Non-negative Wigner-like distributions and Rényi-Wigner entropies of arbitrary non-Gaussian quantum states: The thermal state of the one-dimensional box problem

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Abstract

In this work, we consider the phase-space picture of quantum mechanics. We then introduce non-negative Wigner-like distributions \( \tilde{W}_{\rho,\alpha}(x,p) \)'s corresponding to the density operator \( \hat{\rho} \) and being proportional to \( \{ W_{\rho,2}(x,p) \}^2 \), where \( \{ W_{\rho}(x,p) \}^2 \) denotes the Wigner function. In doing so, we utilize the formal symmetry between the purity measure \( \text{Tr}(\hat{\rho}^2) \) and its Wigner representation \( (2\pi\hbar)^{\frac{1}{2}} \int dxdp \{ W_{\rho}(x,p) \}^2 \) and then consider, as a generalization, such symmetry between the fractional moments \( \text{Tr}(\hat{\rho}^\alpha) \) and their Wigner representations \( (2\pi\hbar)^{\frac{1}{2}} \int dxdp \{ W_{\rho,2}(x,p) \}^2 \). Next, we build up a framework which enables to explicitly evaluate the Rényi-Wigner entropies for the classical-like distributions \( \tilde{W}_{\rho,\alpha}(x,p) \) in a compact way. We also discuss the relationship between the non-negative feature of \( \tilde{W}_{\rho,\alpha}(x,p) \) and the \( x-p \) uncertainty relation with the help of the celebrated Bopp shift, as well as providing a well-defined evaluation scheme of expectation values of observables within this formulation. To illustrate the validity of our framework, we evaluate the distributions \( \tilde{W}_{\beta,\alpha}(x,p) \) corresponding to the (non-Gaussian) thermal state \( \hat{\rho}_\beta \) of a single particle confined by a one-dimensional infinite potential well with either Dirichlet or Neumann boundary condition and then analyze the resulting Rényi entropies. Our phase-space approach will contribute to a deeper understanding of non-Gaussian states and their transitions either in the semiclassical limit (\( h \to 0 \)) or in the high-temperature limit (\( \beta \to 0 \)), as well as enabling to systematically discuss the quantal-classical Second Law of thermodynamics on the single footing.

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I. INTRODUCTION

The Rényi-\(\alpha\) entropy of a probability distribution \(P = \{p_j\}\) has originally been introduced in the classical information theory, explicitly given by \(S_\alpha(P) = (1 - \alpha)^{-1} \ln \{\sum_j (p_j)^\alpha\}\) with order \(\alpha > 0\) \([1, 2]\), as a generalization of the Shannon measure of information (SMI) given by \(S_1(P) = -\sum_j p_j \ln p_j\) (for a deeper conceptual discussion of SMI, see, e.g., \([3]\)). Then, its quantum analog, given by \(S_\alpha(\hat{\rho}) = (1 - \alpha)^{-1} \ln \{\text{Tr}(\hat{\rho}^\alpha)\}\) of a density operator \(\hat{\rho}\), has been studied in various contexts of quantum information theory and quantum thermodynamics \([4–10]\), which is accordingly a generalization of the von Neumann entropy \(S_1(\hat{\rho}) = -\text{Tr}(\hat{\rho} \ln \hat{\rho})\). Obviously, the case of \(\alpha = 2\) gives the well-known quantity \(S_2(\hat{\rho}) = -\ln \{\text{Tr}(\hat{\rho}^2)\}\).

It is true that the quantum-mechanical expectation values of observables \(\hat{A}\) can be calculated independently of the pictures in consideration (i.e., either the operator picture in the Hilbert space or the \(c\)-number picture in the classical phase space), and are required to obey, e.g., the Ehrenfest theorem (as a quantum-classical channel) stating that the classical laws of motion also hold true formally for the quantal expectation values \([11]\). On the other hand, the density operator \(\hat{\rho}\) itself of the Hilbert-space picture can possess genuine quantum features (or non-classicalities) such as coherence and entanglement, which have been attracting considerable interest, as the need for a better theoretical understanding of them increases in response to the experimental manipulation of them in small quantum systems \([12, 13]\). However, when it comes to a systematic study of the canonical quantum-classical transition in the limit of \(\hbar \rightarrow 0\), it would be preferred to take into consideration, instead, the quasi-probability distribution of the \(c\)-number picture, such as the Wigner function \([14–18]\)

\[
W_{\rho}(x, p) = \frac{1}{\pi \hbar} \int_{-\infty}^{\infty} d\xi \langle x + \xi | \hat{\rho} | x - \xi \rangle \exp \left( -\frac{2i}{\hbar} p \xi \right) \tag{1a}
\]

\[
\hat{\rho} = 2 \int d\xi \int dx dp |x + \xi\rangle W_{\rho}(x, p) \exp \left( \frac{2i}{\hbar} p \xi \right) \langle x - \xi| . \tag{1b}
\]

As such, the Wigner function \(W_{\rho}(x, p)\) may be regarded as the direct counterpart to the classical probability distribution \(P(x, p)\) on the same footing, and therefore the quantum-classical channels between the two \(c\)-number distributions could also be explored. However, the Wigner function of a generic quantum state may possess negative values, as is well-known.

Therefore, it would be instructive information-theoretically and thermodynamically to discuss the quantal-classical Second Law on the single footing, i.e., in terms of the Rényi-\(\alpha\)
entropy $S_\alpha(W_\rho)$ for a given distribution $W_\rho(x,p)$, albeit with its negative values, in addition to the First Law in terms of the internal energy $\langle \hat{A} \rangle$ with $\hat{A} \to \hat{H}$, where the expectation value

$$\langle \hat{A} \rangle = \text{Tr}(\hat{\rho} \hat{A}) = \int dx dp \, W_\rho(x,p) \, W_A(x,p)$$

expressed in terms of the Weyl-Wigner representation

$$W_A(x,p) = \int_{-\infty}^{\infty} d\xi \left\langle x + \frac{\xi}{2} \middle| \hat{A} \middle| x - \frac{\xi}{2} \right\rangle \exp \left( -\frac{ip\xi}{\hbar} \right)$$

(cf. $W_A(x,p) \to 1$ for $\hat{A} \to \mathbb{1}$). Thus far, such a unified approach of the Rényi-$\alpha$ entropies has not extensively been discussed, except for either the case of $\alpha = 2$, for which the purity measure $\text{Tr}(\hat{\rho}^2) = (2\pi\hbar) \int dx dp \, \{W_\rho(x,p)\}^2$ given in compact form, or the case of a Gaussian state $\hat{\rho}_G$ (due to its mathematically simple structure) defined as a quantum state, the Wigner function $W_\rho G(x,p)$ of which is Gaussian, such as the canonical thermal equilibrium state $\hat{\rho}_\beta$ (with $\beta = 1/k_B T$) of an $N$-oscillator system (corresponding to its ground state at $T = 0$), the coherent state, and the squeezed state, etc. [19–24]. Further, the entropy $S_2(W_\rho G)$ of a Gaussian state has been shown to coincide with the so-called Wigner entropy $S_W(W_\rho G)$ up to a constant, where $S_W(W_\rho G) := -\int dx dp W_\rho G(x,p) \ln\{2\pi\hbar W_\rho G(x,p)\}$ being well-defined due to the non-negativity of $W_\rho G(x,p)$ over the entire phase space [25, 26].

A framework for exact evaluations of Rényi-$\alpha$ entropies $S_\alpha(W_\rho)$ for given distributions $W_\rho(x,p)$ of non-Gaussian states has finally been provided in [9], but essentially restricted to integer orders $\alpha \to l$ only. Within this framework, the entropies $S_\alpha(W_\rho G)$ of Gaussian states $W_\rho G(x,p)$ for real values of $\alpha > 0$ also have been rediscovered in closed form, but with the help of an additional recurrence relation between two consecutive entropies $S_l$ and $S_{l+1}$ followed by the analytic continuation of $l \to \alpha$. Therefore, it still remains an open question to directly evaluate the entropies $S_\alpha(W_{\rho G})$ of non-Gaussian states $W_{\rho G}(x,p)$ for real values $\alpha$ for which finding such a recurrence relation would be a formidable task.

In this work, we intend to build up another framework, as a generalization of the preceding one, in which a group of Wigner-like distributions denoted by $\tilde{W}_{\rho,\alpha}(x,p)$'s (with $\alpha \in \mathbb{R}^+$) will be introduced, corresponding to the same density operator $\hat{\rho}$, and then the Rényi entropies $S_\alpha(\tilde{W}_{\rho,\alpha})$, being tantamount to $S_\alpha(W_\rho)$, can be evaluated in a compact way for arbitrary non-Gaussian states, actually with no need for the aforesaid recurrence relation and analytic continuation [cf. Eqs. (6) and (9)]. Remarkably, the distributions $\tilde{W}_{\rho,\alpha}(x,p)$'s will be shown to be non-negative over the entire phase space (like the classical
probability distribution) and well-defined in the genuine quantum regime all the way to
the semiclassical limit. Besides, because of the equivalence between \( S_w(W_{\rho G}) \) and \( S_2(W_{\rho G}) \)
(up to a constant) for (non-negative) Gaussian states and also the non-negative feature of
\( \tilde{\mathcal{W}}_{\rho;\alpha}(x, p) \) for non-Gaussian states, it will be legitimate to say that the entropies \( S_{\alpha}(\tilde{\mathcal{W}}_{\rho;\alpha}) \),
called the Rényi-Wigner entropies, may also be regarded as a generalization of the Wigner
entropy \( S_w(W_{\rho G}) \). Subsequently, we will consider a specific non-Gaussian state, which will
be applied for our framework of its Rényi-Wigner entropies; this is the thermal state \( \hat{\rho}_\beta \) of a
single particle confined by a one-dimensional infinite potential well with either Dirichlet or
Neumann boundary condition. Its Wigner function (with its negative values) will be shown
to tend asymptotically to a Gaussian shape in the limit of \( \hbar \to 0 \) only.

The general layout of this paper is as follows: In Sec. II we introduce a group of Wigner-
like distributions as variants of the Wigner function and then provide a generic framework
for the Rényi-Wigner entropies of arbitrary quantum states in the classical phase space. In
Sec. III we explicitly evaluate the Wigner function, and its variants, of the thermal state of
the one-dimensional box problem and then discuss the relevant issues of quantum-classical
transition. In Sec. IV we apply our framework for this thermal state, and discuss some
subjects relevant to the resulting Rényi-Wigner entropies. Finally, we give the concluding
remarks of this paper in Sec. V.

II. NON-NEGATIVE WIGNER-LIKE DISTRIBUTIONS AND ENTROPIES

We first observe that the purity measure, being the first moment of probability \( \langle p \rangle = \sum_n (p_n)^2 \) with the eigenvalues \( p_n \)'s of \( \hat{\rho} \), may be rewritten as
\[
\text{Tr}(\hat{\rho}^2) = \int dx dp \mathcal{W}_{\rho^2}(x, p),
\]
where \( \mathcal{W}_{\rho^2}(x, p) := (2\pi\hbar)^2 \{W_{\rho}(x, p)\}^2 \geq 0 \). This quantity \( \mathcal{W}_{\rho^2}(x, p) \) should be distinguished
from its counterpart \( W_{\rho^2}(x, p) \) which is directly obtained from Eq. (1a) with \( \hat{\rho} \to \hat{\rho}^2 \) and
thus may be negative valued like \( W_{\rho}(x, p) \) itself. However, such formal symmetry between
\( \hat{\rho}^2 \) and \( \mathcal{W}_{\rho^2}(x, p) \) is not available for higher moments, for which \( \text{Tr}(\hat{\rho}^l) \neq \int dx dp \{W_{\rho}(x, p)\}^l \)
with \( l = 3, 4, 5, \cdots \). To directly discuss higher moments \( \text{Tr}(\hat{\rho}^\alpha) \) with \( \alpha \in \mathbb{R}^+ \) in the phase
space, we therefore generalize Eq. (4) in such a way that the \((\alpha - 1)\)th fractional moment
of probability is given by

\[ \langle p^{\alpha - 1} \rangle = \text{Tr}(\hat{\rho}^{\alpha}) = \int dx \, dp \, W_{p^{\alpha}}(x, p), \quad (5) \]

in which the quantity \( W_{p^{\alpha}}(x, p) = (2\pi \hbar)^{2} \{ W_{p^{\alpha/2}}(x, p) \}^{2} \geq 0 \) correspondingly results from Eq. (1a) with \( \hat{\rho} \to \hat{\rho}^{\alpha/2} \). Here, a fractional operator \( \hat{\rho}^{\alpha} \) is obtained from the spectral expansion of \( \hat{\rho} \) by substituting its eigenvalues \( p_{n} \)'s with their positive \( \alpha \)th roots.

Now we introduce the non-negative distributions \( \tilde{W}_{\rho^{\alpha}}(x, p) := W_{p^{\alpha}}(x, p)/N_{p^{\alpha}} \) with the normalizing \( N_{p^{\alpha}} = \int dx dp W_{p^{\alpha}}(x, p) \), all of which correspond to the same density operator \( \hat{\rho} \). Similarly, we also introduce the distributions \( \tilde{W}_{\rho^{\alpha/2}}(x, p) := W_{p^{\alpha/2}}(x, p)/N_{p^{\alpha/2}} \) with \( N_{p^{\alpha/2}} = \int dx dp W_{p^{\alpha/2}}(x, p) \). Let \( \tilde{W}_{\rho} = \{ \tilde{W}_{\rho^{\alpha}}(x, p) | \alpha > 0 \} \). Then the Rényi-Wigner entropy of \( \hat{\rho} \) with order \( \alpha \) can be expressed as the compact form

\[ S_{\alpha}(\tilde{W}_{\rho}) = (1 - \alpha)^{-1} \ln N_{p^{\alpha}} = (1 - \alpha)^{-1} \ln \left\{ (2\pi \hbar)(N_{p^{\alpha/2}}) \langle W_{p^{\alpha/2}} \rangle_{\tilde{W}_{\rho^{\alpha/2}}} \right\}, \quad (6) \]

where the particular selection of \( \tilde{W}_{\rho^{\alpha}}(x, p) \) out of the set \( \tilde{W}_{\rho} \) has been made, with \( \alpha' \to \alpha \), for \( N_{p^{\alpha}} \), and the expectation value \( \langle \cdots \rangle = \int dx dp W_{p^{\alpha/2}}(x, p) \tilde{W}_{\rho^{\alpha/2}}(x, p) \). Eq. (6) is the first central result of this paper. This enables to evaluate the Rényi-\( \alpha \) entropy in the phase space in a more compact way than its counterpart provided in Ref. [9] (cf. Eq. (13) thereof) which has been derived, on the other hand, for positive integers \( \alpha \to l = 2, 3, 4, \cdots \) only and expressed in terms of the product of plain Wigner functions \( W_{\rho}(x, p) \)'s with the Bopp shift; as a result, it turns out that the normalizing \( N_{p^{\alpha}} \) in Eq. (6) now replaces the lengthy expression

\[ (2\pi \hbar)^{l-1} \int dx dp W_{\rho}(x, p) \left\{ W_{\rho} \left( x - \frac{\hbar}{2i} \frac{\partial}{\partial p}, p + \frac{\hbar}{2i} \frac{\partial}{\partial x} \right) \right\}^{l-2} W_{\rho}(x, p) = \text{Tr}(\hat{\rho}^{l}). \quad (7) \]

Then we can compute the entropy with no need for an analytic continuation of \( l \to \alpha \), even for arbitrary non-Gaussian states. We will be interested especially in the case of \( \alpha = 1 \), for which

\[ \tilde{W}_{\rho} \to \tilde{W}_{\rho^{1}}(x, p) = W_{\rho}(x, p) = (2\pi \hbar) \{ W_{\rho^{1/2}}(x, p) \}^{2} \geq 0, \quad (8) \]

obviously with \( W_{\rho}(x, p) \neq W_{\rho}(x, p) \). Then the von-Neumann entropy reduces to

\[ S_{1}(\tilde{W}_{\rho}) = -\partial_{\alpha} \ln \left\{ \int dx dp \, W_{p^{\alpha}}(x, p) \right\}_{\alpha=1} = -(2\pi \hbar)(N_{p^{1/2}}) \langle \partial_{\alpha} (W_{\rho^{\alpha}}) |_{\alpha=1/2} \rangle_{\tilde{W}_{\rho^{1/2}}}, \quad (9) \]

directly obtained without considering any analytic continuation at all. From this, it is easy to see that for a pure state \( \hat{\sigma} \), the quantity \( W_{\sigma^{\alpha}}(x, p) \to W_{\sigma}(x, p) \) and therefore \( \partial_{\alpha}(W_{\sigma^{\alpha}}) \to 0 \), finally leading to the entropy \( S_{1}(\tilde{W}_{\rho}) \to 0 \), as required.

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Now we examine some properties of a distribution $\tilde{W}_{\rho^{\alpha}}(x,p)$. By construction, this distribution is coupled to the density operator $\hat{\rho}$ via Eq. (1b) with $\rho \rightarrow \rho^{\alpha/2}$ followed by the spectral expansion of the resulting operator $\hat{\rho}^{\alpha/2}$. At first sight, its non-negative nature (like that of its classical counterpart) could not suitably reflect the orthogonality relation between any pair $(n,m)$ of two different eigenstates, because of the trace $\int dx dp \tilde{W}_n(x,p) \tilde{W}_m(x,p) > 0$. However, this problem can be remedied with the help of the Bopp shift, like for Eq. (7), such that, with $\hat{\rho}^{\alpha} \rightarrow \hat{\rho}$ for pure states, $\text{Tr}(\hat{\rho}_n \hat{\rho}_m)$ is expressed, instead, as

$$
(2\pi\hbar)^3 \int dx dp W_r(x,p) W_s(x - \frac{\hbar}{2i} \frac{\partial}{\partial p} + \frac{\hbar}{2i} \frac{\partial}{\partial x}) W_u(x - \frac{\hbar}{2i} \frac{\partial}{\partial p} + \frac{\hbar}{2i} \frac{\partial}{\partial x}) W_v(x,p) = \delta_{nm}
$$

(10)

indeed, in which $(r,s,u,v) = (n,n,m,m); (n,m,m,n); (m,m,n,n); (m,n,n,m)$, thus being equivalent to $\text{Tr}\{(\hat{\rho}_n^2)\hat{\rho}_m^2\} = \delta_{nm}$. In the limit of $\hbar \rightarrow 0$, the left-hand side of Eq. (10) would obviously reduce to $\int \tilde{W}_n(x,p) \tilde{W}_m(x,p) \geq 0$ and therefore the orthogonality relation would be gone completely, which is exactly the case for any classical probability distribution $P(x,p)$. For two arbitrary orthogonal mixed states, given by $\hat{\eta} = \sum_n a_n \ket{n}\bra{n}$ and $\hat{\chi} = \sum_m a_m \ket{m}\bra{m}$ with $n \neq m$, the same scenario straightforwardly follows from Eq. (10) with the subscripts $r = s \rightarrow \eta^{\alpha/2}$ multiplied by $(N_{\eta^\alpha})^{-1}$ and $u = v \rightarrow \chi^{\alpha/2}$ multiplied by $(N_{\chi^\alpha})^{-1}$.

Likewise, the purity measure of $\tilde{W}_{\rho_{\alpha}}(x,p)$ can also be in consideration for comparison, in addition to Eq. (4) (or Eq. 6), such that

$$\text{Tr}(\hat{\rho}^{2}) = (2\pi\hbar)^3 (N_{\rho^\alpha})^{-2} \int dx dp W_{\rho^{\alpha}/2}(x,p) W_{\rho^{\alpha}/2}(x - \frac{\hbar}{2i} \frac{\partial}{\partial p} + \frac{\hbar}{2i} \frac{\partial}{\partial x}) \times W_{\rho^{\alpha}/2}(x - \frac{\hbar}{2i} \frac{\partial}{\partial p} + \frac{\hbar}{2i} \frac{\partial}{\partial x}) W_{\rho^{\alpha}/2}(x,p).$$

(11)

This is in exactly the same form as Eq. (11) of Ref. [9] for $\text{Tr}(\hat{\rho}^{4})$, up to the subscripts $\rho \rightarrow \rho^{\alpha/2}$ and the normalizing $(N_{\rho^\alpha})^2$. Applying the same technique as for Eq. (13) of Ref. [9] with the help of the Fourier transform $\mathcal{F}_{\rho^\alpha}(\mathbf{r}, \mathbf{p}) = (2\pi\hbar)^{-1} \int dx dp W_{\rho^\alpha}(x,p) \exp\{i(x\mathbf{p} + p\mathbf{q})/\hbar\}$, this purity measure (11) will finally be transformed, after some algebraic manipulations, into

$$\text{Tr}(\hat{\rho}^{2}) = (N_{\rho^\alpha})^{-2} \int_{-\infty}^{\infty} dx dp dx_1 dp_1 dx_2 dp_2 dx_3 dp_3 \times$$

$$W_{\rho^{\alpha}/2}(x,p) \exp\left\{-\frac{i}{\hbar} (x_1 + x_2 + x_3) \right\} W_{\rho^{\alpha}/2}(x + (x_2 + x_3)/2, p_1) \exp\left(\frac{i}{\hbar} x_1 p_1\right) \times$$

$$W_{\rho^{\alpha}/2}(x - (x_1 - x_3)/2, p_2) \exp\left(\frac{i}{\hbar} x_2 p_2\right) W_{\rho^{\alpha}/2}(x - (x_1 + x_2)/2, p_3) \exp\left(\frac{i}{\hbar} x_3 p_3\right),$$

(12)
which is another phase-space representation of the purity measure (cf. Eq. (33) for actual evaluation of this with respect to a specific state). It is also worthwhile to point out that the Wigner entropy given by $S_W(\tilde{W}_\rho) = -\int dxdp \tilde{W}_{\rho,\alpha}(x,p) \log\{(2\pi\hbar) \tilde{W}_{\rho,\alpha}(x,p)\}$ is ill-defined, though $\tilde{W}_{\rho,\alpha}(x,p) \geq 0$, because the Bopp shift has not been employed at all and thus this entropy can, e.g., not appropriately distinguish pure states from mixed states [cf. Eqs. (34a)-(34d) and the discussion thereafter].

Next, let us consider the expectation value of an observable $\hat{A}$ within our formulation. We begin with the case of $\alpha = 1$. Following the idea developed in the preceding paragraphs, it is straightforward to show that $\text{Tr}(\hat{\rho}\hat{A}) \neq \int dxdp \tilde{W}_{\rho,1}(x,p) W_A(x,p)$ but the expression

$$\text{Tr}(\hat{\rho}\hat{A}) = \text{Tr}(\hat{\rho}^{1/2}\hat{\rho}^{1/2}) = (2\pi\hbar) \int dxdp W_{\rho^{1/2}}(x,p) W_A\left(x - \frac{\hbar}{2i} \frac{\partial}{\partial p}, p + \frac{\hbar}{2i} \frac{\partial}{\partial x}\right) W_{\rho^{1/2}}(x,p)$$

(also note the standard form, Eq. (2) for comparison). We can easily confirm Eq. (13), by taking into consideration the cases of $\hat{A} \to 1; \hat{x}, \hat{p}; \hat{x}^2, \hat{p}^2, \hat{x}\hat{p} + \hat{p}\hat{x}; \cdots$. This result reminds the expression $\langle \hat{A} \rangle_{\psi} = \int dx \psi^*(x) A(x, -i\hbar \partial_x) \psi(x)$ in formal similarity [27]. Then we apply the same technique as for Eq. (12) with the help of the Fourier transform $W_A(x,p) = (2\pi\hbar)^{-1} \int dxdp W_A(x,p) \exp\{i(xp + px)/\hbar\}$, which will enable Eq. (13) to have the form

$$\text{Tr}(\hat{\rho}\hat{A}) = (4\pi\hbar)^{-1} \int_{-\infty}^{\infty} dx dp dx_1 dp_1 dx_2 dp_2 W_{\rho^{1/2}}(x/2,p) \exp\left\{-i\hbar (x_1 - x_2) p\right\} \times W_A(x/2, p_1) \exp\left\{-i\hbar (x_2 - x) p_1\right\} W_{\rho^{1/2}}(x/2, p_2) \exp\left\{-i\hbar (x - x_1) p_2\right\}.$$  

(14)

It is straightforward to verify Eq. (14) with the help of Eq. (1a); for $\hat{A} \to 1$, this is shown to reduce to unity. Considering in Eq. (14) the diagonal terms with $x = x_1 = x_2$ and $p = p_1 = p_2$ only, then Eq. (14) would simply reduce to $\text{Tr}(\hat{\rho}\hat{A}) \propto \int dxdp \tilde{W}_{\rho,1}(x,p) W_A(x,p)$ indeed. In fact, all off-diagonal terms play a critical role in exact evaluation of the expectation value, which is not the case for the standard form, Eq. (2). As a result, we have a real-valued quantity $(2\pi\hbar) W_{\rho^{1/2}}(x,p) W_{\rho^{1/2}}(x',p')$ whose diagonal elements each, being non-negative, represent the probability distributions of staying at $(x,p)$, like the classical probability distribution $P(x,p)$, while its off-diagonal elements each, allowed to be negative valued, are responsible for jumps between $(x,p)$ and $(x',p')$. This is the second central result of this paper. The verification for the case of $\hat{A} \to -i [\hat{x}, \hat{p}]$ also implies that the $\hat{x}\hat{p}$ uncertainty cannot at all break the non-negative feature of the corresponding distribution $\tilde{W}_{\rho,1}(x,p)$. Further, we may generalize Eq. (13) into the cases of $0 < \alpha < 1$ such that the
symmetrized form

\[
\text{Tr}(\hat{\rho} \hat{A}) = (\pi \hbar) \int dx dp \left\{ W_{\rho^0}(x, p) W_A \left( x - \frac{\hbar}{2i} \frac{\partial}{\partial p}, p + \frac{\hbar}{2i} \frac{\partial}{\partial x} \right) W_{\rho^{1-\alpha}}(x, p) + W_{\rho^{1-\alpha}}(x, p) W_A \left( x - \frac{\hbar}{2i} \frac{\partial}{\partial p}, p + \frac{\hbar}{2i} \frac{\partial}{\partial x} \right) W_{\rho^\alpha}(x, p) \right\}. 
\]

However, the corresponding distribution \( \tilde{W}_{\rho^\alpha}(x, p) := (2\pi \hbar) W_{\rho^\alpha}(x, p) W_{\rho^{1-\alpha}}(x, p) \) with \( \int dx dp \tilde{W}_{\rho^\alpha}(x, p) = 1 \) is not guaranteed to be non-negative for \( \alpha \neq 1/2 \).

Now we consider the canonical thermal equilibrium state \( \hat{\rho}_\beta \) for explicit evaluation of \( \tilde{W}_{\rho^\alpha}(x, p) \). First, its Wigner function is given by \( W_\beta(x, p) = \{(2\pi \hbar) Z_\beta\}^{-1} \text{Num}(\beta) \), where the partition function \( Z_\beta \) and

\[
\text{Num}(\beta) := (2\pi \hbar) \sum_n \exp(-\beta E_n) W_n(x, p).
\]

By noting that \( \text{Tr}\{(\hat{\rho})^n\} = Z_{\alpha^n}/(Z_\beta)^\alpha \), it is straightforward to show that \( \tilde{W}_{\rho^\alpha}(x, p) =: \tilde{W}_\beta; \alpha(x, p) = (2\pi \hbar) \{W_{\rho^{n/2}}(x, p)\}^2 \{\text{Tr}(\rho^\alpha)\}^{-1} = \{(2\pi \hbar) Z_{\alpha}\}^{-1} \{\text{Num}(\alpha\beta/2)\}^2 \geq 0 \), where \( W_{\rho^n}(x, p) = (Z_\beta)^{-\alpha} (Z_{\alpha\beta}) W_{\alpha\beta}(x, p) \). As a simple example, the thermal state of a single linear oscillator, being Gaussian, is considered such that \( Z_\beta = 2^{-1} \text{csch}(\beta \hbar \omega/2) \) \cite{28}, and

\[
W_\beta(x, p) = \text{sech}(\beta \hbar \omega/2) \frac{(2\pi \hbar) Z_\beta}{\text{sech}(\beta \hbar \omega/4)} \exp \left[ \left( \tanh \frac{\beta \hbar \omega}{2} \right) \left\{ \kappa_x^2 + \frac{p^2}{\hbar^2} \right\} \right] \geq 0 \quad (17a)
\]

\[
\tilde{W}_{\beta;1}(x, p) = \frac{\text{sech}(\beta \hbar \omega/4)}{(2\pi \hbar) Z_\beta} \exp \left[ -2 \left( \tanh \frac{\beta \hbar \omega}{4} \right) \left\{ \kappa_x^2 + \frac{p^2}{\hbar^2} \right\} \right] \geq 0 \quad (17b)
\]

where \( \kappa = m \omega/\hbar \), as well as the Wigner entropy \( S_W(W_\beta) = S_2(W_\beta) + 1 - \ln(2) \neq S_1(W_\beta) \). It is then straightforward to verify Eqs. \([6]\) and \([9]\) for this system.

Finally, we stress that our formulation for the study of non-Gaussian states, consisting of the non-negative phase-space distributions and Rényi-Wigner entropies, essentially differs from the approach based on the (non-negative) Husimi functions \( Q_\rho(x, p) = \langle \gamma | \hat{\rho} | \gamma \rangle / \pi \) and the resulting Wehrl entropies defined as \( -1 \int dq dp \ Q_\rho(x, p) \ln\{Q_\rho(x, p)\} \); this entropy has been known to have the conceptual weakness, resulting from the non-orthogonality \( |\langle \gamma_1 | \gamma_2 \rangle|^2 = e^{-|\gamma_1 - \gamma_2|^2} \) (e.g., \cite{24} 29).

III. WIGNER FUNCTION OF THERMAL STATE FOR ONE-DIMENSIONAL BOX PROBLEM

The system under consideration is a single particle confined in the region of \(-a \leq x \leq a\) (with \( a > 0 \)) by a one-dimensional infinite potential well with either Dirichlet boundary
condition $\Psi(a) = \Psi(-a) = 0$ (Dbc) or Neumann boundary condition $\Phi'(a) = \Phi'(-a) = 0$ (Nbc). As is well-known, its $n$th eigenstate for Dbc is given by \[ \psi_n(x) = \left( \frac{1}{a} \right)^{1/2} \sin \left\{ \frac{n\pi}{2} \left( 1 + \frac{x}{a} \right) \right\} , \] where $n = 1, 2, 3, \cdots$ and $|x| \leq a$, while the eigenvalue for Nbc is given by \[ \phi_n(x) = \left( \frac{1}{a} \right)^{1/2} \cos \left\{ \frac{n\pi}{2} \left( 1 + \frac{x}{a} \right) \right\} , \] where $n = 1, 2, 3, \cdots$ and $|x| \leq a$, and $\phi_0(x) = (2a)^{-1/2}$; therefore, $\phi_n(x)$ is discontinuous at $x = \pm a$ if the analytic continuation is under consideration that $\phi_n(x) \equiv 0$ for $|x| \leq a$. The corresponding energy eigenvalue is $E_n(L) = (p_n)^2/(2m)$ for both Dbc and Nbc, where $m$ is the mass of the particle, and $p_n = \hbar k_n$ with $k_n = \pm n\pi/L$; here $L = 2a$ denotes the width of the potential well (note that $E_0 = 0$ for Nbc \[31\]). Then the Wigner function corresponding to the eigenstate $|n\rangle$ can be acquired to be, for Dbc, \[ W_{n,D}(x,p) = \frac{1}{\pi \hbar} \int_{-\xi_s}^{\xi_s} d\xi \psi_n(x+\xi) \psi_n(x-\xi) e^{-2ip\xi/\hbar} = \frac{1}{4\pi a} \left[ \left\{ \sin \left( \frac{2\pi}{\hbar} x(p+p_n) \right) \times \left( \frac{1}{p+p_n} - \frac{1}{p} \right) + \{p_n \rightarrow -p_n\} \right\} \right] \] (cf. \[16\] \[32\] \[33\]) while for Nbc, \[ W_{n,N}(x,p) = \frac{1}{\pi \hbar} \int_{-\xi_s}^{\xi_s} d\xi \phi_n(x+\xi) \phi_n(x-\xi) e^{-2ip\xi/\hbar} = \frac{1}{4\pi a} \left[ \left\{ \sin \left( \frac{2\pi}{\hbar} x(p+p_n) \right) \times \left( \frac{1}{p+p_n} + \frac{1}{p} \right) + \{p_n \rightarrow -p_n\} \right\} \right] \] where $n = 1, 2, 3, \cdots$ and $W_{n,N}(x,p) = (2\pi a p)^{-1} \sin(2\xi_x p/\hbar)$; here, $\xi_x = a - |x|$ is required by the boundary condition of $|x+\xi| \leq a$ and $|x-\xi| \leq a$. Therefore, $W_n(\pm a, p) = 0$ for both Dbc and Nbc, as required (cf. Ref. \[33\]). We observe that Eqs. (19a) and (19b), as well as $W_{n,N}(x,p)$, are even functions of both $x$ and $p$, non-Gaussian, and can be negative valued indeed (cf. Figs. 1 and 2).

It is also instructive, for later purpose, to consider Eqs. (19a) and (19b) in the limit of $\hbar \rightarrow 0$, in particular the respective ground states. First, with the help of the identity $\delta(p) = \lim_{\epsilon \rightarrow 0} (\pi p)^{-1} \sin(p/\epsilon)$ \[34\], it is easy to show that $W_{0,N}(x,p) \rightarrow (2a)^{-1} \delta(p)$ in this limit. It is also straightforward to observe that $W_{1,D}(x,p) \rightarrow 0$ for $p \neq 0$ and $W_{1,D}(x,0) \rightarrow \infty$, thus yielding $W_{0,D}(x,p) \rightarrow (2a)^{-1} \delta(p)$ as well.
Now we are ready to discuss the thermal Wigner function of this system, which is given for Dbc and Nbc by [cf. Eq. (16)]

\[
W_{\beta,D}(x,p) = \frac{1}{(Z_{\beta})_{D}} \sum_{n=1}^{\infty} \exp \left( -\lambda n^{2} \right) W_{n,D}(x,p), \tag{20a}
\]

\[
W_{\beta,N}(x,p) = \frac{1}{(Z_{\beta})_{N}} \sum_{n=0}^{\infty} \exp \left( -\lambda n^{2} \right) W_{n,N}(x,p) \tag{20b}
\]

with \( \lambda = \beta \hbar^{2} \pi^{2} (8ma^{2})^{-1} \) and \((Z_{\beta})_{N} = (Z_{\beta})_{D} + 1 \), respectively. These can also be expressed as the integral form

\[
W_{\beta}(x,p) = \frac{1}{(2\pi \hbar)^{1/2} Z_{\beta}} \left\{ B \left( \frac{\hbar}{2p} \right) \sin \left( \frac{2\xi p}{\hbar} \right) \vartheta_{4} \left( \frac{\pi p}{2a}, \exp (-\lambda) \right) + \int_{0}^{\xi/a} d\xi \cos \left( \frac{2\xi p}{\hbar} \right) \vartheta_{3} \left( \frac{\pi \xi}{2a}, \exp (-\lambda) \right) \right\} \tag{21}
\]

in terms of the Jacobi theta functions \( \vartheta_{3}, \vartheta_{4} \)

\[
\vartheta_{3}(z,q) = 1 + 2 \sum_{n=1}^{\infty} q^{n^{2}} \cos(nz) ; \quad \vartheta_{4}(z,q) = 1 + 2 \sum_{n=1}^{\infty} (-1)^{n} q^{n^{2}} \cos(nz) ; \tag{22}
\]

here, \( Z_{\beta} \rightarrow (Z_{\beta})_{D} = 2^{-1} \{ \vartheta_{3}(0, e^{-\lambda}) - 1 \} \) and \( B = -1 \) for \( W_{\beta,D}(x,p) \) while \( Z_{\beta} \rightarrow (Z_{\beta})_{N} = 2^{-1} \{ \vartheta_{3}(0, e^{-\lambda}) + 1 \} \) and \( B = 1 \) for \( W_{\beta,N}(x,p) \).

To study the quantum-classical transition, we rewrite Eqs. (20a) and (20b) as

\[
W_{\beta}(x,p) = \frac{1}{(2\pi \hbar) Z_{\beta}} \int_{0}^{y_{e}} dy \cos \left( \frac{2apy}{\hbar} \right) \sum_{n=-\infty}^{\infty} \exp(-\lambda n^{2}) \left\{ \cos(n\pi y) + B \cos(n\pi y_{e}) \right\} , \tag{23}
\]

where \( y = \xi/a \). Employing the Poisson summation rule \( \sum_{n=-\infty}^{\infty} \exp(-\lambda n^{2}) \cos(n\pi \kappa) = \left( \frac{\pi}{\lambda} \right)^{1/2} \sum_{\nu=-\infty}^{\infty} \exp \left\{ -\frac{\pi^{2} (\kappa + 2\nu)^{2}}{4\lambda} \right\} \) \( \tag{24} \)

and then with the help of the identity \( \int dn \exp(-an^{2} - 2bn) = \frac{1}{\sqrt{a}} \exp \left( \frac{b^{2}}{a} \right) \erf \left( a^{1/2} n + a^{-1/2} b \right) , \) \( \tag{25} \)

Eq. (23) will be transformed into

\[
W_{\beta}(x,p) = \frac{1}{(2\pi \hbar) Z_{\beta}} \left( \frac{\pi}{\lambda} \right)^{1/2} \sum_{\nu=-\infty}^{\infty} \left[ \int_{0}^{y_{e}} \cos \left( \frac{2apy}{\hbar} \right) \exp \left\{ -\frac{\pi^{2} (y + 2\nu)^{2}}{4\lambda} \right\} dy + \frac{B\hbar}{2ap} \sin \left( \frac{2apy_{e}}{\hbar} \right) \exp \left\{ -\frac{\pi^{2} (y_{e} + 2\nu)^{2}}{4\lambda} \right\} \right] \tag{26}
\]
Performing the integration over \( y \) by applying the identity (25) with \( n \to y \) and then after some algebraic manipulations, we can finally arrive at the expression

\[
W_\beta(x, p) = \frac{1}{(2\pi\hbar)} Z_\beta \left[ \exp \left( -\frac{\beta p^2}{2m} \right) \sum_{\nu=-\infty}^{\infty} \Re \left\{ \exp \left( \frac{2ip\nu L}{\hbar} \right) \left[ \erf \left( \frac{2m}{\beta\hbar^2} \right)^{1/2} (\xi_x + \nu L) \right] \right\} \right. \\
+ \left. \left( \frac{\beta}{2m} \right)^{1/2} \right) \right) - \erf \left( \frac{2m}{\beta\hbar^2} \nu L + \left( \frac{\beta}{2m} \right)^{1/2} \right) \right) \left\} \right\} \\
+ \frac{BZ_{\beta,cl}}{2\pi a} \sin \left( \frac{2\xi_x p}{\hbar} \right) \sum_{\mu=-\infty}^{\infty} \exp \left\{ -\frac{2m}{\beta\hbar^2} (\xi_x + \mu L)^2 \right\} \right] (27)
\]

in terms of the error function \( \erf(z) \), where the width \( L = 2a \) and the classical partition function \( Z_{\beta,cl} = (8\pi ma^2/\beta)^{1/2} \) for both Dbc and Nbc; here we also used, with the help of Poisson’s sum rule, the relation

\[
(2\pi\hbar) Z_\beta = 2\pi\hbar \sum_{n=1}^{\infty} \exp \left( -\lambda n^2 \right) = B\pi\hbar + Z_{\beta,cl} \sum_{\nu=-\infty}^{\infty} \exp \left( -\frac{8ma^2\nu^2}{\beta\hbar^2} \right), \quad (28)
\]

which reduces to \( Z_{\beta,cl} \) in the limit of \( \hbar \to 0 \) indeed. It is then straightforward to observe that in the classical limit, Eq. (27) reduces to its classical counterpart \( P_\beta(x, p) = (Z_{\beta,cl})^{-1} e^{-\beta p^2/2m} > 0 \), being Gaussian, which results from the term of \( \nu = 0 \) (with \( \hbar \to 0 \)). Eq. (27) is the third central result of this paper.

Comments are deserved here. First, we observe that \( W_\beta(\pm a, p) = 0 \) and thus \( W_\beta(x, p) \) is continuous in the entire phase space (in particular for Nbc). On the other hand, \( P_\beta(\pm a, p) \neq 0 \) and thus \( P_\beta(x, p) \) is discontinuous at both boundary points. This discontinuity also implies the disappearance of the wave properties. Second, the classical probability distribution \( P_\beta(x, p) \) further reduces to \( (2a)^{-1} \delta(p) \) at \( T = 0 \), in accordance with both \( W_{1,D}(x, p) \) and \( W_{0,N}(x, p) \) within \( \hbar \to 0 \), as discussed after Eq. (19b). Third, all other terms of \( \nu \neq 0 \) of Eq. (27) will then represent the purely quantum correction; the value \( 2L \) denotes the length of an arbitrary primitive periodic orbit (i.e., a closed path traversed only once from an arbitrary phase-space position \( (x_0, p_0) \) to itself after a couple of reflections on the potential walls at \( x = \pm a \) \cite{36, 38}. In fact, if an index \( \nu = \nu_e \) (or \( \mu = \mu_e \)) is even, then it represents a periodic orbit with its length \( \nu_e L \) (or \( \mu_e L \)), corresponding to \( \nu_e/2 \) (or \( \mu_e/2 \)) repetitions of its primitive periodic orbit. On the other hand, if an index \( \nu = \nu_o \) (or \( \mu = \mu_o \)) is odd, then it represents an orbit moving from \( (x_0, p_0) \) to \( (-x_0, -p_0) \) with its length \( \nu_o L \) (or \( \mu_o L \)), which is also needed due to the even parity of this system; note that the cases of \( \nu, \mu < 0 \) simply denote periodic orbits initially moving in the negative direction.

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To explicitly discuss Eq. (27) in the high-temperature regime, we employ both identities 
\[ \text{erf} = 1 - \text{erfc} \quad \text{and} \quad \sum_{k=0}^{\infty} (-2z_2)^k i^k \text{erfc}(z_1) \] 
which will yield the exact expression

\[ W_\beta(x, p) = \frac{1}{(2\pi \hbar) Z_\beta} \left[ \exp \left( -\frac{\beta p^2}{2m} \right) - \cos \left( \frac{2\xi_x p}{\hbar} \right) \sum_{k=0}^{\infty} \left( -\frac{2\beta p^2}{m} \right)^k \times \right. \]
\[ \sum_{\nu=1}^{\infty} \left\{ i^{2k} \text{erfc} \left\{ \left( \frac{2m}{\beta \hbar^2} \right)^{1/2} (\xi_x + (\nu - 1)L) \right\} - i^{2k} \text{erfc} \left\{ \left( \frac{2m}{\beta \hbar^2} \right)^{1/2} (\nu L - \xi_x) \right\} \right\} - \]
\[ \frac{Z_{\beta,cl}}{4\pi^{1/2} ap} \sin \left( \frac{2\xi_x p}{\hbar} \right) \sum_{k=1}^{\infty} \left( -\frac{2\beta p^2}{m} \right)^k \times \]
\[ \sum_{\nu=1}^{\infty} \left\{ i^{2k-1} \text{erfc} \left( \left( \frac{2m}{\beta \hbar^2} \right)^{1/2} (\xi_x + (\nu - 1)L) \right) + i^{2k-1} \text{erfc} \left( \left( \frac{2m}{\beta \hbar^2} \right)^{1/2} (\nu L - \xi_x) \right) \right\} + \]
\[ \frac{BZ_{\beta,cl}}{2\pi ap} \sin \left( \frac{2\xi_x p}{\hbar} \right) \sum_{\mu=1}^{\infty} \left\{ \exp \left\{ -\frac{2m}{\beta \hbar^2} (\xi_x + (\mu - 1)L)^2 \right\} + \exp \left\{ -\frac{2m}{\beta \hbar^2} (\mu L - \xi_x)^2 \right\} \right\} \right] . \]

With the help of \( i^k \text{erfc}(0) = \{ 2^k \Gamma(k/2 + 1) \}^{-1} \) with \( i^{-1} \text{erfc}(z) = (2/\sqrt{\pi}) \exp(-z^2) \), the boundary condition, \( W_\beta(\pm a, p) = 0 \), can be confirmed. Here, the classical Gaussian part and the quantal non-Gaussian part compete with each other, which is not the case for a single linear oscillator, Eq. (17a). This non-Gaussian part is actually expressed as two different kinds of contributions; the sums over the periodic orbits \((\nu, \mu)\) are responsible for the purely quantum effect (i.e., temperature-independent) while the sums of \( k \) for the thermal effect (also note, for comparison, that \( \hbar \) and \( \beta \) are always non-separable in form of \( \beta \hbar \omega \) for Eq. (17a)). As is well-known, the sums over periodic orbits with non-zero lengths are responsible for the stepwise nature of the spectral staircase \( N(E) = \sum_n \Theta(E - E_n) \) while the trivial orbits with zero lengths solely contribute to the smooth increase of \( N(E) \) with \( E \). Therefore, it would be interesting to consider two different limits of Eq. (29) separately; first, the purely semiclassical limit by neglecting all periodic orbits with non-zero lengths (i.e., weakening the oscillatory quantum correction), and second, the high-temperature limit \((\beta \to 0)\).
First, in the semiclassical limit, Eq. (29) easily reduces to

\[ W_\beta(x, p) \approx \frac{1}{N_\beta} \left[ \exp \left( -\frac{\beta p^2}{2m} \right) - \cos \left( \frac{2 \xi_x p}{\hbar} \right) \sum_{k=0}^{\infty} \left( -\frac{2 \beta p^2}{m} \right)^k i^{2k} \text{erfc} \left\{ \left( \frac{2m}{\beta \hbar^2} \right)^{1/2} \xi_x \right\} - \left( \frac{m}{2 \beta} \right)^{1/2} \frac{1}{p} \sin \left( \frac{2 \xi_x p}{\hbar} \right) \sum_{k=1}^{\infty} \left( -\frac{2 \beta p^2}{m} \right)^k i^{2k-1} \text{erfc} \left\{ \left( \frac{2m}{\beta \hbar^2} \right)^{1/2} \xi_x \right\} + \left( \frac{2m}{\pi \beta} \right)^{1/2} B \sin \left( \frac{2 \xi_x p}{\hbar} \right) \exp \left\{ -\frac{2m}{\beta \hbar^2} (\xi_x)^2 \right\} \right] \]

(30)

with the corresponding normalizing \( N_\beta \). Eq. (30) actually meets the boundary condition \( W_\beta(\pm a, p) = 0 \) as long as \( \hbar \) is finite, albeit sufficiently small. Then, Figs. 3 and 4 show that even this semiclassical result with the weakened oscillatory quantum correction can possess negative values indeed. On the other hand, in the high-temperature limit, Eq. (29) turns out to be

\[ W_\beta(x, p) \bigg|_{\beta \to 0} = \frac{1}{Z_{\beta,c1}} \left[ \exp \left( -\frac{\beta p^2}{2m} \right) + \text{QF}_\beta(x, p) \right] , \]

(31)

where the quantum fluctuation

\[ \text{QF}_\beta(x, p) = \frac{B}{(\pi \beta / 2m)^{1/2} p} \left\{ 1 + \mathcal{O}(\beta) \right\} \sin \left( \frac{2 \xi_x p}{\hbar} \right) \times \sum_{\mu=1}^{\infty} \left[ \exp \left\{ -\frac{2m}{\beta \hbar^2} (\xi_x + (\mu - 1)L)^2 \right\} + \exp \left\{ -\frac{2m}{\beta \hbar^2} (\mu L - \xi_x)^2 \right\} \right] \]

(32)

with \( \int dx dp \text{QF}_\beta(x, p) = 0 \). Eq. (31) also can be negative valued indeed, as long as \( \beta \) is finite, albeit sufficiently small. This cannot meet the boundary condition. (cf. Fig. 5).

As a result, the non-negative distributions \( \tilde{W}_{\beta,\alpha}(x, p) = (2\pi \hbar)(Z_{\alpha\beta/2})^2 \{W_{\alpha\beta/2}(x, p)\}^2/Z_{\alpha\beta} \) [cf. Eq. (16)] can directly be evaluated, with the help of Eqs. (27) and (29).

IV. EVALUATIONS OF RÉNYI-WIGNER ENTROPIES IN THE PHASE SPACE

Now it is straightforward to compute the entropies \( S_\alpha(\tilde{W}_{\beta,\alpha}) \) in Eqs. (6) and (9) for given distributions \( \tilde{W}_{\beta,\alpha}(x, p) \). We numerically observe good agreement between \( S_\alpha(\tilde{W}_{\beta,\alpha}) = (1 - \alpha)^{-1} \ln[\{2\pi \hbar\}^2(Z_{\beta})^{-\alpha}(Z_{\alpha\beta/2})^2 \int dx dp \{W_{\alpha\beta/2}(x, p)\}^2] \) and \( S_\alpha(\hat{\rho}_\beta) = (1 - \alpha)^{-1} \{\ln Z_{\alpha\beta} \} - \alpha(\ln Z_{\beta}) \} \) (in the high-temperature regime) (cf. Fig. 6). It is also interesting to compare Eq. (4) (or Eq. (6) with \( \alpha = 2 \)) and Eq. (12) by performing their actual evaluations with the ground state \( \tilde{W}_{\alpha,N}(x, p) = (2\pi \hbar) \{W_{0,N}(x, p)\}^2 \) for Nbc as a simple illustration of our formulation, where \( W_{0,N}(x, p) = (2\pi \alpha p)^{-1} \sin(2(a - |x|)p/\hbar); \) for Eq. (4), \( \text{Tr}(\hat{\rho}^2) = \)
(2\pi \hbar) \int_{-a}^{a} dx \int_{-\infty}^{\infty} dp \{ W_{o,N}(x,p) \}^2 = 1 \text{ and thus } S_2(\tilde{W}_{o,N}) = 0, \text{ as is easily shown. On the other hand, Eq. (12) will take the form, after some steps of algebraic manipulations, of}

\[(4\pi a)^{-4} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dx_3 \int_{-\infty}^{\infty} p^{-1} \left[ \left\{ \sin \frac{2}{\hbar} (a - |y_1|) p \right\} + \{ y_1 \to y_4 \} \right] \times \]

\[\left( p_1 \right)^{-1} \left[ \left\{ \sin \frac{2}{\hbar} (a - |y_1|) p_1 \right\} + \{ y_1 \to y_2 \} \right] \left( p_2 \right)^{-1} \left[ \left\{ \sin \frac{2}{\hbar} (a - |y_2|) p_2 \right\} + \{ y_2 \to y_3 \} \right] \times \]

\[\left( p_3 \right)^{-1} \left[ \left\{ \sin \frac{2}{\hbar} (a - |y_3|) p_3 \right\} + \{ y_3 \to y_4 \} \right] \quad (33)\]

as long as \( |a - (\cdots)| \leq a \) in the argument of \( \sin \), where \( y_1 := x + (x_1 + x_2 + x_3)/2; y_2 := x - (x_1 - x_2 - x_3)/2; y_3 := x - (x_1 + x_2 - x_3)/2; y_4 := x - (x_1 + x_2 + x_3)/2 \). Then we will have \( \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dx_3 \to \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2 \int_{-\infty}^{\infty} dy_3 \), which will finally lead to \( \text{Tr}(\hat{\rho}^2) = 1 \). As is explicitly shown here, an evaluation of \( S_2 \) via Eq. (6) considered one of our central results is much simpler than employing Eq. (12) for the same quantity. Therefore, we already notice that it would be a formidable task to find the recurrence relation between entropies \( S_l \) and \( S_{l+1} \), with \( l = 2, 3, 4, \cdots \) for a given distribution \( \tilde{W}_{\rho(a)}(x,p) \) (or \( W_\rho(x,p) \)) [cf. Eqs. (27) and (29)], if needed for the analytic continuation of \( l \to \alpha \).

For comparison, we briefly discuss other “entropies” as well, without considering the Bopp shift. First, some moments of the Wigner function \( W_{n;D}(x,p) \) for Dbc can explicitly be evaluated such that

\[(2\pi \hbar) \int dx dp \{ W_{n,D}(x,p) \}^2 = 1 \quad (34a)\]

\[(2\pi \hbar)^2 \int dx dp \{ W_{n,D}(x,p) \}^3 = \frac{1}{4} + \frac{1}{(n\pi)^2} \left\{ \frac{15}{4} - \frac{20}{3}(-1)^n \right\} \quad (34b)\]

\[(2\pi \hbar)^3 \int dx dp \{ W_{n,D}(x,p) \}^4 = \frac{2}{3} + \frac{25}{2(n\pi)^2} \quad (34c)\]

\[(2\pi \hbar)^4 \int dx dp \{ W_{n,D}(x,p) \}^5 = \frac{23}{192} + \frac{1}{(n\pi)^2} \left\{ \frac{475}{192} - \frac{4462}{135}(-1)^n \right\} + \frac{1}{(n\pi)^4} \left\{ \frac{11275}{256} + \frac{1091816}{10125}(-1)^n \right\} \quad (34d)\]

Because of \( n \)-dependence, Eqs. (34b)-(34d) cannot appropriately reflect the higher moments \( \text{Tr}(\hat{\rho}^3) = \text{Tr}(\hat{\rho}^4) = \text{Tr}(\hat{\rho}^5) = 1 \), as expected. For \( W_{n,N}(x,p) \) of the Nbc case, similar results will come out. Therefore, it is obvious that the Wigner entropy given by \( S_w(\tilde{W}_{n,D}) = -\int dx dp \tilde{W}_{n,D}(x,p) \ln \{(2\pi \hbar) \tilde{W}_{n,D}(x,p)\} \) will be \( n \)-dependent and so cannot at all be used as an appropriate entropy for our study. This confirms that the same story will also apply for the resulting Wigner entropy \( S_w(\tilde{W}_\beta) = -\int dx dp \tilde{W}_\beta(x,p) \ln \{(2\pi \hbar) \tilde{W}_\beta(x,p)\} \) of the
thermal state. Finally, the Wigner entropy of the classical thermal distribution $W_\beta(x, p) \to P_\beta(x, p) = (Z_{\beta,\text{cl}})^{-1} e^{-\beta p^2/2m}$ with $|x| < a$ is given by the closed form

$$S_W(P_\beta) = -\int dx dp P_\beta(x, p) \ln\{(2\pi\hbar) P_\beta(x, p)\} = \ln(Z_{\beta,\text{cl}}) + 1/2 + \ln(2\pi\hbar).$$

(35)

Likewise, by applying Eq. (9) with substitution of $(2\pi\hbar) Z_\beta \to Z_{\beta,\text{cl}}$ and $W_\rho^\alpha(x, p) \to (2\pi\hbar)^{\alpha-1}(Z_{\beta,\text{cl}})^\alpha e^{-\alpha\beta p^2/2m}$, it is straightforward to obtain the entropy $S_1(P_\beta) \to \ln(Z_{\beta,\text{cl}}) + 1/2 - \ln(2\pi\hbar)$. By setting $(2\pi\hbar) \to 1$, we see that $S_W(P_\beta)$ and $S_1(P_\beta)$ become identical.

V. CONCLUSIONS

We have introduced a group of Wigner-like distributions $\{\tilde{W}_\rho^\alpha(x, p)\}$ in the classical phase space, all of which are non-negative and well-defined over the entire phase space, by utilizing the properties of fractional moments $\text{Tr}(\hat{\rho}^\alpha)$ with $\alpha > 0$ of the density operator $\hat{\rho}$. Then we have provided a framework for exact evaluations of Rényi-Wigner entropies for the classical-like distributions $\tilde{W}_\rho^\alpha(x, p)$, in particular for arbitrary non-Gaussian states. This result can be regarded as a generalization of the preceding one developed in Ref. [9], which has enabled to evaluate the entropies but essentially restricted to integer values of $\alpha$ only. Within this formulation, we have also provided a well-defined evaluation scheme of expectation values of observables [cf. Eq. (14)], which differs from the standard form [cf. Eq. (2)].

Subsequently, we have rigorously evaluated the Wigner function $W_\rho(x, p)$, directly leading to $\tilde{W}_\rho^\alpha(x, p)$, of the thermal state of a single particle confined by a one-dimensional infinite potential well with either Dirichlet or Neumann boundary condition. This has been useful in particular for the study of $W_\rho(x, p)$’s behaviors in the quantal-classical transition. We have successfully applied our framework for this non-Gaussian state.

Our study will contribute to a better understanding of non-Gaussian states and their transitions either in the semiclassical limit ($\hbar \to 0$) or in the high-temperature limit ($\beta \to 0$). This phase-space approach will be useful information-theoretically and thermodynamically for deeper discussions of the quantal-classical Second Law on the single footing. We also expect that our approach will straightforwardly apply for other billiard systems (i.e., confined systems with different boundary shapes in two dimensions), which are well-known to have interesting properties in the semiclassical regime.
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Fig. 1: (Color online) Wigner functions $y = W_{n,D}(x,p)$ for Dbc versus (dimensionless) momentum $p \equiv ap/\hbar$ at (dimensionless) position $x \equiv x/a = 0$ with $n = 1, 2, 3, 4, 5$, each of which demonstrates negative values as its non-Gaussian feature [cf. Eqs. (19a)]. The values $n = 3, 4, 1, 2, 5$, in sequence from top to bottom at $p = 5$. cf. For $W_{1,D}(x,p)$ versus $(x,p)$, see Ref. [32].
Fig. 2. (Color online) Wigner functions $y = W_{n;N}(x, p)$ for Nbc versus momentum $p$ at $x = 0$ with $n = 0, 1, 2, 3, 4$, each of which demonstrates negative values as its non-Gaussian feature [cf. Eqs. (19b)]. The values $n = 3, 1, 4, 0, 2$, in sequence from top to bottom at $p = 5$. 
Fig. 3: (Color online) The semiclassical Wigner function $W_\beta(x,p)$ for Dbc versus (dimensionless) position $x \equiv x/a$ and (dimensionless) momentum $p \equiv ap/\hbar$ [cf. Eq. (30)], re-scaled to $20 W_\beta(x,p)$, with the (dimensionless) temperature $\beta \equiv \beta \hbar^2/(ma^2) = 1$. We see that $W_\beta(a,p) = 0$ (also $W(-a,p) = 0$ due to the symmetry of this system). Its negative values emerge from the oscillatory behaviors around $x = 0$ (cf. Fig. 4). Here, we have used 50 orbits by using the sum over $k$ with $0 \leq k \leq 50$, with good numerical convergence. A similar result will come out for Nbc.
Fig. 4: (Color online) The semiclassical Wigner function \( y = W_\beta(0, p) \) for Dbc [cf. Eq. (30)], re-scaled to \( 20W_\beta(0, p) \), which explicitly shows its negative values; e.g., \( W_\beta(0, 3) = -0.0710 \). Otherwise, the same parameters as for Fig. 3.
Fig. 5: (Color online) The Wigner function $W_\beta(x,p)$ for Dbc versus (dimensionless) position $x \equiv x/a$ and (dimensionless) momentum $p \equiv ap/\hbar$ in the high-temperature limit [cf. Eq. (31)], re-scaled to $20 W_\beta(x,p)$, with the (dimensionless) temperature $\beta \equiv \beta h^2/(ma^2) = 0.1$, which is very high. We see that its negative values still emerge from the highly oscillatory behaviors in the vicinity of $x = \pm a$. This comes primarily from the contribution of the zero-length trivial orbit corresponding to the first exponential function with $\mu = 1$ in Eq. (32). We also observe that the boundary condition $W_\beta(\pm a, p) = 0$ does not hold any longer. Here, we have used 50 orbits by using the sum over $\mu$ with $0 \leq \mu \leq 50$, with good numerical convergence. A similar result will come out for Nbc.
Fig. 6: (Color online) Comparison between $y_1 = \int dx dp \{ W_{\alpha/2}(x,p) \}^2$, exactly computable using Eq. (31), (solid curves) and its exact value $y_2 = (2\pi\hbar)^{-1}(Z_{\alpha\beta})/(Z_{\alpha\beta/2})^2$ (dash curves) for given orders $\alpha$ for Dbc in the high-temperature limit, which is equivalent to the comparison between $y_1 = S_{\alpha}(\tilde{W}_{\beta;\alpha})$ and its counterpart $y_2 = S_{\alpha}(\hat{\rho}_{\beta})$ in the same limit (before Eq. (33)); 1) the solid curves with $\beta = 3, 1, 0.5$, in sequence from top to bottom; 2) the dash curves in the same way. For sufficiently small values of $\alpha\beta$, we have good agreement between the two curves for each $\beta$. Here, we have used 15 orbits by using the sum over $\mu$ with $0 \leq \mu \leq 15$ in Eq. (32), already with good numerical convergence. A similar result will come out for Nbc. This analysis will be useful for a study of the high-temperature approximation in the quantum-classical transition.