Wigner function’s negativity demystified

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(Dated: February 17, 2012)

As early as 1932 Wigner defined the joint distribution for the coordinate and momentum of a quantum particle. Despite a drawback of being sometimes negative, the Wigner distribution has stood the test of time and found many applications. Having demonstrated that the Wigner function of a pure quantum state is a wave function in a standard tool for establishing the quantum-to-classical interface [3, 4], and has a broad range of applications in optics and signal processing [5]. Techniques for the experimental measurement of the Wigner function are also developed [6–8]. Despite its ubiquity, the Wigner function is a probability amplitude for the quantum particle to be at a certain point of the classical phase space. Since probability amplitude need not be positive, our findings elucidate the long-standing mystery of the Wigner function’s negativity. Additionally, we establish that in the classical limit, the Wigner function transforms into a classical Koopman-von Neumann wave function rather than into a classical probability distribution. As a result, contrary to widespread beliefs, the volume of negative regions in the Wigner distribution cannot quantify the degree of quantum character.

In his seminal work [1], Wigner defined the combined distribution of the quantum particle’s coordinate and momentum in terms of the wave function. Since then, this function, bearing his name, plays a paramount role in the phase space formulation of quantum mechanics [2], is a standard tool for establishing the quantum-to-classical interface [3, 4], and has a broad range of applications in optics and signal processing [5]. Techniques for the experimental measurement of the Wigner function are also developed [6–8]. Despite its ubiquity, the Wigner function is a probability amplitude for the quantum particle to be at a certain point of the classical phase space. Since probability amplitude need not be positive, our findings elucidate the long-standing mystery of the Wigner function’s negativity. Additionally, we establish that in the classical limit, the Wigner function transforms into a classical Koopman-von Neumann wave function rather than into a classical probability distribution. As a result, contrary to widespread beliefs, the volume of negative regions in the Wigner distribution cannot quantify the degree of quantum character.

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In this Letter we clarify the origin of the negativity by advocating the following interpretation: The Wigner function is a probability amplitude for a quantum particle to be at a certain point of the classical phase space, i.e., the Wigner function is a wave function analogous to the Koopman-von Neumann (KvN) wave function of a classical particle.

Around the time the Wigner distribution was conceived, Koopman and von Neumann [13–16] recast classical mechanics in a form similar to quantum mechanics by introducing classical complex valued wave functions and representing associated physical observables by means of commuting self-adjoint operators. In particular, it was postulated that the wave function \(|\Psi(t)\rangle\) of a classical particle obeys the following equation of motion:

\[
i \frac{d}{dt} |\Psi(t)\rangle = \hat{L} |\Psi(t)\rangle,
\]

\[
\hat{L} = \frac{\hat{p}}{m} \hat{\lambda}_x - U'(\hat{x}) \hat{\lambda}_p,
\]

where \([\hat{x}, \hat{\lambda}_x] = [\hat{p}, \hat{\lambda}_p] = i\) and \([\hat{x}, \hat{p}] = [\hat{\lambda}_x, \hat{\lambda}_p] = 0\).

Without loss of generality one-dimensional systems are considered throughout. Since the self-adjoint operators representing the classical observables of coordinate \(\hat{x}\) and momentum \(\hat{p}\) commute, they share a common set of orthogonal eigenvectors \(|p\rangle\) such that \(1 = \int dpdx |p\rangle \langle p|\). In the KvN classical mechanics, all observables are functions of \(\hat{x}\) and \(\hat{p}\). The expectation value of an observable \(\hat{F} = F(\hat{x}, \hat{p})\) at time \(t\) equals to \(|\langle \Psi(t) | \hat{F} | \Psi(t) \rangle|\). The probability amplitude \(|\langle p | \psi(t) \rangle|\) for a classical particle to be at point \(x\) with momentum \(p\) at time \(t\) is found to satisfy

\[
\left[ \frac{\partial}{\partial t} + \frac{p}{m} \frac{\partial}{\partial x} - U'(x) \frac{\partial}{\partial p} \right] |\langle p | \psi(t) \rangle| = 0.
\]

This is the evolution equation for the classical wave function in the \(xp\)-representation, where \(\hat{x} = x\), \(\hat{\lambda}_x = -i\partial/\partial x\), \(\hat{p} = p\), and \(\hat{\lambda}_p = -i\partial/\partial p\) in order to satisfy the commutation relations \([\hat{x}, \hat{p}] = i\). Utilizing the chain rule and equation (3), we obtain the well known classical Liouville equation for the phase-space probability distribution \(\rho(x, p; t) = |\langle p | \psi(t) \rangle|^2\),

\[
\left[ \frac{\partial}{\partial t} + \frac{p}{m} \frac{\partial}{\partial x} - U'(x) \frac{\partial}{\partial p} \right] \rho(x, p; t) = 0.
\]

Note that the classical wave function and the classical probability distribution satisfy the same dynamical equation, which reflects the physical irrelevance of the phase of a classical wave function.

In recent work [17], we put forth the Ehrenfest quantization as a systematic theoretical framework for deducing equations of motion from the evolution of average values.
First, starting from the Ehrenfest theorems, we obtained the Schrödinger equation if the momentum and coordinate operators obeyed the canonical commutation relation, and the KvN equation \cite{1} if the momentum and coordinate operators commuted. Then, applying the same technique to the Ehrenfest theorems, 
\begin{align}
 m \frac{d}{dt} \langle \Psi_\kappa(t) | \dot{x}_q | \Psi_\kappa(t) \rangle &= \langle \Psi_\kappa(t) | \dot{\rho}_q | \Psi_\kappa(t) \rangle, \\
 \frac{d}{dt} \langle \Psi_\kappa(t) | \dot{\rho}_q | \Psi_\kappa(t) \rangle &= \langle \Psi_\kappa(t) | -U'(\dot{x}_q) | \Psi_\kappa(t) \rangle, \end{align}
with a generalization \( \dot{x}_q, \dot{\rho}_q = i\hbar \kappa (0 \leq \kappa \leq 1) \) and demanding a smooth classical limit \( \kappa \to 0 \), we have shown that 
\begin{align}
 i\hbar \frac{d}{dt} | \Psi_\kappa(t) \rangle &= \mathcal{H}_{qc} | \Psi_\kappa(t) \rangle, \\
 \mathcal{H}_{qc} &= \frac{\hbar}{m} \hat{p} \hat{\lambda}_x + \frac{1}{\kappa} U \left( \hat{x} - \frac{\hbar \kappa}{2} \hat{\lambda}_p \right) - \frac{1}{\kappa} U \left( \hat{x} + \frac{\hbar \kappa}{2} \hat{\lambda}_p \right),
\end{align}
where \( \hat{x}_q, \hat{\rho}_q \) represent the quantum coordinate and momentum respectively, \( \hat{x}, \hat{\rho}, \hat{\lambda}_x, \hat{\lambda}_p \) are the same classical operators as in equation \( \frac{d}{dt} \), and \( \kappa \) denotes the degree of quantumness/commutativity: \( \kappa \to 1 \) corresponds to quantum mechanics whereas \( \kappa \to 0 \) recovers classical mechanics, \( \lim_{\kappa \to 0} \mathcal{H}_{qc} = \hbar L \). See figure \( \ref{fig:1} \) for a pictorial summary of these derivations thoroughly presented in \cite{17}.

A crucial point for our current discussion is that this unified wave function \( | \Psi_\kappa \rangle \) (t is dropped henceforth) in the \( xp \)-representation is proportional to the Wigner function \( W \), 
\begin{align}
 \langle p,x | \Psi_\kappa \rangle &= \sqrt{2\pi \hbar \kappa} W(x,p), \\
 W(x,p) &= \int \frac{dy}{2\pi \hbar \kappa} \rho_\kappa \left( x - \frac{y}{2}, x + \frac{y}{2} \right) e^{ipy/(\hbar \kappa)}, \end{align}
where \( \rho_\kappa \) denotes the density matrix with \( \hbar \) replaced by \( \hbar \kappa \). \cite{17} Straightforward calculations show that the normalization condition for the unified wave function implies that the density matrix must correspond to a pure state, 
\begin{align}
 \langle \Psi_\kappa | \Psi_\kappa \rangle = 1 \iff \rho_\kappa^2 = \hat{\rho}_\kappa.
\end{align}

\begin{align}
 \langle \Psi_\kappa | G(\hat{x}_q) F(\hat{\rho}_q) | \Psi_\kappa \rangle &= \langle \phi_\kappa | G(\hat{x}_q) F(\hat{\rho}_q) | \phi_\kappa \rangle,
\end{align}
where \( G(\hat{x}_q) \) and \( F(\hat{\rho}_q) \) are arbitrary functions of the quantum position and momentum, respectively.

Equations \cite{8} and \cite{9} reveal that the Wigner distribution of a pure state indeed behaves like a wave function. As shown in figure \( \ref{fig:1} \) the Wigner function’s dynamical equation \cite{6} transforms into the evolution equation for a classical KvN wave function \cite{7}. Hence, in the classical limit, the Wigner function maps a quantum wave function into a corresponding KvN classical wave function rather than a classical phase space distribution. Since the vectors \( | p,x \rangle \) are identical in both KvN and Wigner representations, \( W(x,p) \) is proportional to the probability amplitude that a quantum particle is located at a point \( (x,p) \) of the classical phase space. Note it is important to distinguish the classical \( (\hat{x},\hat{\rho}) \) and quantum \( (\hat{x}_q,\hat{\rho}_q) \) phase spaces because the notion of a phase-space point arises naturally only in the commutative classical variables \( (\hat{x},\hat{p}) \). One may take this distinction further and interpret the Wigner function as the KvN wave function of a classical counterpart of the analogous quantum system. In any case, the Wigner function, as any other wave function, need not be strictly positive, and its negativity does not necessarily imply the quantum nature of either the system or dynamics.

The following statement, proven in \cite{17}, serves as an illustration of the interpretation above: The equality \( \mathcal{H}_{qc} = \hbar L \) holds solely for a quadratic potential; namely, quantum and classical harmonic oscillators with the identical spring constant share the same eigenstates. Hence, the Wigner and KvN wave functions of these eigenstates coincide.

Acknowledgments. The authors acknowledge financial support from DARPA QuBE, NSF, and ARO.

\begin{thebibliography}{99}
[1] E. Wigner. On the quantum correction for thermodynamic equilibrium. Phys. Rev., 40(5):749–759, 1932. [doi:10.1103/PhysRev.40.749].
[2] C. Zachos, D. Fairlie, and T. Curtright. Quantum Mechanics in Phase Space. World Scientific, Singapore, 2005.
[3] A. O. Bolivar. Quantum-classical correspondence: dynamical quantization and the classical limit. Springer, Berlin: New York, 2004.
[4] W. H. Zurek. Sub-Planck structure in phase space and its relevance for quantum decoherence. Nature, 412(6848):712–717, 2001. [doi:10.1038/35089017].
[5] D. Dragoman. Applications of the Wigner Distribution Function in Signal Processing. EURASIP Journal on Advances in Signal Processing, 2005(10):1520–1534, 2005. [doi:10.1155/ASP:2005.1520].
[6] S. Deléglise, I. Dotsenko, C. Sayrin, J. Bernu, M. Brune, J.-M. Raimond, and S. Haroche. Reconstruction of non-classical cavity field states with snapshots of their decoherence. Nature, 455(7212):510–514, 2008.
\end{thebibliography}
FIG. 1: The derivation of quantum mechanics, classical mechanics, and quantum mechanical phase space representation within the Ehrenfest quantization proposed in [17].