# Linear entropy in quantum phase space

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(Received 16 June 2011; published 17 October 2011)

We calculate the quantum Renyi entropy in a phase-space representation for either fermions or bosons. This can also be used to calculate purity and fidelity, or the entanglement between two systems. We show that it is possible to calculate the entropy from sampled phase-space distributions in normally ordered representations, although this is not possible for all quantum states. We give an example of the use of this method in an exactly soluble thermal case. The quantum entropy cannot be calculated at all using sampling methods in classical symmetric (Wigner) or antinormally ordered (Husimi) phase spaces, due to inner-product divergences. The preferred method is to use generalized Gaussian phase-space methods, which utilize a distribution over stochastic Green's functions. We illustrate this approach by calculating the reduced entropy and entanglement of bosonic or fermionic modes coupled to a time-evolving, non-Markovian reservoir.

DOI: 10.1103/PhysRevA.84.042114 PACS number(s): 03.65.Ca, 05.30.−d, 05.10.Ln

## I. INTRODUCTION

Quantum dynamics and thermal equilibrium states in large many-body systems have been widely investigated using phase-space representations [1–4]. Applications of these methods [5] include Einstein-Podolsky-Rosen (EPR) correlations in parametric amplifiers, quantum soliton propagation [6], nonequilibrium quantum criticality [7], quantum dynamics of Bose-Einstein condensates in two [8] and three dimensions [9,10], molecular down-conversion [11], and many other problems. Gaussian operator expansions [12–15] are an important extension to these phase-space mappings. Unlike earlier methods, Gaussian phase-space methods can be applied to either fermionic or bosonic quantum many-body systems [16,17]. These methods employ a representation as a distribution over stochastic Green's functions. They have the essential property that they are probabilistic, allowing them to scale to large-sized systems without the exponential complexity of the usual orthogonal basis-set methods. Such methods have proved useful for treating the ground state of the fermionic Hubbard model [18–20], and dynamical cases where quantum Monte Carlo (QMC) techniques are impractical [21,22].

Yet one of the most fundamental properties of quantum systems, entropy [23], has not been treated using this approach. In ultracold atomic physics it is usually the entropy that is directly measurable, rather than the temperature [24]. This is because there is no traditional thermal reservoir, so that to measure thermal effects, it is often necessary to use an entropy-conserving adiabatic passage to a state of known entropy. While some QMC methods can calculate entropy [25], standard phase-space simulations have not yet done this. Similarly, in quantum information, entropic concepts like entanglement of formation [26] and the quantum discord [27] are important measures of quantum behavior. This leads to the question: can phase-space methods be used to calculate entropy, which is not a typical quantum observable?

In this paper we investigate quantum entropy calculations using phase-space representations. Such calculations can be used, for example, to determine thermodynamics and entanglement of a many-body system [28] or to calculate the fidelity of a quantum memory [29]. Alternatively, they can be utilized to assess how close a calculated state is to a known state, or to check that unitary evolution preserves the entropy. This is essential in computationally demanding problems, where it is important to be able to check the validity of a given quantum simulation. More generally, such investigations throw light on one of the fundamental problems of quantum statistical physics. This is the well-known paradox that unitary evolution leaves the quantum entropy unchanged while apparently introducing disorder through collisions and mixing.

For probabilistically sampled distributions, we show that the preferred method for entropy calculations is a Gaussian phase-space representation. In this approach, the operator basis is comprised of Gaussian operators, and the corresponding variance or Green's function is used as a stochastic phase-space variable [12]. For ease of computation we treat the simplest entropy measure, the Renyi or linear entropy [30,31]. An essential ingredient in sampled linear entropy calculations is a knowledge of the inner products of the generating operators of the phase-space representation. We calculate these inner products for phase-space representations of either bosonic [15] or fermionic [13] fields. In the case of fermionic operators, the results come from an elegant application of the Grassmann integration in a Grassmann space.

This method is directly useful for calculating a coarse-grained or localized entropy [32]. Coarse-grained entropy can increase even when the fundamental quantum entropy is invariant, and is a fundamental entanglement measure. Coarse-graining is then carried out simply by restricting or projecting the stochastic Green's function onto a subspace of system modes. As physical applications of these methods, the coarse-grained partial entropy is calculated for systems of either bosonic or fermionic modes that are coupled to a general, non-Markovian reservoir. These cases cannot be treated using master equation methods and have applications to many current nanoscale systems in quantum information. These can be readily solved for the entanglement between the system and reservoir using the phase-space entropy approach.

By comparison, the commonly used Wigner [1] and Husimi $Q$ function [2] expansions are not directly useful in entropy calculations. In the $Q$-function case, the inner products of the generating operators are not defined. In the Wigner distribution

 

case, the entropy obtained from a sampled phase-space distribution is singular. For normally ordered distributions, such as the Glauber-Sudarshan $P$ distribution [3,33], the sampled quantum entropy is well behaved, but the distribution is singular, except for classical-like states. This rules out the use of traditional, classical phase-space mappings for entropy calculations using probabilistic sampling. The positive-$P$ distribution [4,34,35], defined on a double-dimension phase space, has a well-defined positive distribution with nonsingular inner products. Even in this case, entropy calculations are nontrivial since, for some quantum states, the sampling error for entropy calculations diverges.

This paper is organized as follows. In the next section, we describe the definition of quantum entropy and describe the phase-space representations that we will treat in this paper. We also give a general expression of entropy in terms of phase-space representations and discuss the evaluation of the sampled entropy. In Sec. III we discuss coarse graining and reduced entropy and give their expressions in terms of phase-space projections. In Sec. IV we describe sampled entropy calculations using fixed-variance phase-space methods, for instance, the general Cahill-Glauber distribution, as well as the Husimi, Wigner, Glauber-Sudarshan, and positive-$P$ representations. In Secs. V and VI we discuss general Gaussian phase-space representations for bosons and fermions, respectively. The evaluation of inner products of Gaussian operators is presented, which allows us to evaluate the linear entropy and the reduced coarse-grained entropy. We evaluate the linear entropy analytically for thermal states and a comparison with the sampled entropy using the Glauber-Sudarshan representation is made. Finally, as physically relevant examples, we evaluate the coarse-grained entropy for both bosons and fermions in the important case of a system of particles linearly coupled to a non-Markovian reservoir. Section VII gives a summary of our results and conclusions.

## II. ENTROPY AND OPERATOR REPRESENTATIONS

Entropy is a conserved quantity for unitary evolution in quantum mechanics. Intuitively, entropy [23,36] is a measure of loss of information about a physical system. It is invariant for unitary quantum evolution, and only changes when one considers a subsystem coupled to a reservoir. Physically, quantum pure state evolution involves no intrinsic information loss. Of course, this is somewhat counterintuitive. One might expect the mixing effects of nonlinear evolution to reduce information. But this is only true if a restricted or coarse-grained set of measurements is used; in principle, there is no information loss in pure state evolution, and information or entropy should be invariant in any simulation of unitary quantum dynamics. Thus, a pure state will remain a pure state, implying that state purity is a completely general benchmark for the accuracy of a quantum simulation.

### A. Quantum entropy

Quantum entropy is most commonly defined using the von Neumann [23] or Shannon entropy [37]:

$$S = -\mathrm{Tr}(\widehat{\rho}\ln\widehat{\rho}) \ . \tag{2.1}$$

This is an important physical quantity, related to both information content and thermodynamic behavior. However, there are many other conserved entropic quantities. The existence of these can be thought of as related to general information conservation. These were recently discussed [38] in relation to the Wigner function, where it was pointed out that any quantity like $S_F = \mathrm{Tr}[F(\widehat{\rho})]$ is also conserved. In particular, the linear entropy [39], which we normalize following Renyi [30], is defined as

$$S_2 = -\ln \mathrm{Tr}(\widehat{\rho}^2) \ . \tag{2.2}$$

This has similar properties to the entropy, and measures state purity, since $S_2 = 0$ for a pure state, while $S_2 > 0$ for a mixed state. In this article, we focus on the linear entropy, which is simplest to calculate using phase-space methods. This is also true for the fidelity of $\widehat{\rho}$ to a fiduciary state $\widehat{\rho}_0$,

$$F = \mathrm{Tr}(\widehat{\rho}\widehat{\rho}_0) \ , \tag{2.3}$$

which is a closely related concept. Such fidelity measures [40] are useful in evaluating the accuracy of information storage in a quantum network [41], quantum computer [42], or quantum memory [43].

The most general class of entropies normally studied in this way are the general Renyi entropies [30,31], defined for $p > 1$ as

$$S_p = \frac{1}{1-p}\ln \mathrm{Tr}(\widehat{\rho}^p) \ . \tag{2.4}$$

It is known that $S = \lim_{p\to 1} S_p$, so the conventional von Neumann or Shannon entropy can be regained from the general Renyi entropy in the appropriate limit.

### B. Phase-space representations

A general phase-space representation can be written as [4,44]

$$\widehat{\rho} = \int P(\boldsymbol{\lambda})\widehat{\Lambda}(\boldsymbol{\lambda})\, d\boldsymbol{\lambda} \ , \tag{2.5}$$

where $P(\boldsymbol{\lambda})$ is the probability density over the phase space, $\boldsymbol{\lambda}$ is a real or complex vector parameter in a general phase space, $d\boldsymbol{\lambda}$ is the integration measure, and $\widehat{\Lambda}(\boldsymbol{\lambda})$ is the representation kernel or operator basis. For simplicity, we exclude phase spaces that involve Grassmannian degrees of freedom [45,46]. These can be extremely useful in analytic calculations but are not readily sampled computationally, since the vector parameter $\boldsymbol{\lambda}$ is not a real or complex vector.

We consider a bosonic or fermionic quantum field theory with an $M$-dimensional set of mode operators $\hat{\boldsymbol{a}}^\dagger \equiv [\hat{a}_1^\dagger, \hat{a}_2^\dagger, \ldots, \hat{a}_M^\dagger]$. In the bosonic case, we can define $\delta\hat{\boldsymbol{a}} = \hat{\boldsymbol{a}} - \boldsymbol{\alpha}$ and $\delta\hat{\boldsymbol{a}}^\dagger = \hat{\boldsymbol{a}}^\dagger - \boldsymbol{\beta}^\dagger$ as operator displacements, where in general $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}^\dagger$ are independent complex vectors. In the fermionic case we set these displacements to zero. The annihilation and creation operators satisfy (anti)commutation relations, with $(+)$ for fermions and $(-)$ for bosons:

$$[\hat{a}_i, \hat{a}_j^\dagger]_\pm = \delta_{ij}. \tag{2.6}$$

The phase-space representations we will treat in this paper use a general number-conserving Gaussian operator basis [13–15], in which any density matrix $\hat{\rho}$ is expanded in terms

of a basis of Gaussian operators, defined as exponentials of quadratic operator forms $\widehat{\Lambda}(\boldsymbol{\lambda})$, where

$$\widehat{\Lambda}(\boldsymbol{\lambda}) = \frac{1}{\mathcal{N}}\hat{\Lambda}_u(\boldsymbol{\lambda}) = \frac{1}{\mathcal{N}} : \exp[-\delta\hat{\boldsymbol{a}}^\dagger \underline{\boldsymbol{\mu}}\delta\hat{\boldsymbol{a}}] : \tag{2.7}$$

Here, $\underline{\boldsymbol{\mu}}$ is a complex $M \times M$ matrix so that $\boldsymbol{\lambda} = [\boldsymbol{\alpha}, \boldsymbol{\beta}^\dagger, \underline{\boldsymbol{\mu}}]$, $\mathcal{N} = \mathrm{Tr}[\widehat{\Lambda}_u(\boldsymbol{\lambda})]$ is a normalizing factor, and : : indicates normal ordering. The normalizing factor has two forms for bosons and fermions, respectively:

$$\begin{aligned} \mathcal{N}_b &= \det[\underline{\boldsymbol{\mu}}]^{-1}, \\ \mathcal{N}_f &= \det[2\underline{\boldsymbol{I}} - \underline{\boldsymbol{\mu}}]. \end{aligned} \tag{2.8}$$

The interpretation as a stochastic Green's function comes from the identification that $\underline{\boldsymbol{\mu}}$ is closely related to a correlation function of each basis member $\widehat{\Lambda}(\boldsymbol{\lambda})$:

$$\begin{aligned} \underline{\boldsymbol{n}}_b &= \underline{\boldsymbol{\mu}}^{-T} - \underline{\boldsymbol{I}}, \\ \underline{\boldsymbol{n}}_f &= [2\underline{\boldsymbol{I}} - \underline{\boldsymbol{\mu}}]^{-T}. \end{aligned} \tag{2.9}$$

In either case, the stochastic average of $\underline{\boldsymbol{n}}$ over the distribution $P$ is physically a normally ordered many-body Green's function, so that

$$\langle \hat{a}_i^\dagger \hat{a}_j \rangle = \langle n_{ij} + \beta_i^* \alpha_j \rangle_P . \tag{2.10}$$

In traditional, classical types of phase space—for example, the Wigner function approach—the random variable or phase-space coordinate is a stochastic position or momentum. In the case of a general Gaussian phase space, the random variable is a stochastic correlation function.

We see immediately, from Eq. (2.2), that the Renyi entropy in a phase-space representation is

$$S_2 = -\ln \int\int P(\boldsymbol{\lambda})P(\boldsymbol{\lambda}')\mathrm{Tr}[\widehat{\Lambda}(\boldsymbol{\lambda})\widehat{\Lambda}(\boldsymbol{\lambda}')]\, d\boldsymbol{\lambda}\, d\boldsymbol{\lambda}' . \tag{2.11}$$

The evaluation of inner products of Gaussian operators of form $\mathrm{Tr}[\widehat{\Lambda}(\boldsymbol{\lambda})\widehat{\Lambda}(\boldsymbol{\lambda}')]$ is therefore a central task in calculations of linear entropy using phase-space representations.

### C. Sampled entropy

For computational purposes, distributions always exist such that $P(\boldsymbol{\lambda})$ has positive values, and it can be interpreted as a probability in these cases. One can then sample the distribution $N$ times to obtain a sampled estimate $\widehat{\rho}_S$, such that

$$\widehat{\rho} \approx \widehat{\rho}_S = \frac{1}{N}\sum_{j=1}^{N} \widehat{\Lambda}(\boldsymbol{\lambda}_j) . \tag{2.12}$$

This approximation becomes an exact equality in the limit of $N \to \infty$, provided the sampling is unbiased. Given a set of samples $\boldsymbol{\lambda}_i$, we can now calculate the linear entropy as follows:

$$S_2 \approx -\ln\left\{ \frac{1}{N^2}\sum_{i,j=1}^{N} \mathrm{Tr}[\widehat{\Lambda}(\boldsymbol{\lambda}_i)\widehat{\Lambda}(\boldsymbol{\lambda}'_j)] \right\}. \tag{2.13}$$

This, however, requires a double sampling of the population. In phase-space representations the kernel of the representation consists of nonorthogonal operators, so the operator inner product $\mathrm{Tr}[\widehat{\Lambda}(\boldsymbol{\lambda}_i)\widehat{\Lambda}(\boldsymbol{\lambda}_j)]$ is nonvanishing even if $\boldsymbol{\lambda}_i \neq \boldsymbol{\lambda}_j$. It is desirable that the two sets of samples $\boldsymbol{\lambda}_i, \boldsymbol{\lambda}'_j$ are independent of each other, to prevent sampling biases. The above result has obvious extensions to other entropies. For example, the general Renyi entropy involves a $p$-fold summation over sampling indices:

$$S_p \approx \frac{1}{1-p}\ln\left\{ \frac{1}{N^p}\sum_{\mathbf{j}=1}^{N} \mathrm{Tr}[\widehat{\Lambda}(\boldsymbol{\lambda}_{j_1})\cdots\widehat{\Lambda}(\boldsymbol{\lambda}'_{j_p})] \right\}, \tag{2.14}$$

but clearly the linear entropy is computationally the simplest. In the remainder of this paper, we focus on the question of how to evaluate the inner products of the Gaussian phase-space basis set, which is the essential ingredient in calculating a linear entropy or fidelity measure, and how to apply this in physically relevant situations. We note that for some calculations it is useful to allow $P(\boldsymbol{\lambda})$ to have complex values [47], in which cases the entropy is best calculated analytically.

## III. COARSE GRAINING AND REDUCED ENTROPY

There is a fundamental paradox in understanding quantum entropy. For an isolated quantum system, all of the entropies defined above are invariant under unitary evolution, even including particle-particle interactions. This appears to defy conventional wisdom, which is that for a many-body system the effect of particle collisions is to cause mixing, and hence increase disorder. Thus, collisions appear to increase the entropy. Such expectations contradict the entropy invariance of unitary evolution, which is at the heart of such famous controversies as the Bekenstein-Hawking black-hole information loss paradox [48,49].

However, these paradoxes are easily resolved at a practical level. Typically, in many experiments only part of the density matrix is measurable. For example, one may only have experimental access to measurements of the low-momentum modes. Under these conditions, one can separate the Hilbert space into a measured part $\mathcal{H}_A$ and unmeasured part $\mathcal{H}_B$, so that the entire Hilbert space is $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. Other separations of measured and unmeasured operations are also possible, using the method of communication alphabets [50]. An interesting recent proposal of this type is to employ the many-body energy eigenstates as a communication alphabet to define entropy [51].

Here, for definiteness, we focus on a division of the Hilbert space into measured and unmeasured single-particle modes. These could, for example, correspond to a physical partition into distinct spatial locations. The two parts of the quantum wave function then become entangled during time evolution under a Hamiltonian that couples the two parts. This means that part of the quantum information is only accessible through measurement of correlations. An estimate of this relative entropy [52] based on measurements reveals an apparent increase in entropy, or loss of information due to entanglement [26].

If we trace out the unmeasured part of Hilbert space, denoting this trace over $\mathcal{H}_B$ as $\mathrm{Tr}_B$, we obtain the reduced density matrix that corresponds to operational measurement on $A$:

$$\hat{\rho}_A = \mathrm{Tr}_B(\hat{\rho}). \tag{3.1}$$

Such a reduced density matrix can experience increased entropy, called "entanglement entropy," even when the total entropy is conserved. The corresponding reduced entropy is then

$$S_p^{\rm red} = \frac{1}{1-p}\ln {\rm Tr}_A(\widehat{\rho}_A^p)\ . \tag{3.2}$$

This reduced entropy is an important measure of quantum entanglement. In the case of a pure state, $S_p^{\rm red} > 0$ is both necessary and sufficient for entanglement. This can also be extended to the case of mixed states. In this case, one must generalize the approach, to take into account the possibility that the original state was a mixed state [26].

### A. Phase-space projections

In the case of Gaussian phase-space expansions, all our entropy results are also applicable to the reduced entropy, in which case we must replace the phase-space basis $\widehat{\Lambda}(\boldsymbol{\lambda})$ by

$$\widehat{\Lambda}^A(\boldsymbol{\lambda}) = {\rm Tr}_B[\widehat{\Lambda}(\boldsymbol{\lambda})]. \tag{3.3}$$

With such a replacement, the trace used in the following calculations must be replaced by a reduced trace over $\mathcal{H}_A$ for consistency. If coarse graining is carried out on a modal basis, we can divide up the modes into two sets: $\hat{\boldsymbol{a}} \equiv [\hat{a}_1,\hat{a}_2,\ldots,\hat{a}_M] \equiv [\hat{\boldsymbol{a}}^A,\hat{\boldsymbol{a}}^B]$. Here the modes $\hat{\boldsymbol{a}}^A$ may comprise only low-momentum modes or, alternatively, only modes localized to part of an apparatus.

In such cases, $\widehat{\Lambda}^A(\boldsymbol{\lambda})$ depends on a new set of parameters $\boldsymbol{\lambda}^A \equiv (\boldsymbol{\alpha}^A,\boldsymbol{\beta}^{A\dagger},\underline{\boldsymbol{\mu}}^A)$. The reduced displacements are just the projection of the full displacements onto the reduced Hilbert space, while the reduced covariance can be evaluated using standard trace identities. We first write the original matrix $\underline{\boldsymbol{\mu}}$ in a block form as

$$\underline{\boldsymbol{\mu}} = \begin{bmatrix} \underline{\boldsymbol{\mu}}^{AA} & \underline{\boldsymbol{\mu}}^{AB} \\ \underline{\boldsymbol{\mu}}^{BA} & \underline{\boldsymbol{\mu}}^{BB} \end{bmatrix}, \tag{3.4}$$

so that the Gaussian exponent term becomes

$$\delta\hat{\boldsymbol{a}}^\dagger\underline{\boldsymbol{\mu}}\delta\hat{\boldsymbol{a}} = \delta\hat{\boldsymbol{a}}^{A\dagger}\underline{\boldsymbol{\mu}}^{AA}\delta\hat{\boldsymbol{a}}^A + \delta\hat{\boldsymbol{a}}^{A\dagger}\underline{\boldsymbol{\mu}}^{AB}\delta\hat{\boldsymbol{a}}^B + (A\leftrightarrow B). \tag{3.5}$$

Next, the relevant traces over the unobserved subspace $B$ are evaluated using coherent state identities:

$$\begin{aligned} {\rm Tr}_b[\hat{O}] &= \frac{1}{\pi^M}\int d^{2M}\boldsymbol{\alpha}\langle\boldsymbol{\alpha}|\hat{O}|\boldsymbol{\alpha}\rangle, \\ {\rm Tr}_f[\hat{O}] &= \int d^{2M}\boldsymbol{\alpha}\langle-\boldsymbol{\alpha}|\hat{O}|\boldsymbol{\alpha}\rangle. \end{aligned} \tag{3.6}$$

This gives the result that the reduced basis set remains Gaussian, but with a modified covariance:

$$\widehat{\Lambda}^A(\boldsymbol{\lambda}) = \widehat{\Lambda}^A(\boldsymbol{\alpha}^A,\boldsymbol{\beta}^{A\dagger},\underline{\boldsymbol{\mu}}^A), \tag{3.7}$$

where the reduced covariance matrix $\underline{\boldsymbol{\mu}}^A$ is given, for bosons and fermions, respectively, by

$$\begin{aligned} \underline{\boldsymbol{\mu}}_b^A &= \underline{\boldsymbol{\mu}}^{AA} - \underline{\boldsymbol{\mu}}^{AB}\left[\underline{\boldsymbol{\mu}}^{BB}\right]^{-1}\underline{\boldsymbol{\mu}}^{BA}, \\ \underline{\boldsymbol{\mu}}_f^A &= \underline{\boldsymbol{\mu}}^{AA} + \underline{\boldsymbol{\mu}}^{AB}\left[2\underline{\boldsymbol{I}} - \underline{\boldsymbol{\mu}}^{BB}\right]^{-1}\underline{\boldsymbol{\mu}}^{BA}. \end{aligned} \tag{3.8}$$

The important result here is that for a Gaussian basis, coarse graining via mode projection leaves the phase-space representation invariant. Just as for the full Gaussian expansion, there is a reduced Green's function for these Gaussian operators in the subspace. From Eq. (2.9) in the previous section, this must have the standard form of

$$\begin{aligned} \underline{\boldsymbol{n}}_b^A &= [\underline{\boldsymbol{\mu}}^A]^{-T} - \underline{\boldsymbol{I}}^A, \\ \underline{\boldsymbol{n}}_f^A &= [2\underline{\boldsymbol{I}}^A - \underline{\boldsymbol{\mu}}^A]^{-T}. \end{aligned} \tag{3.9}$$

The results for the reduced stochastic Green's function for bosons and fermions can now be written, using standard matrix block reduction algebra, in terms of the block representation of the original stochastic matrix $\underline{\boldsymbol{n}}$, which also has a decomposition:

$$\underline{\boldsymbol{n}} = \begin{bmatrix} \underline{\boldsymbol{n}}^{AA} & \underline{\boldsymbol{n}}^{AB} \\ \underline{\boldsymbol{n}}^{BA} & \underline{\boldsymbol{n}}^{BB} \end{bmatrix}. \tag{3.10}$$

We find that the trace reduction simply gives the diagonal block in the first quadrant.

$$\underline{\boldsymbol{n}}_b^A = \underline{\boldsymbol{n}}_b^{AA}, \quad \underline{\boldsymbol{n}}_f^A = \underline{\boldsymbol{n}}_f^{AA}. \tag{3.11}$$

This has a simple physical explanation. We naturally expect that any correlation function that is restricted just to the $A$ Hilbert space will have no dependence on measurable correlations of the $B$ Hilbert space. This physical property of the full Green's function also holds for the stochastic Green's functions.

The basis is mapped to new values, and the reduced density matrix $\widehat{\rho}^A = {\rm Tr}_B[\hat{\rho}]$ of Eq. (3.2) can be written in the reduced Gaussian representation in terms of the reduced Green's function as

$$\widehat{\rho}^A = {\rm Tr}_B\int P(\underline{\boldsymbol{n}})\Lambda(\underline{\boldsymbol{n}})\,d\underline{\boldsymbol{n}} = \int P(\underline{\boldsymbol{n}})\Lambda^A(\underline{\boldsymbol{n}}^A)\,d\underline{\boldsymbol{n}}. \tag{3.12}$$

Next, we can introduce the corresponding reduced distribution function

$$P^A(\underline{\boldsymbol{n}}^A) \equiv \left[\int P(\underline{\boldsymbol{n}})d\underline{\boldsymbol{n}}^{\backslash A}\right], \tag{3.13}$$

where $\underline{\boldsymbol{n}}^{\backslash A}$ is the relative complement of $\underline{\boldsymbol{n}}^A$, i.e., the set of all variables in $\underline{\boldsymbol{n}}$ that are not included in $\underline{\boldsymbol{n}}^A$.

Using the definition of the reduced density matrix, the linear coarse-grained entropy, Eq. (3.2), for $p = 2$, is

$$\begin{aligned} S_2^{\rm red} = -\ln\int\int P^A(\underline{\boldsymbol{n}}^A)P^A(\underline{\boldsymbol{n}}'^A){\rm Tr}_A \\ \times[\widehat{\Lambda}^A(\underline{\boldsymbol{n}}^A)\widehat{\Lambda}^A(\underline{\boldsymbol{n}}'^A)]\,d\underline{\boldsymbol{n}}^A d\underline{\boldsymbol{n}}'^A. \end{aligned} \tag{3.14}$$

## IV. FIXED-VARIANCE PHASE SPACES

To evaluate the entropy from a set of phase-space samples, we need the inner product of the kernel members. This depends on how the phase space is parametrized, either through changing the displacement or the variance or both. Traditional phase spaces for bosons utilize a displacement-based approach, which is the most similar to classical phase-space ideas. In the case of fermions, the displacements must be Grassmann variables, not $c$ numbers [45], which means that only the *variances* can be readily sampled computationally. In

this section, we treat fixed-variance phase spaces, which are therefore bosonic.

### A. Cahill-Glauber phase space

The traditional mappings of bosonic fields to a classical phase space utilize a single classical displacement. These can all be written in a unified form as [15]

$$\widehat{\Lambda}_s(\boldsymbol{\lambda}) = \frac{1}{\mathcal{N}} : \exp[-(\widehat{\boldsymbol{a}}^\dagger - \boldsymbol{\alpha}^\dagger)\underline{\boldsymbol{\mu}}(\widehat{\boldsymbol{a}} - \boldsymbol{\alpha})] : \tag{4.1}$$

Here $\boldsymbol{\alpha}$,$\boldsymbol{\alpha}^\dagger$ are complex vectors, and $\underline{\boldsymbol{\mu}}$ is held constant so that $\boldsymbol{\lambda} = \boldsymbol{\alpha}$. There are three famous cases, corresponding to different values of $\underline{\boldsymbol{\mu}} = 2\underline{\boldsymbol{I}}/(s+1)$, where $s = 0, \pm 1$. Cahill and Glauber [53] have calculated the inner product for these $s$-ordered representations, which includes the diagonal $P$ representation ($s = 1$) and the Wigner representation ($s = 0$), as special cases. Their results are that, for $s > 0$,

$$\mathrm{Tr}[\widehat{\Lambda}_s(\boldsymbol{\alpha})\widehat{\Lambda}_s(\boldsymbol{\alpha}')] = \frac{1}{s}\exp[-|\boldsymbol{\alpha} - \boldsymbol{\alpha}'|^2/s]. \tag{4.2}$$

We note that the Husimi representation with $s = -1$ has no well-defined inner product for its basis set members, as the product trace is divergent. Thus, a point-sampled $Q$ function is not a useful way to calculate the entropy, without additional assumptions. More sophisticated techniques would be needed in this case. One could, for example, expand the $Q$ function using Gaussian wavelets, instead of $\delta$ functions, so that the sampling expansion uses smoother functions. However, since different types of $s$ ordering are interrelated through Gaussian convolutions, this simply generates another member of the class of Gaussian operator expansions.

### B. Wigner representation

Strictly speaking, the only positive Wigner distributions are the Gaussian ones that represent certain special cases, including thermal, coherent, and squeezed states. Nevertheless, one often wishes to use a truncated Wigner time-evolution equation, which generates positive Wigner distributions as an approximation to the full time evolution. This has a close analogy with a classical phase space, for which entropy can also be calculated in the classical sense.

One can treat the Wigner case as the Cahill-Glauber representation in the limit of $s \to 0$, where

$$\mathrm{Tr}[\widehat{\Lambda}_0(\boldsymbol{\alpha})\widehat{\Lambda}_0(\boldsymbol{\alpha}')] = \pi^M \delta^M(\boldsymbol{\alpha} - \boldsymbol{\alpha}')\,, \tag{4.3}$$

which is highly singular. As in the Husimi case, point sampling does not provide a useful estimate of the purity. Two distinct samples will not have identical points in phase space, except for points of measure zero where the samples are equal. This demonstrates the nontrivial nature of estimating quantum entropy in sampled phase-space representations. One can understand this from the perspective that the coherent states are the only pure states with a positive Wigner function. These have a finite distribution variance, but a zero quantum entropy.

This result is consistent with other calculations. It is known that one can estimate $S_2$ in a Wigner representation through [38]

$$S_2 = -\ln \pi^M \int W^2(\boldsymbol{\alpha}) d^{2M}\boldsymbol{\alpha}\,, \tag{4.4}$$

which is identical with the $\delta$-correlated trace result given above. This can be used when $W$ is known analytically, but it is not computationally useful when we only have access to a sampled estimate of $W(\boldsymbol{\alpha})$.

### C. Glauber-Sudarshan

In the case of the normally ordered Glauber-Sudarshan representation, $s = 1$. This corresponds to an expansion in coherent-state projectors, so that $\widehat{\Lambda}_1(\boldsymbol{\alpha}) \equiv |\boldsymbol{\alpha}\rangle\langle\boldsymbol{\alpha}|$, where $|\boldsymbol{\alpha}\rangle$ is a coherent state, and

$$\mathrm{Tr}[\widehat{\Lambda}_1(\boldsymbol{\alpha})\widehat{\Lambda}_1(\boldsymbol{\alpha}')] = \exp[-|\boldsymbol{\alpha} - \boldsymbol{\alpha}'|^2]. \tag{4.5}$$

Here the linear entropy is well behaved, and both linear coupling and damping can be treated exactly. However, there is no corresponding stochastic process in this case, for nonlinear evolution of an interacting system, and many nonclassical states involve a nonpositive or singular distribution. For a positive distribution, the only pure states in this representation are coherent states. Provided a Glauber-Sudarshan distribution exists, a direct point sampling is enough to obtain the entropy. One can easily obtain the entropy of a noninteracting thermal state, which always has a well-defined Glauber-Sudarshan distribution. For example, the vacuum state has a $\delta$-function distribution, and so clearly one has $\mathrm{Tr}[\widehat{\Lambda}_1(\boldsymbol{\alpha})\widehat{\Lambda}_1(\boldsymbol{\alpha}')] = 1$, and hence $S_2 = S_p = 0$ as expected.

For a thermal case with

$$\hat{\rho}_{\mathrm{th}} \propto \exp[-\widehat{\boldsymbol{a}}^\dagger\widehat{\boldsymbol{a}}/k_B T] =: \exp\left[-\widehat{\boldsymbol{a}}^\dagger[1 + \underline{\boldsymbol{n}}]^{-1}\widehat{\boldsymbol{a}}\right] : \tag{4.6}$$

where $\underline{\boldsymbol{n}}$ is the thermal Bose-Einstein occupation number, clearly

$$n_{kk'} \equiv \frac{\delta_{kk'}}{e^{E_k/k_B T} - 1}, \tag{4.7}$$

where $k_B$ is the Boltzmann constant.

Here one finds that in the Glauber-Sudarshan representation, one has

$$P(\boldsymbol{\alpha}) = \exp[-\boldsymbol{\alpha}^\dagger \underline{\boldsymbol{n}}^{-1}\boldsymbol{\alpha}']. \tag{4.8}$$

Therefore we can use the results of $P(\boldsymbol{\alpha})$ in order to sample the entropy for the thermal states. In Fig. 1 we show the results of the sampled linear entropy as a function of the number of samples $N$ for different values of the thermal Bose-Einstein occupation number $\underline{\boldsymbol{n}}$, compared with exact results obtained in the next section.

The generators in this case are coherent-state projection operators, which means that obtaining a coarse-grained entropy is straightforward. On dividing the modes into two groups, $A$ and $B$, one can simply write the coherent state as an outer product

$$|\boldsymbol{\alpha}\rangle = |\boldsymbol{\alpha}^A\rangle|\boldsymbol{\alpha}^B\rangle,$$

so that

$$\widehat{\Lambda}_1(\boldsymbol{\alpha}) = \widehat{\Lambda}_1(\boldsymbol{\alpha}^A)\widehat{\Lambda}_1(\boldsymbol{\alpha}^B),$$

where $\widehat{\Lambda}_1(\boldsymbol{\alpha}^A) \equiv |\boldsymbol{\alpha}^A\rangle\langle\boldsymbol{\alpha}^A|$ is a coherent-state projector in the reduced Hilbert space.

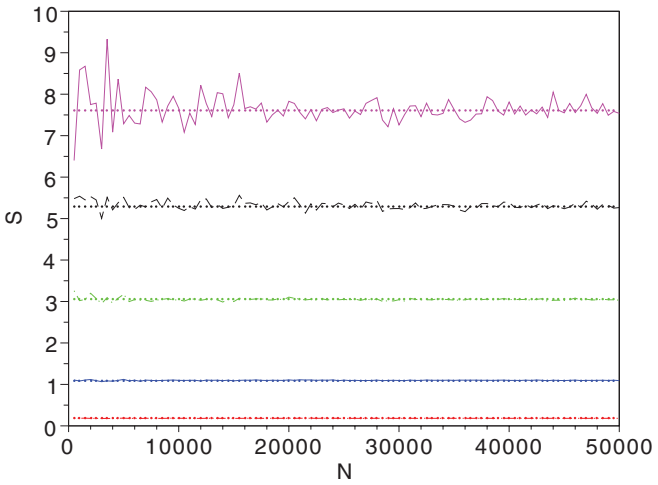


FIG. 1. (Color online) Comparison of the linear entropy for thermal states using the Glauber-Sudarshan representation and the Gaussian representation for bosons. The dotted line is the exact result using the Gaussian representation for bosons for $\underline{n} = 0.1, 1, 10, 100, 1000$, with the smallest occupation numbers having the lowest entropy. Here $N$ is the number of samples used.

### D. Positive-*P* representation

The positive-$P$ representation extends the Glauber-Sudarshan representation into a space of double the classical dimension, with $\boldsymbol{\lambda} = (\boldsymbol{\alpha}, \boldsymbol{\beta})$. This has the advantage that any state or density matrix has a positive probability expansion. Unlike the Husimi $Q$ function, the basis set has a nonsingular inner product, which allows the entropy to be calculated through sampling techniques. The kernel can be written in an alternate form as a Hermitian projection operator [4,44]:

$$\widehat{\Lambda}(\boldsymbol{\lambda}) = \frac{|\boldsymbol{\alpha}\rangle\langle\boldsymbol{\beta}|}{\langle\boldsymbol{\beta}|\boldsymbol{\alpha}\rangle}. \tag{4.9}$$

Just as in the Glauber-Sudarshan case, the issue of coarse graining is a straightforward one of simply dividing the modes into two groups and replacing $\widehat{\Lambda}(\boldsymbol{\lambda})$ by its reduced version, $\widehat{\Lambda}(\boldsymbol{\lambda}^A)$. The inner product is always well defined, being just a Gaussian form in the displacement vectors:

$$\begin{aligned}\mathrm{Tr}[\widehat{\Lambda}(\boldsymbol{\lambda})\widehat{\Lambda}(\boldsymbol{\lambda}')] &= \frac{\langle\boldsymbol{\beta}|\boldsymbol{\alpha}'\rangle\langle\boldsymbol{\beta}'|\boldsymbol{\alpha}\rangle}{\langle\boldsymbol{\beta}|\boldsymbol{\alpha}\rangle\langle\boldsymbol{\beta}'|\boldsymbol{\alpha}'\rangle} \\ &= \exp[-(\boldsymbol{\beta}-\boldsymbol{\beta}')^{\dagger}(\boldsymbol{\alpha}-\boldsymbol{\alpha}')]\,. \end{aligned} \tag{4.10}$$

In all cases, a highly localized distribution is guaranteed to exist from the fundamental existence theorem of the positive-$P$ representation. This states that at least one canonical, positive distribution $P(\boldsymbol{\alpha}, \boldsymbol{\beta})$ always exists for any $\hat{\rho}$, with

$$P(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \frac{1}{(2\pi)^{2M}} e^{-|\boldsymbol{\alpha}-\boldsymbol{\beta}|^2/4} \left\langle \frac{\boldsymbol{\alpha}+\boldsymbol{\beta}}{2} \middle| \widehat{\rho} \middle| \frac{\boldsymbol{\alpha}+\boldsymbol{\beta}}{2} \right\rangle. \tag{4.11}$$

While this distribution always exists, and is suitable for calculating moments, it generally leads to large sampling errors when calculating the entropy. This is because when $|\alpha_i - \beta_i|^2 \gg 1$, in Eq. (4.10), the cross terms can become exponentially large, because these are not sufficiently bounded by the exponentials in the canonical form, Eq. (4.11).

In summary, we see that calculating entropies using a displacement-based phase-space expansion with point sampling is nontrivial. With traditional phase-space expansions, either the basis has singular inner products or the distribution is nonpositive or both. For the Glauber-Sudarshan representation of a thermal state, the distribution is well behaved and the linear entropy can be computed. In the positive-$P$ case, a positive distribution always exists, and the basis has nonsingular inner products. However, even in this case the entropic sampling error can diverge for nonclassical states.

## V. GAUSSIAN REPRESENTATIONS FOR BOSONS

An alternative way to represent quantum states in phase space is to use a general representation in terms of Gaussian operators. These types of phase spaces can in principle combine the displacement- and variance-based approaches. However, for definiteness, in this section we will treat the case where the representation is entirely variance based. Such an approach has a clear intuitive meaning. In this approach, the physical many-body system is treated as a distribution over stochastic Green's functions, whose average is the observed Green's function or correlation function. We note that the basis set includes non-Hermitian terms for completeness, which means that the stochastic Green's functions themselves can be non-Hermitian.

### A. Un-normalized Gaussians

For the bosonic case, we must evaluate the trace of the product of two un-normalized bosonic Gaussian operators, $B(\underline{\mu}, \underline{\nu}) = \mathrm{Tr}[\hat{\Lambda}_u(\underline{\mu})\hat{\Lambda}_u(\underline{\nu})]$ for the M-mode case:

$$B(\underline{\mu}, \underline{\nu}) = \mathrm{Tr}[: e^{-\hat{\boldsymbol{a}}^{\dagger}\underline{\mu}\hat{\boldsymbol{a}}} :: e^{-\hat{\boldsymbol{a}}^{\dagger}\underline{\nu}\hat{\boldsymbol{a}}} :], \tag{5.1}$$

Using the expressions for the trace of an operator, Eq. (3.6) and the expansion of the identity operator in terms of the bosonic coherent states

$$\frac{1}{\pi^M}\int d^{2M}\boldsymbol{\alpha}|\boldsymbol{\alpha}\rangle\langle\boldsymbol{\alpha}| = \hat{I}, \tag{5.2}$$

we obtain

$$\begin{aligned} B(\underline{\mu}, \underline{\nu}) = \frac{1}{\pi^{2M}}\int d^{2M}\boldsymbol{\alpha} d^{2M}\boldsymbol{\beta}\langle\boldsymbol{\alpha}| : e^{-\hat{\boldsymbol{a}}^{\dagger}\underline{\mu}\hat{\boldsymbol{a}}} : \\ \times|\boldsymbol{\beta}\rangle\langle\boldsymbol{\beta}| : e^{-\hat{\boldsymbol{a}}^{\dagger}\underline{\nu}\hat{\boldsymbol{a}}} : |\boldsymbol{\alpha}\rangle. \end{aligned} \tag{5.3}$$

Expanding the normal-ordered exponential, and using the standard eigenvalue properties for the bosonic coherent states $\hat{\boldsymbol{a}}|\boldsymbol{\alpha}\rangle = \boldsymbol{\alpha}|\boldsymbol{\alpha}\rangle$ gives

$$\begin{aligned} B(\underline{\mu}, \underline{\nu}) = \frac{1}{\pi^{2M}}\int d^{2M}\boldsymbol{\alpha} d^{2M}\boldsymbol{\beta}\langle\boldsymbol{\alpha}|e^{-\boldsymbol{\alpha}^{\dagger}\underline{\mu}\boldsymbol{\beta}} \\ \times|\boldsymbol{\beta}\rangle\langle\boldsymbol{\beta}|e^{-\boldsymbol{\beta}^{\dagger}\underline{\nu}\boldsymbol{\alpha}}|\boldsymbol{\alpha}\rangle. \end{aligned} \tag{5.4}$$

From the inner product of two coherent states, we finally obtain a Gaussian integral over $2M$ complex coordinates:

$$B(\underline{\mu}, \underline{\nu}) = \frac{1}{\pi^{2M}}\int d^{2M}\boldsymbol{\alpha}\, d^{2M}\boldsymbol{\beta}\, e^{-\boldsymbol{\alpha}^{\dagger}\underline{\mu}\boldsymbol{\beta}-\boldsymbol{\beta}^{\dagger}\underline{\nu}\boldsymbol{\alpha}-|\boldsymbol{\alpha}-\boldsymbol{\beta}|^2}. \tag{5.5}$$

Next, introducing a double-dimension vector

$$\boldsymbol{\gamma} = \begin{bmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{bmatrix}, \tag{5.6}$$

we can write this as

$$B(\underline{\boldsymbol{\mu}},\underline{\boldsymbol{\nu}}) = \frac{1}{\pi^{2M}}\int d^{4M}\boldsymbol{\gamma}\, e^{-\boldsymbol{\gamma}^{\dagger}\underline{\boldsymbol{\Gamma}}\boldsymbol{\gamma}} = \det[\underline{\boldsymbol{\Gamma}}]^{-1}, \tag{5.7}$$

where we use the standard identity [54] for an $N$-dimensional Gaussian complex integral and introduce a double-dimension matrix

$$\underline{\boldsymbol{\Gamma}} = \begin{bmatrix} \underline{\boldsymbol{I}} & \underline{\boldsymbol{\mu}} - \underline{\boldsymbol{I}} \\ \underline{\boldsymbol{\nu}} - \underline{\boldsymbol{I}} & \underline{\boldsymbol{I}} \end{bmatrix}. \tag{5.8}$$

Therefore, on simplifying the determinant, we obtain

$$B(\underline{\boldsymbol{\mu}},\underline{\boldsymbol{\nu}}) = \det[\mathbf{I} - (\underline{\boldsymbol{\mu}} - \underline{\boldsymbol{I}})(\underline{\boldsymbol{\nu}} - \underline{\boldsymbol{I}})]^{-1}. \tag{5.9}$$

### B. Normalized Gaussians

It is useful to rewrite these expressions in terms of the underlying stochastic Green's functions. These are the normally ordered correlations of the basis sets, defined so that

$$n_{ij} = \mathrm{Tr}[\widehat{\Lambda}(\mathbf{n})\hat{a}_i^{\dagger}\hat{a}_j]. \tag{5.10}$$

Using this definition, the normalized Gaussian generators are

$$\widehat{\Lambda}(\mathbf{n}) = \frac{1}{\det[\underline{\mathbf{I}} + \underline{\mathbf{n}}]} : \exp[-\hat{\boldsymbol{a}}^{\dagger}(\underline{\mathbf{I}} + \underline{\mathbf{n}})^{-1}\hat{\boldsymbol{a}}] : . \tag{5.11}$$

We note that there is a restriction on the values of $\underline{\mathbf{n}}$, which is that $\mathrm{Re}\{\underline{\mathbf{I}} + \underline{\mathbf{n}}\}$ must have positive-definite eigenvalues in order for the basis operators to be normalizable, and hence for the Gaussian generators to be in the Hilbert space.

Applying this normalization to the results given above, one finds that

$$\mathrm{Tr}[\widehat{\Lambda}(\mathbf{n})\widehat{\Lambda}(\mathbf{m})] = \det[\underline{\mathbf{I}} + \underline{\mathbf{n}} + \underline{\mathbf{m}}]^{-1}. \tag{5.12}$$

For Renyi entropy calculations there is another restriction: all pairs of stochastic samples must have the property that $\mathrm{Re}\{\underline{\mathbf{I}} + \underline{\mathbf{n}} + \underline{\mathbf{m}}\}$ has positive-definite eigenvalues to calculate the entropy using sampling methods. Under this restriction, the inner products are well defined.

To illustrate the technique of the Gaussian representation for bosons in the evaluation of the linear entropy and coarse-grained entropy, respectively, in the next two sections we will evaluate the linear entropy of thermal states and the coarse-grained entropy of a system coupled to a non-Markovian reservoir.

### C. Thermal linear entropy for bosons

The linear entropy for thermal states is evaluated as previously, using Eq. (2.13) and the result of Eq. (5.12) for the single-mode case. When the density matrix is thermal, only a single basis-set member is required, and

$$S_2 = -\ln \mathrm{Tr}[\widehat{\Lambda}^2(\mathbf{n}_{\mathrm{th}})] = \ln \det[\underline{\mathbf{I}} + 2\underline{\mathbf{n}}_{\mathrm{th}}]. \tag{5.13}$$

For the single-mode case we know that the thermal Green's function is a scalar: $\underline{\mathbf{n}}_{\mathrm{th}} = n_{\mathrm{th}}$, where $n_{\mathrm{th}}$ is the Bose-Einstein occupation number at a given temperature. In Table I we show the results for the linear entropy using the Gaussian representation for bosons. In Fig. 1 we show the comparison of the results obtained using the Gaussian phase-space representation, the results of Table I, and the results from the sampling using the Glauber-Sudarshan representation as a function of the number of samples, giving excellent agreement in the limit of large numbers of samples.

TABLE I. Linear entropy for thermal states using the Gaussian representation for bosons.

| $n_{\mathrm{th}}$ | $S_2$ |
|---|---|
| 0.01 | 0.0198 |
| 0.1 | 0.1823 |
| 1 | 1.0986 |
| 10 | 3.0445 |
| 100 | 5.3033 |
| 1000 | 7.6014 |

Clearly there is a great improvement in efficiency in this case, relative to the Glauber-Sudarshan approach. Only one Gaussian phase-space sample is needed, instead of up to 50 000 samples using more traditional phase-space methods.

### D. Coarse-grained entropy for bosons

We now consider a practical example of considerable physical applicability. In much of modern physics a bosonic mode is coupled to a reservoir, with which it can exchange particles. The traditional example of this is a single-mode interferometer [55]. In current applications relevant to quantum information, one may have a localized photonic waveguide mode [56], an ultracold Bose condensate [57], or a nanomechanical oscillator [58]. These exchange photons, atoms, or phonons, respectively, with their environments. In nearly all of these recent applications, one is interested in evolution with non-Markovian reservoirs.

To model such physically important examples and evaluate the coarse-grained entropy, we consider the following non-Markovian system. A set of bosonic modes (the *system*) is coupled to a large number of other modes (the *reservoir*). The total Hamiltonian can be written, on introducing $\hat{n}_{ij} = \hat{a}_i^{\dagger}\hat{a}_j$, as

$$\hat{H} = \hbar\sum_{ik}\omega_{ik}\hat{n}_{ik}, \tag{5.14}$$

where $\omega_{ik} = \delta_{ik}\nu_k + g_{ik}$. Here $\nu_k$ denotes the resonant frequencies of the modes, $g_{kj}$ denotes the couplings between the modes. We assume that the modes for $k = 1, \ldots S$ are system modes ($A$), while the remainder are the reservoir ($B$). We note that we make no assumptions concerning their relative sizes or quantum states. We suppose that the initial density matrix at time $t = 0$ has the general number-conserving form

$$\widehat{\rho}^{0} = \int P^{0}(\underline{\boldsymbol{n}})\Lambda(\underline{\boldsymbol{n}})\, d\underline{\boldsymbol{n}}. \tag{5.15}$$

The Gaussian representation provides a form to express the real or imaginary time evolution of the density matrix of either fermions or bosons into a set of phase-space stochastic equations [12,14,15], the mappings are given by [14,15]

$$\begin{aligned} \hat{n}_{ik}\hat{\rho} &\to \left[n_{ik} - \frac{\partial}{\partial n_{\ell m}}(1 \pm n_{im})n_{\ell k}\right]P, \\ \hat{\rho}\hat{n}_{ik} &\to \left[n_{ik} - \frac{\partial}{\partial n_{\ell m}}n_{im}(1 \pm n_{\ell k})\right]P, \end{aligned} \tag{5.16}$$

Here the $+(-)$ sign corresponds to the bosonic (fermionic) case, and we will use the bosonic identities here.

The real time evolution of the density matrix is given, as usual, by

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}]. \tag{5.17}$$

Using Eqs. (5.17) and (5.16) we obtain that the time evolution equation of the stochastic Green's function in matrix form is

$$\dot{\underline{\boldsymbol{n}}} = i[\underline{\boldsymbol{\omega}}, \underline{\boldsymbol{n}}]. \tag{5.18}$$

The solution of Eq. (5.18) is simply

$$\underline{\boldsymbol{n}}(t) = e^{i\underline{\boldsymbol{\omega}}t}\,\underline{\boldsymbol{n}}(0)\,e^{-i\underline{\boldsymbol{\omega}}t}. \tag{5.19}$$

The reduced linear entropy for this system is evaluated using Eq. (3.14) and the result for the time evolution of the stochastic Green's functions, Eq. (5.19). In this case we will trace over the system $A$. Therefore, the expression for the reduced entropy is

$$S_2^{\rm red} = -\ln \iint P^0(\underline{\boldsymbol{n}})P^0(\underline{\boldsymbol{n}}')\det[1 + \underline{\boldsymbol{n}}^A(t) + \underline{\boldsymbol{n}}'^A(t)]^{-1} d\underline{\boldsymbol{n}}\, d\underline{\boldsymbol{n}}'. \tag{5.20}$$

### E. Example of bosonic entropy

To illustrate the time evolution of the coarse-grained entropy of Eq. (5.20), we will consider the following model for the Hamiltonian of Eq. (5.14). The bosonic system will be a single mode ($j = 1$) and the reservoir will be modeled as a Lorentzian distribution of couplings, with

$$g_j = \frac{C}{\nu_j^2 + s^2}, \tag{5.21}$$

where $C$ is the strength of the coupling, $\nu_j = \pm j d\omega$ are the resonant frequencies of the modes, and $s$ describes the non-Markovian reservoir width. For this model, the time evolution of the stochastic Green's function of Eq. (5.19) is written assuming that $\underline{\boldsymbol{n}}(0)$ describes the thermal state at $t = 0$, with a system occupation of $n = 1$, and all the other modes unoccupied. Here $\underline{\boldsymbol{\omega}}$ is an $M \times M$ matrix, and $M$ is the total number of modes, so that

$$\underline{\boldsymbol{\omega}} = \begin{pmatrix} \nu_{11} & g_{21} & \cdots & \cdots & \cdots & g_{1M} \\ g_{12} & \ddots & 0 & \cdots & 0 & \vdots \\ \vdots & 0 & \ddots & 0 & \vdots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 & \vdots \\ \vdots & 0 & \cdots & 0 & \ddots & \\ g_{M1} & \cdots & \cdots & \cdots & & \nu_{MM} \end{pmatrix}. \tag{5.22}$$

In Fig. 2, we show the time evolution of the coarse-grained entropy. We use the following parameters: $M = 100$, $s = 0.5$, $C = 0.05$. The frequency spacing of the modes is $d\omega = 0.04$. We observe the non-Markovian behavior of the reservoir, as shown in the increase and decrease of the entropy with time.

In summary, to solve for the coarse-grained entropy one must take the partial determinant of a block reduced form $\underline{\boldsymbol{n}}^A$ of the time-evolved stochastic Green's function, then average over the initial ensemble. Apart from the limitation to linear couplings needed to obtain an exactly soluble form, there are no restrictions to the state, the type of coupling, or the subdivision between the system and the reservoir in this calculation.

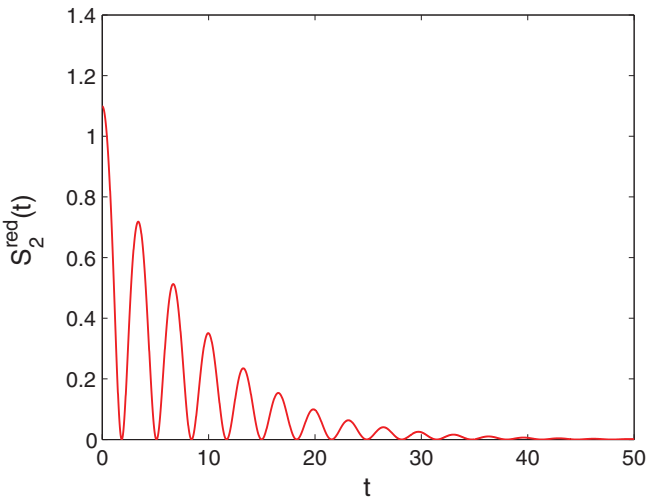


FIG. 2. (Color online) Time evolution of the coarse-grained entropy for a bosonic thermal state coupled to a non-Markovian reservoir.

## VI. GAUSSIAN REPRESENTATIONS FOR FERMIONS

The fermionic case is similar, except that one must use fermionic coherent states [45] and Grassmann integrals to carry out the trace calculations. Just as with bosons, this has a clear intuitive meaning. In this approach, the physical many-body system is treated as a distribution over fermionic Green's functions, whose average is the observed Green's function or correlation function. As with the bosonic case, the stochastic Green's functions themselves can be non-Hermitian.

### A. Un-normalized Gaussians

Here we must evaluate the trace of the product of two un-normalized fermionic Gaussian operators, $F(\underline{\boldsymbol{\mu}}, \underline{\boldsymbol{\nu}}) = \mathrm{Tr}[\hat{\Lambda}_u(\underline{\boldsymbol{\mu}})\hat{\Lambda}_u(\underline{\boldsymbol{\nu}})]$ for the M-mode case:

$$F(\underline{\boldsymbol{\mu}}, \underline{\boldsymbol{\nu}}) = \mathrm{Tr}[: e^{-\hat{\boldsymbol{a}}^\dagger \underline{\boldsymbol{\mu}}\hat{\boldsymbol{a}}} :: e^{-\hat{\boldsymbol{a}}^\dagger \underline{\boldsymbol{\nu}}\hat{\boldsymbol{a}}} :], \tag{6.1}$$

For fermions [45], the trace of an operator using fermionic coherent states $|\boldsymbol{\alpha}\rangle$ in terms of Grassmann variables $\boldsymbol{\alpha}$ is

$$\mathrm{Tr}[\hat{O}] = \int d^{2M}\boldsymbol{\alpha}\langle -\boldsymbol{\alpha}|\hat{O}|\boldsymbol{\alpha}\rangle, \tag{6.2}$$

and the identity operator is

$$\int d^{2M}\boldsymbol{\alpha}|\boldsymbol{\alpha}\rangle\langle\boldsymbol{\alpha}| = 1. \tag{6.3}$$

Therefore, we have

$$F(\underline{\boldsymbol{\mu}}, \underline{\boldsymbol{\nu}}) = \frac{1}{\pi^{2M}} \int d^{2M}\boldsymbol{\alpha}\, d^{2M}\boldsymbol{\beta}\langle -\boldsymbol{\alpha}| : e^{-\hat{\boldsymbol{a}}^\dagger \underline{\boldsymbol{\mu}}\hat{\boldsymbol{a}}} : \times |\boldsymbol{\beta}\rangle\langle\boldsymbol{\beta}| : e^{-\hat{\boldsymbol{a}}^\dagger \underline{\boldsymbol{\nu}}\hat{\boldsymbol{a}}} : |\boldsymbol{\alpha}\rangle. \tag{6.4}$$

Expanding the normal-ordered exponential and using the standard eigenvalue properties for the fermionic coherent states $\hat{\boldsymbol{a}}|\boldsymbol{\alpha}\rangle = \boldsymbol{\alpha}|\boldsymbol{\alpha}\rangle$ gives

$$F(\underline{\boldsymbol{\mu}},\underline{\boldsymbol{\nu}}) = \int d^{2M}\boldsymbol{\alpha} d^{2M}\boldsymbol{\beta}\langle -\boldsymbol{\alpha}|e^{\boldsymbol{\alpha}^\dagger \underline{\boldsymbol{\mu}}\boldsymbol{\beta}}|\boldsymbol{\beta}\rangle\langle\boldsymbol{\beta}|e^{-\boldsymbol{\beta}^\dagger \underline{\boldsymbol{\nu}}\boldsymbol{\alpha}}|\boldsymbol{\alpha}\rangle. \quad (6.5)$$

From the inner product of two fermion coherent states, we note that

$$\langle\boldsymbol{\alpha}|\boldsymbol{\beta}\rangle = e^{\boldsymbol{\alpha}^\dagger\boldsymbol{\beta}-(\boldsymbol{\alpha}^\dagger\boldsymbol{\alpha}+\boldsymbol{\beta}^\dagger\boldsymbol{\beta})/2}, \quad (6.6)$$

Next, introducing a double-dimension Grassmann vector

$$\boldsymbol{\gamma} = \begin{bmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{bmatrix}, \quad (6.7)$$

we finally obtain a Gaussian Grassmann integral over $2M$ complex coordinates, which we can write as

$$\begin{aligned} F(\underline{\boldsymbol{\mu}},\underline{\boldsymbol{\nu}}) &= \int d^{4M}\boldsymbol{\gamma}\, e^{\boldsymbol{\alpha}^\dagger\underline{\boldsymbol{\mu}}\boldsymbol{\beta}-\boldsymbol{\beta}^\dagger\underline{\boldsymbol{\nu}}\boldsymbol{\alpha}-\boldsymbol{\alpha}^\dagger\boldsymbol{\beta}+\boldsymbol{\beta}^\dagger\boldsymbol{\alpha}^\dagger-(\boldsymbol{\alpha}^\dagger\boldsymbol{\alpha}+\boldsymbol{\beta}^\dagger\boldsymbol{\beta})} \\ &= \int d^{4M}\boldsymbol{\gamma}\, e^{-\boldsymbol{\gamma}^\dagger\underline{\boldsymbol{\Gamma}}\boldsymbol{\gamma}} = \det[\underline{\boldsymbol{\Gamma}}]. \end{aligned} \quad (6.8)$$

Here we have used the standard identity [54] for an $N$-dimensional Gaussian complex Grassmann integral and introduced a double-dimension matrix

$$\underline{\boldsymbol{\Gamma}} = \begin{bmatrix} \underline{\boldsymbol{I}} & \underline{\boldsymbol{I}}-\underline{\boldsymbol{\mu}} \\ \underline{\boldsymbol{\nu}}-\underline{\boldsymbol{I}} & \underline{\boldsymbol{I}} \end{bmatrix}. \quad (6.9)$$

Therefore, on simplifying the determinant, we obtain

$$F(\underline{\boldsymbol{\mu}},\underline{\boldsymbol{\nu}}) = \det[\mathbf{I} + (\underline{\boldsymbol{I}}-\underline{\boldsymbol{\mu}})(\underline{\boldsymbol{I}}-\underline{\boldsymbol{\nu}})]. \quad (6.10)$$

### B. Normalized Gaussians

Just as in the bosonic case, it is useful to rewrite these expressions in terms of the normally ordered Green's functions or correlations of the basis sets, defined so that

$$n_{ij} = \mathrm{Tr}[\widehat{\Lambda}(\mathbf{n})\hat{a}_i^\dagger\hat{a}_j]. \quad (6.11)$$

Here, introducing the hole Green's function, $\underline{\tilde{\mathbf{n}}} = [\underline{\mathbf{I}} - \underline{\mathbf{n}}]$, and $\underline{\tilde{\mathbf{m}}} = [\underline{\mathbf{I}} - \underline{\mathbf{m}}]$, the normalized generators are

$$\widehat{\Lambda}(\mathbf{n}) = \Omega\det[\underline{\tilde{\mathbf{n}}}] : \exp[\hat{\boldsymbol{a}}^\dagger(\underline{\tilde{\mathbf{n}}}^{-1} - 2\underline{\mathbf{I}})^T\hat{\boldsymbol{a}}] : , \quad (6.12)$$

and therefore,

$$\underline{\boldsymbol{\nu}}^T = 2\underline{\mathbf{I}} - \underline{\tilde{\mathbf{n}}}^{-1}, \quad (6.13)$$

$$\underline{\boldsymbol{\mu}}^T = 2\underline{\mathbf{I}} - \underline{\tilde{\mathbf{m}}}^{-1}. \quad (6.14)$$

Hence,

$$\underline{\tilde{\mathbf{n}}}(\underline{\boldsymbol{I}} - \underline{\boldsymbol{\nu}})^T = \underline{\mathbf{n}}, \quad (6.15)$$

which leads to the following result for the normalized inner product:

$$\mathrm{Tr}[\widehat{\Lambda}(\mathbf{m})\widehat{\Lambda}(\mathbf{n})] = \det[\underline{\tilde{\mathbf{n}}}\underline{\tilde{\mathbf{m}}} + \underline{\mathbf{n}}\underline{\mathbf{m}}]. \quad (6.16)$$

We note that this has some obvious properties. Suppose that $\underline{\mathbf{n}}$ and $\underline{\mathbf{m}}$ are each diagonal in the same basis, with real eigenvalues $n_i$ such that $0 \leqslant n_i \leqslant 1$. Then one obtains

$$\mathrm{Tr}[\widehat{\Lambda}(\mathbf{m})\widehat{\Lambda}(\mathbf{n})] = \prod_{i=1}^{M}(\tilde{n}_i\tilde{m}_i + n_i m_i). \quad (6.17)$$

Thus, the two generators are orthogonal if, in any mode, one generator has a vanishing particle population while the other has a vanishing hole population. The overlap is maximized if the generators both have a unit hole population or a unit particle population in all modes.

For the thermal case, the entropy can be evaluated in other ways, but here we demonstrate the technique using the Gaussian operator method, which will be useful in evaluating the entropy of other systems.

### C. Thermal linear entropy for fermions

We can now apply these inner products to the evaluation of the linear entropy of a thermal Fermi-Dirac state. When the density matrix is thermal, only a single basis-set member is required, and

$$S_2 = -\ln\mathrm{Tr}[\widehat{\Lambda}^2(\mathbf{n}_{\mathrm{th}})] = -\ln\det\left[\underline{\mathbf{I}} - 2\underline{\mathbf{n}}_{\mathrm{th}} + 2\underline{\mathbf{n}}_{\mathrm{th}}^2\right]. \quad (6.18)$$

Just as with bosons, for the thermal case we know that the thermal Green's function is a scalar: $\underline{\mathbf{n}}_{\mathrm{th}} = n_{\mathrm{th}}$, where $n_{\mathrm{th}}$ is now the Fermi-Dirac occupation number at a given temperature, so that $0 \leqslant n_{\mathrm{th}} \leqslant 1$. Here the results are asymptotically equal to the bosonic case as expected for $n_{\mathrm{th}} \ll 1$ or for $\tilde{n}_{\mathrm{th}} \ll 1$ . Typical results are shown in Table II, showing the particle-hole symmetry. The greatest entropy is at $n_{\mathrm{th}} = 0.5$, corresponding to infinite temperature, while mirror states with small hole occupations can be thought of as having negative temperatures or negative Hamiltonians.

### D. Coarse-grained entropy for fermions

Just as in the case of bosons, we now consider an example of physical applicability for the case of fermions that is a fermionic mode coupled to a reservoir. An example of such a system is a quantum dot coupled to a fermionic reservoir [59], or a fermionic atomtronic circuit [60]. This system can be considered as an example of solid-state quantum physics and has potential applications in quantum-information processing. In such hybrid quantum systems, long-range interactions can be important. Here we neglect this in order to obtain analytic results, although these can be added if necessary.

We consider a Hamiltonian identical to that of the bosonic case in the last section. Similar to the bosonic case, we assume that the modes for $k = 1,\ldots,S$ are system modes ($A$), while the remainder are for the reservoir ($B$) and the initial density matrix at time $t = 0$ has the general number-conserving form of Eq. (5.15). Using the identities of Eqs. (5.16) and (5.17) we obtain the time-evolution equation of the stochastic Green's

TABLE II. Linear entropy for thermal states using the Gaussian representation for fermions.

| $n_{\mathrm{th}}$ | $S_2$ |
|---|---|
| 0.01 | 0.02 |
| 0.1 | 0.1984 |
| 0.5 | 0.6931 |
| 0.9 | 0.1984 |
| 0.99 | 0.02 |

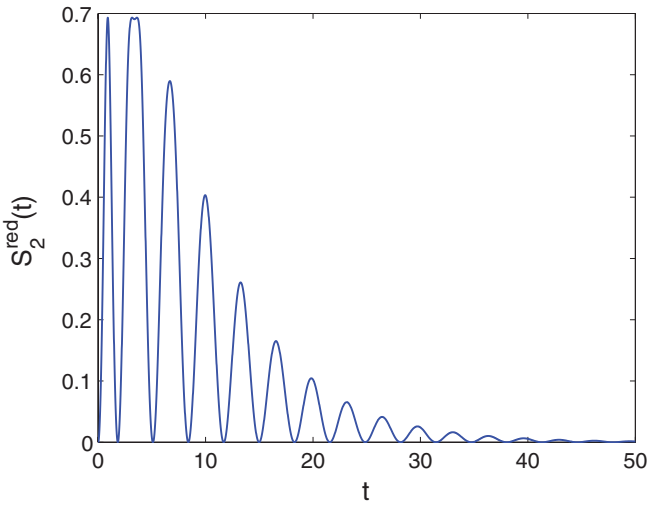


FIG. 3. (Color online) Time evolution of the coarse-grained entropy using the fermionic Gaussian representation, for a pure fermionic number state coupled to a non-Markovian reservoir.

function, which is identical to the bosonic case. Therefore, the expression for the reduced linear entropy for fermions is

$$S_2^{\rm red} = -\ln \int\int P^0(\underline{\boldsymbol{n}})P^0(\underline{\boldsymbol{n}}')\det[\tilde{\underline{\boldsymbol{n}}}^A(t)\tilde{\underline{\boldsymbol{n}}}'^A(t) + \underline{\boldsymbol{n}}^A(t)\underline{\boldsymbol{n}}'^A(t)]\,d\underline{\boldsymbol{n}}\,d\underline{\boldsymbol{n}}'. \quad (6.19)$$

This has a very simple physical interpretation. The linear entropy and hence the fermionic entanglement can be calculated completely from the local stochastic Green's functions in the system of interest. However, one must average over all possible initial states defined by the complete initial phase-space distribution $P^0(\underline{\boldsymbol{n}})$. This is necessary, since the correlations and initial states of the reservoir can change the final system properties.

### E. Example of fermionic entanglement

Similar to the bosonic case, we will illustrate the time evolution of the coarse grained entropy of Eq. (6.19). We will consider a pure fermionic number state. The $\underline{\boldsymbol{\omega}}$ matrix of time evolution of the stochastic Green's function has the same form as the bosonic case, Eq. (5.22). We also model the reservoir with a Lorentzian distribution described by Eq. (5.21).

In Fig. 3, we show the time evolution of the coarse-grained entropy, Eq. (6.19), using a model and parameters identical to those for the bosonic case. However, there is a large physical difference, because a fermionic state with $n = 1$ is a pure number state. We observe an initial increase of entropy, which means that the entropy is measuring the entanglement of the system with the reservoir. As before, the non-Markovian behavior of the system is shown in the increase and decrease of the coarse-grained entropy, which in this case corresponds to entanglement oscillations.

## VII. SUMMARY

We have calculated the linear entropy for sampled phase-space representations of bosonic and fermionic quantum many-body systems. The crucial element to the calculation is an evaluation of the inner products of the phase-space basis elements. Traditional displacement-based phase-space methods have a range of pathologies. In the Wigner and Husimi cases, the inner products are singular or divergent, while in the Glauber-Sudarshan case, the representation is not well defined in all cases. Even the positive-$P$ distribution, which exists and has well-defined inner products, is found to have a sampling convergence problem. By comparison, Gaussian phase-space representations for fermions and bosons are much more suitable for the task. For thermal states, only a single basis element is needed, and the inner products are well behaved.

There is a counterintuitive element to the idea that entropy is conserved in quantum dynamics; but this must be the case when simulating time-reversible, unitary quantum dynamics. We show how, in the case of reduced entropy of a subsystem, the linear entropy can and does evolve in time. We give an exact calculation of couplings of Fermi and Bose systems to a non-Markovian quantum reservoir. Such phase-space methods appear useful for investigating the fundamental paradox of entropy invariance in unitary quantum dynamics. They are equally applicable to entire system evolution and to the evolution of the density matrix for a coarse-grained subspace.

## ACKNOWLEDGMENTS

L.E.C.R.Z. acknowledges financial support from CONACYT-Mexico. P.D.D. acknowledges financial support from the Australian Research Council and Swinburne University of Technology, as well as the generous hospitality of the Aspen Center for Physics.

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