rangle \langle n_2 | \beta \rangle$. Defining Wigner eigenfunctions as $W_{\alpha,\beta}(\mathbf{m}) = T_W \rho_{\alpha,\beta}(\mathbf{n})$, we have for the Wigner propagator

$$K_{\mathbf{W}}(\mathbf{m}'', t''; \mathbf{m}', t') = N^{-1} \sum_{\alpha, \beta} e^{-i(E_{\alpha} - E_{\beta})(t'' - t')/\hbar} W_{\alpha, \beta}^{*}(\mathbf{m}'') W_{\alpha, \beta}(\mathbf{m}'). \tag{4}$$

Equation (4) allows for an easy direct numerical access to the propagator once enough eigenfunctions, e.g., in position representation, are known.

3 Wigner eigenfunctions and propagator for the quantum baker map

The baker transformation [7] is arguably the simplest example of a fully chaotic map of the unit square to itself. A quantum version has been suggested in

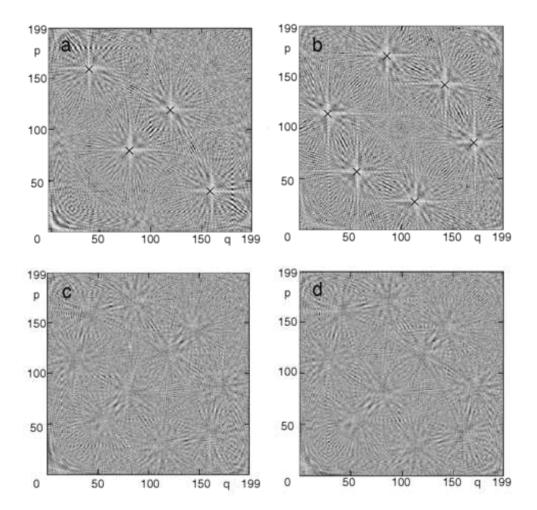


Fig. 1. Wigner functions according to Eq. (1) for eigenstates of the quantum baker map, Eq. (5). Panels a,b show diagonal Wigner eigenfunctions $W_{\alpha,\alpha}$ for (a) $\alpha=88$ and (b) 159. Panels c,d are real and imaginary parts, respectively, of the off-diagonal Wigner eigenfunction $W_{88,129}$. Hilbert-space dimension is N=200. Greyscale ranges from negative (dark) to positive (bright) values. Unstable periodic orbits of the corresponding classical map underlying the scars have been marked with crosses.

Ref. [7] in terms of Fourier transformations F_M , $(F_M)_{m,n} = M^{-1/2}e^{-2\pi i m n/M}$ of sizes M = N and N/2, where N (even) denotes the Hilbert-space dimension, as follows,

$$B_N = F_N^{-1} \begin{pmatrix} F_{N/2} & 0 \\ 0 & F_{N/2} \end{pmatrix}, \tag{5}$$

so that wavefunctions map $\psi'(n') = \sum_{n=0}^{N-1} (B_N)_{n'n} \psi(n)$, and the density operator accordingly. We have calculated diagonal Wigner eigenstates $W_{\alpha,\alpha}$ and off-diagonal ones $W_{\alpha,\beta}$ and used them to construct the Wigner propagator equivalent to the unitary map (5) according to Eq. (4). The eigenstates $\alpha = 88$

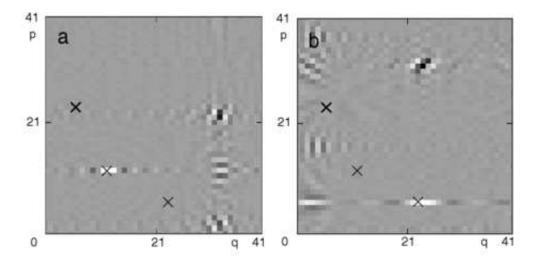


Fig. 2. Propagator of the Wigner function according to Eq. (4) for initial condition $\mathbf{m}' = (6, 25)$ (bold cross) on the period-3 unstable periodic orbit as marked in Fig. 1, after (a) 1 and (b) 2 applications of the same quantum baker map as in Fig. 1. Hilbert-space dimension is N = 42. Other parameters and greyscale as in Fig. 1.

(Fig. 1a) and 129 (1b) clearly show scars of classical unstable periodic orbits (crosses) which up to now could be identified only in the corresponding Husimi functions [9], with considerably inferior resolution. Figures 1 c,d show, respectively, the real and imaginary part of the off-diagonal eigenstate $W_{88,129}$, scarred simultaneously by both orbits that appear in the eigenstates $W_{88,88}$ and $W_{129,129}$.

The Wigner propagator is depicted in Fig. 2, for fixed initial $\mathbf{m}' = (6, 25)$ at t' = 0, the leftmost point of one of the period-3 orbits scarring $W_{129,129}$ (Fig. 1b), at final times t'' = 1 (panel a) and t'' = 2 (b). The strong localization of the propagator on the underlying classical orbit is evident, as are quantum coherence effects reflected in oscillatory patterns far off the classical orbit.

4 Conclusion

The redundance-free Wigner function for discrete phase spaces proposed here enables to identify classical and other phase-space structures in states and time evolution of quantum systems with finite-dimensional Hilbert space, without being marred by artificial ghost images. It facilitates developing and assessing semiclassical approximations for the propagator in such systems [10], providing an alternative point of view for the analysis of coherent structures like "quantum carpets" [11,12].

The method allows to represent signals simultaneously in time and in fre-

quency space, in all applications where data are both discrete and periodic in time (or space) such as in optics, acoustics, or other fields possibly far away from quantum mechanics.

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