# Nonequilibrium Dynamics of Renyi Entropy for Bosonic Many-Particle Systems

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We propose a new field theoretic method for calculating Renyi entropy of a subsystem of many interacting bosons without using replica methods. This method is applicable to dynamics of both open and closed quantum systems starting from arbitrary initial conditions. Our method identifies the Wigner characteristic of a reduced density matrix with the partition function of the whole system with a set of linear sources turned on only in the subsystem, and uses this to calculate the subsystem's Renyi entropy. We use this method to study the evolution of Renyi entropy in a noninteracting open quantum system starting from an initial Fock state. We find a relation between the initial state and final density matrix which determines whether the entropy shows nonmonotonic behavior in time. For non-Markovian dynamics, we show that the entropy approaches its steady-state value as a power law with exponents governed by nonanalyticities of the bath. We illustrate that this field-theoretic method can be used to study large bosonic open quantum systems.

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A quantum state of a many-body system encodes phase relations between spatially separated degrees of freedom. When this distributed information is erased by tracing out a set of degrees of freedom, the remaining subsystem is described by a reduced density matrix, which mixes quantum probability amplitudes with classical probabilities [1]. The Renyi entanglement entropy of the subsystem is the entropy of the resultant classical probability distribution. It indicates nonseparability of the quantum state between the traced out and remaining degrees of freedom 2]]. Renyi entropy of subsystems has been used to study quantum phase transitions [3–5] and many-body localization transition [6–10] in interacting disordered systems. It has been measured experimentally in ultracold atomic systems [11].

The simplest method for calculating entanglement entropy numerically diagonalizes the many-body Hamiltonian [12,13]. While this works for fermions and spin systems of reasonable sizes [14], the large local Hilbert space of bosons makes this method useless, unless one imposes hard-core constraints to whittle down the Hilbert space [15]. The problem becomes harder when one considers open quantum systems where the number of particles is not conserved, and hence one cannot consider a truncated Hilbert space. Field-theoretic methods, on the other hand, either use conformal invariance [16–18] or require correlation functions evaluated in replicated space-time sheets with branch cuts along the subsystem [19]. In this Letter, we present a new method for calculating Renyi entropy of bosonic many-body systems, which can work without complicated manifolds and in the absence of conformal invariance. Our method is applicable to systems both in and out of thermal equilibrium. It can describe the evolution of Renyi entropy in non-Markovian open quantum systems (OQS) starting from arbitrary initial conditions.

The Renyi entropy of a density matrix can be written as an integral of the square of its Wigner quasiprobability distribution (WQD) [20], which is the closest approximation to a "phase-space distribution function" for quantum systems [20–22]. The Wigner function has been measured in different single mode quantum systems [23–28]. In this letter, we show that the Wigner characteristic function (WCF) of a reduced density matrix is equal to the partition function of the full system in the presence of a particular set of sources turned on only in the subsystem. For systems out of thermal equilibrium, we use Schwinger Keldysh (SK) field theory to calculate this partition function, with recently proposed modifications to take care of arbitrary initial conditions [29]. The Wigner characteristics can then be used to calculate the Renyi entropy. We note that our formalism is quite different from earlier attempts to calculate WQDs [30–34] within path integral approaches.

We use this formalism to study the evolution of Renyi entropy of bosonic systems coupled to external baths, which are initialized to a Fock state with 0 initial entropy. For a single mode system coupled to Markovian as well as non-Markovian baths [35], the entanglement entropy shows nonmonotonic evolution in time in some cases. We find an explicit relation between the initial particle number and final density which determines whether the entropy evolution is nonmonotonic. To illustrate the power of this new method, we then study the evolution of Renyi entropy in a linear chain of 12 sites coupled to external non-Markovian baths. We recover the nonmonotonic time dependence of the Renyi entropy of the subsystems. We have also used this method to calculate Renyi entropies of large interacting thermal systems of bosons in one and two dimensions, which is presented in a separate paper [36]. Thus, our method can be used to calculate Renyi entropy of bosonic many-body systems in versatile circumstances not accessible by existing methods [37–44].

*Wigner function, Renyi entropy, and Keldysh partition function.*—For a many-body bosonic system, the WCF $\chi_W$ is given by [20].

$$\chi_W(\{\beta_j\},t) = \mathrm{Tr}[\hat{\rho}(t)e^{\sum_j \beta_j a_j^\dagger - \beta_j^* a_j}] \tag{1}$$

where $a_j^\dagger$ is the creation operator for the $j$th site, and $\hat{\rho}(t)$ is the density matrix of the system. The reduced density matrix of the subsystem $A$ (of size $\Omega_A$), $\hat{\rho}_A(t) = Tr_B\hat{\rho}(t)$ is obtained by tracing over the sites in the rest of the system ($B$). The WCF $\chi_W^A$ of $\hat{\rho}_A(t)$ can be obtained from Eq. (1) by restricting the $\beta_j$s to the sites in $A$. The second Renyi entropy $S^{(2)} = -\log Tr[\hat{\rho}_A^2(t)]$ is [20]

$$S^{(2)}(t) = -\log\left[\int \prod_{i\in A} \frac{d^2\beta_i}{\pi^{\Omega_A}} |\chi_W^A(\{\beta_i\},t)|^2\right]. \tag{2}$$

The time evolution of the density matrix, $\hat{\rho}(t) = U(t,0)\hat{\rho}(0)U^\dagger(t,0)$, can be described by a SK path integral with two copies of fields, $\phi_+(j,t)$ and $\phi_-(j,t)$, corresponding to the forward and backward evolution in time, shown in Fig. 1. We decompose the displacement operator $D(\{\beta_j\}) = e^{\sum_j \beta_j a_j^\dagger - \beta_j^* a_j}$ in Eq. (1), into $D \to D^{1/2} \times D^{1/2}$, with each of the $D^{1/2}$ placed on the $+$ and $-$ contour; i.e.,

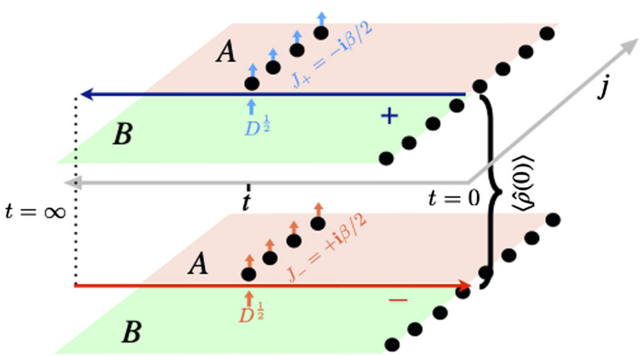


FIG. 1. Two contour ($\pm$) evolutions of the density matrix $\hat{\rho}(t)$ in SK field theory. For calculating $\chi_W(\beta_j,t)$, the displacement operator, $D(\{\beta_j\})$ is decomposed into $D \to D^{1/2}D^{1/2}$ with each $D^{1/2}$ inserted on the $+$ and $-$ contour at time $t$. For the WCF $\chi_W^A(\beta_j,t)$ of the reduced density matrix in subsystem $A$, this insertion is equivalent to turning on sources $J_+(j) = -\mathbf{i}\beta_j/2$ (shown by blue upward arrows) and $J_-(j) = +\mathbf{i}\beta_j/2$ (shown by orange upward arrows) only at the time of measurement $t$, and only on the lattice sites $j \in A$. The resultant partition function gives the WCF $\chi_W^A(\beta_j,t)$ from which $S^{(2)}(t)$ can be calculated using Eq. (2).

$$\chi_W = Tr[U(\infty,t)D^{1/2}U(t,0)\hat{\rho}(0)U^\dagger(t,0)D^{1/2}U^\dagger(\infty,t)]. \tag{3}$$

The insertion of $D^{1/2} = e^{\frac{1}{2}\sum_j \beta_j a_j^\dagger - \beta_j^* a_j}$ corresponds to turning on sources $J_+(j,t') = -\mathbf{i}(\beta_j/2)\delta(t-t')$ and $J_-(j,t') = \mathbf{i}(\beta_j/2)\delta(t-t')$ coupled linearly to the fields, and evaluating the SK partition function in the presence of these sources (see Appendix A [45]). Working with the classical and quantum fields, $\phi_{\mathrm{cl}} = (\phi_+ + \phi_-)/\sqrt{2}$ and $\phi_q = (\phi_+ - \phi_-)/\sqrt{2}$, the WCF is the Keldysh partition function $Z$ with the classical source turned off throughout the evolution, and a quantum source $J_q(j,t') = [J_+(j,t') - J_-(j,t')]/\sqrt{2} = -\mathbf{i}\beta_j/\sqrt{2}\delta(t-t')$, turned on only at the time of measurement, i.e.,

$$\chi_W(\{\beta_j\},t) = Z\left[J_{\mathrm{cl}} = 0, J_q(j,t') = -\mathbf{i}\frac{1}{\sqrt{2}}\beta_j\delta(t-t')\right]. \tag{4}$$

This is the main result of this Letter, which is valid for generic nonequilibrium dynamics of interacting bosons.

In this formalism, integrating out modes without turning on a source traces over those degrees of freedom, while integrating out a mode after turning on a quantum source calculates the WCF. Hence $\chi_W^A$ can be obtained by restricting the quantum sources $\beta_j$ only to the modes in subsystem $A$ (see Fig. 1). This simplification allows us to study Renyi entropy for the arbitrary geometry of subsystems.

*Renyi entropy in nonequilibrium dynamics.*—We consider a lattice system of bosons initialized in a Fock state and coupled to an external bath. It evolves to a long time steady state under a nonunitary dynamics.

This dynamics can be treated within a recent extension of SK field theory [29]. For an initial $\hat{\rho}(0) = |\{n_i\}\rangle\langle\{n_i\}|$, where $|\{n_i\}\rangle = |n_1, n_2 \ldots\rangle$, with $n_\nu$ the occupation number of the $\nu$th mode, the extended SK formalism adds to the Keldysh action a source $-\mathbf{i}(1+u_\nu)/(1-u_\nu)$ coupled to the bilinear $\phi_q^*(\nu,0)\phi_q(\nu,0)$, i.e., it is turned on only at the initial time $t=0$. The WCF $\chi_W(\beta_j,t,\vec{u})$ can then be calculated as the partition function in the presence of both the linear quantum sources $\beta_j$, turned on at time of measurement $t$, and the initial bilinear sources $u_\nu$ turned on at $t=0$. The physical WCF corresponding to the particular initial state is then obtained from

$$\chi_W(\{\beta_j\},t) = \prod\nolimits_\nu \frac{1}{n_\nu!}\left(\frac{\partial}{\partial u_\nu}\right)^{n_\nu} \chi_W(\beta_j,t,\vec{u})\bigg|_{u=0}. \tag{5}$$

For a noninteracting system of bosons coupled to noninteracting bosonic baths, $\chi_W(\beta_j,t,\vec{u})$, after integrating out the bath, is given by

$$\chi_W(\beta_j,t,\vec{u}) = e^{-\frac{1}{2}\beta_i^*\beta_j\Lambda_{ij}^0(t)} \prod_\nu \frac{e^{-\beta_i^*\beta_j\Lambda_{ij}^\nu(t)\frac{u_\nu}{1-u_\nu}}}{1-u_\nu}, \tag{6}$$

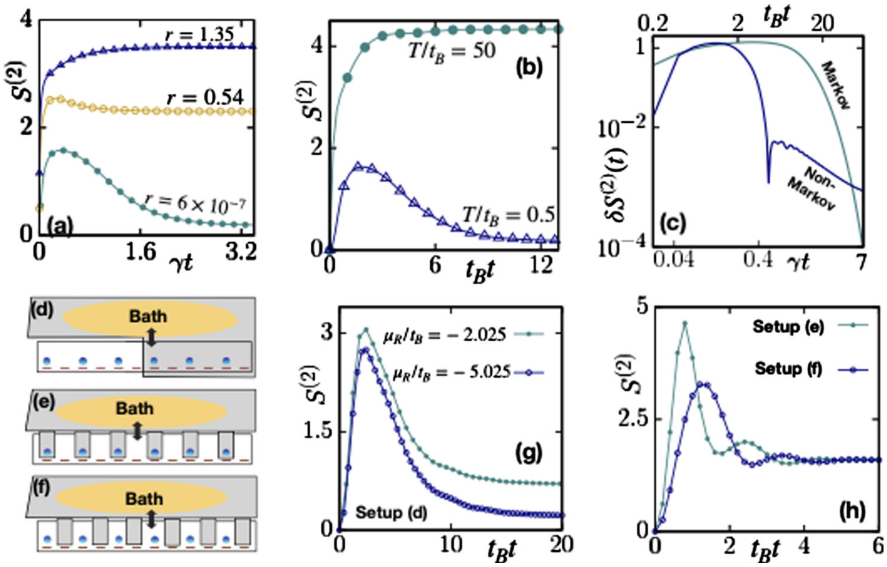


FIG. 2. (a)–(b) Evolution of $S^{(2)}$ of a 1 mode system starting from $|n_i = 6\rangle$ coupled to (a) a Markovian bath with increasing final number $n_f = 0.1$ and $r = 6 \times 10^{-7}$, $n_f = 4.5$ and $r = 0.54$, and $n_f = 16.2$ and $r = 1.35$. Here $r = n_f^{n_i}/(1+n_f)^{(n_i+1)}(1+2n_f)$; when $r < 1$, $S^{(2)}$ shows nonmonotonic behavior in time. (b) A non-Markovian bath with $T/t_B = 0.5$, showing a peak in $S^{(2)}$ and $T/t_B = 50$ showing the monotonic evolution of $S^{(2)}$. In general increasing $n_f$ with respect to $n_i$ leads to the disappearance of peaks in $S^{(2)}(t)$. (c) $\delta S^{(2)}(t) = |S^{(2)}(t) - S^{(2)}(\infty)|$ as a function of $t$ in a log-log plot. $S^{(2)}$ approaches its steady-state value exponentially for a Markovian bath and as a power law ($\sim t^{-3/2}$) for a non-Markovian bath. (d)–(f) Schematic representation of 12-site linear chain initialized to $|101010\ldots\rangle$ coupled to external bath. The gray shaded regions are integrated out to compute the Renyi entropy. (g) $S^{(2)}(t)$ for the setup of (d) where the right half of the system is integrated out. The two graphs correspond to a steady state with a finite current ($\mu_L/t_B = -2.025, \mu_R/t_B = -5.025$) and with zero current ($\mu_L/t_B = \mu_R/t_B = -2.025$). (h) $S^{(2)}(t)$ for the setups of (e) and (f) where the subsystem initialized to 1 and 0 particles in the initial state is integrated out respectively. $S^{(2)}(t)$ shows damped out-of-phase oscillations as the density imbalance between the sublattices is wiped out by the bath. Unless otherwise mentioned, the external bath has $T/t_B = 0.5$ and $\mu/t_B = -2.025$. The non-Markovian bath has a bandwidth $t_B = 2$ and a system bath coupling $\epsilon = 1$.

where $\Lambda^0_{ij}(t) = \langle \phi_{\rm cl}(i,t)\phi^*_{\rm cl}(j,t)\rangle_0$ is the equal time classical correlator in a system that starts from the vacuum state with 0 particles, and $\Lambda^\nu_{ij}(t) = G^R_{i\nu}(t)G^{R*}_{j\nu}(t)$, where the retarded Green's function $G^R_{i\mu}(t)$ is the probability amplitude of finding a particle in mode $i$ at time $t$ if it was initially in mode $\mu$. Our formalism can treat open and closed quantum systems, as well as Markovian and non-Markovian dynamics on equal footing. After taking the $\vec{u}$ derivatives [46], the physical WCF is given by

$$\chi_W(\beta_j, t) = e^{-\frac{1}{2}\beta^*_i\beta_j\Lambda^0_{ij}(t)}\prod_\nu L_{n_\nu}[\beta^*_i\beta_j\Lambda^\nu_{ij}(t)] \tag{7}$$

where $L_n(x)$ is the Laguerre polynomial of order $n$.

The effect of the bath on the system dynamics is incorporated through the retarded self-energy $\Sigma^R(i,j,\omega)$ (real part of $\Sigma^R$ controls the dressing of the system spectrum, and its imaginary part controls the dissipation in the system) and the Keldysh self-energy $\Sigma^K(i,j,\omega)$ (related to the stochastic noise from the bath and controls the steady state of the system). Inverting the Dyson equation, the correlators, and hence the evolution of the Renyi entanglement entropy can be computed (see Appendix B [45]).

Note that this method can be easily generalized to interacting systems to start making approximations for entanglement entropy of interacting OQS (see Appendixes A and C [45]).

*Single mode coupled to bath.*—We first consider a single mode with $H = \omega_0 a^\dagger a$, initialized in the number state $\hat{\rho}(0) = |n_i\rangle\langle n_i|$, and coupled to an external bath. The time-evolving Renyi entropy is given by

$$e^{-S^{(2)}(t)} = \frac{{}^{2n_i}C_{n_i}[\tilde{\Lambda}]^{2n_i}}{[\Lambda^0]^{2n_i+1}}\,{}_2F_1\left[-n_i, -n_i, -2n_i, \frac{-\Lambda^0[\Lambda - \tilde{\Lambda}]}{[\tilde{\Lambda}]^2}\right] \tag{8}$$

where $\tilde{\Lambda}(t) = \Lambda^0(t) - \Lambda(t)$ and ${}_2F_1$ is the hypergeometric function. Here, as time increases $\Lambda(t)$ decays from 1 to 0 due to dissipation, while the stochastic contribution $\tilde{\Lambda}(t)$ increases from 0 to a finite value determined by the bath parameters.

The simplest bath is a Markovian Langevin type bath, characterized by a frequency independent $\Sigma^R(\omega) = \mathbf{i}\gamma$, where $\gamma$ is the dissipation scale, and a frequency independent $\Sigma^K(\omega) = -\mathbf{i}D$ where $D$ is the noise scale. The steady-state average number in the system is controlled by $1 + 2n_f = D/2\gamma$. The correlators in this case can be found analytically: $\Lambda^0(t) = e^{-2\gamma t} + (D/2\gamma)[1 - e^{-2\gamma t}]$ and $\Lambda(t) = e^{-2\gamma t}$. Figure 2(a) shows $S^{(2)}(t)$ for this OQS starting from $n_i = 6$ for three different values of $n_f = 0.1$, 4.5, and 16.2. $S^{(2)}(t)$ shows nonmonotonic evolution with a peak at $t_{\rm peak} \sim 1/2\gamma$ for $n_f = 0.1$ and $n_f = 4.5$, while the evolution is monotonic for $n_f = 16.2$. A peak in $S^{(2)}$ implies that at $t \sim t_{\rm peak}$, the initial delta function distribution of $\rho_{nn}$ spreads to a distribution which is wider than the final thermal distribution.

We next consider coupling the same system to a non-Markovian bath of bandwidth $t_B$ characterized by a spectral density $\mathcal{J}(\omega) = \Theta(4t_B^2 - \omega^2)(2/t_B)\sqrt{1 - (\omega^2/4t_B^2)}$, temperature $T$, and chemical potential $\mu$ with coupling strength $\epsilon$ [35]. In this case, $\Sigma^R(\omega) = \mathbf{i}\epsilon^2\mathcal{J}(\omega)$ and $\Sigma^K(\omega) = -\mathbf{i}\epsilon^2\mathcal{J}(\omega)\coth[(\omega - \mu)/2T]$. Figure 2(b) shows the evolution of $S^{(2)}(t)$ for this OQS for $T/t_B = 0.5$ where we see a nonmonotonic time dependence with a peak at a timescale $\sim t_B/\epsilon^2$ and $T/t_B = 50$ where the peak has disappeared. We note that contrary to previous predictions [49,50], the presence of the peak in $S^{(2)}(t)$ is not related to the non-Markovian nature of the dynamics. The key difference between the Markovian and non-Markovian dynamics is manifested in how $S^{(2)}(t)$ approaches its steady-state value. As shown in Fig. 2(c), the Markovian approach is exponential while that for the non-Markovian case has a power law tail ($t^{-3/2}$) at long times [35].

To understand why the time evolution is nonmonotonic in some cases, and monotonic in others, we use the ansatz $\hat{\rho}(t) = A(t)|n_i\rangle\langle n_i| + B(t)\hat{\rho}(\infty)$, where the first term denotes the forward time propagation (decay) of the initial state due to dissipation and the second term can be viewed as the backward time propagation of the steady-state density matrix of the system $\hat{\rho}(\infty)$. For the Langevin bath, we can obtain exact expressions, $A(t) = |G^R(t,0)|^2 = e^{-2\gamma t}$ and $B(t) = 1 - e^{-2\gamma t}$. While similar expressions for the non-Markovian bath can only be written in terms of multiple integrals, it is easy to see that in both cases $A(t) \sim 1 - at$ and $B(t) \sim bt$ for short times, where $a$ and $b$ are rates that can be computed from a Fermi golden rule calculation. Also $A(t) \to 0$ and $B(t) \to 1$ as $t \to \infty$ to obtain the correct steady-state density matrix. We can then obtain the time dependent Renyi entropy

$$e^{-S^{(2)}(t)} = A^2(t) + B^2(t)e^{-S^{(2)}(\infty)} + 2A(t)B(t)\rho_{n_i,n_i}(\infty), \quad (9)$$

where $\rho_{n_i,n_i}(\infty)$ is the diagonal matrix element of $\hat{\rho}(\infty)$ in the initial state $|n_i\rangle$.

The initial rise of the entanglement is controlled by the rates $a$ and $b$ with $e^{-S^{(2)}(t)} \sim 1–2at(1 - \rho_{n_i,n_i}(\infty)b/a)$. Interestingly this rate is neither controlled by the initial state, nor the final density matrix, but a cross term between them. For an heuristic argument, we can compare the entropy at a time $t_0 \sim (2a)^{-1}$, $e^{-S^{(2)}(t_0)} \sim \rho_{n_i,n_i}(\infty)b/a$, with its steady-state value $e^{-S^{(2)}(\infty)}$ and say that a peak occurs if $\rho_{n_i,n_i}(\infty)b/a < e^{-S^{(2)}(\infty)}$. For the Langevin bath $b = a = 2\gamma$, so this criterion reduces to $\rho_{n_i,n_i}(\infty) < e^{-S^{(2)}(\infty)} = (1 + 2n_f)^{-1}$, which gives $r < 1$, where $r = n_f^{n_i}/(1 + n_f)^{(n_i+1)}(1 + 2n_f)$. We also find the peak condition for the Langevin bath from an exact calculation involving the maxima of Eq. (9) (see Appendix D [45]) and get the same result. Increasing average density in a thermal system leads to a broader distribution of $\rho_{nn}(\infty)$, and hence a decrease in $\exp[-S^{(2)}(\infty)]$. Thus, a general conclusion from this is that increasing $n_f$ keeping $n_i$ fixed leads to the disappearance of the peak in $S^{(2)}$.

*Entanglement dynamics of a many-body system.*—For a single or two mode system the dynamics of Renyi entropy can in principle be studied by more direct means like quantum master equations [37–44]. However, these methods are not easy to generalize to many-body bosonic systems due to the infinite size of the local Hilbert space. Our method, however, is easily generalizable to dynamics of many-body open quantum systems initialized to nonthermal states. The truncation of the Hilbert space in the existing methods is specially problematic for open quantum systems where the particle number is not conserved. While methods like time evolving density matrix using orthogonal polynomials algorithm chain mapping [51] try to get around this by working with a finite sized bath, our method can easily incorporate infinite baths.

To show the power of this method, we consider a linear chain of bosons described by the Hamiltonian

$$H = -g\sum_j a_{j+1}^\dagger a_j + \mathrm{H.c.}, \quad (10)$$

with the nearest neighbor hopping $g = 0.5t_B$. This system is made of the even ($E$) and odd ($O$) sublattices and is initialized to a Fock state with 0 and 1 number of particles on the $E$ and $O$ sublattices, respectively [see Figs. 2(d)–2(f)]. Each site of the system is coupled to the non-Markovian bath described earlier. The temperature of the baths is set to $T/t_B = 0.5$. We treat two different cases: (i) when the baths have the same $T$ and $\mu$, leading to thermalization at long times, and (ii) when $\mu$ of the baths coupled to neighboring sites have a fixed difference of chemical potential, leading to steady states with finite currents. In this case,

$$e^{-S^{(2)}(t)} = \int \prod_{i\in A} \frac{d^2\beta_i}{\pi^{\Omega_A}} e^{-\sum_{i,j\in A}\beta_i^*\beta_j\Lambda_{ij}^0(t)} \prod_{\nu\in O} L_1^2[\beta_i^*\beta_j\Lambda_{ij}^\nu(t)], \quad (11)$$

where $A$ denotes the reduced subsystem and $O$ denotes the initially filled sublattice [52].

In a many-body system, we can trace out a part of the system, together with the bath, to construct the subsystem for which we consider Renyi entropy. Figure 2(g) shows the evolution of $S^{(2)}(t)$ of the subsystem which occupies the left half of the linear chain [see setup in Fig. 2(d)]. The chemical potential for the leftmost bath is set to be $\mu_L/t_B = -2.025$, so the graph for $\mu_R/t_B = -2.025$ corresponds to identical baths, while the graph for $\mu_R/t_B = -5.025$ corresponds to a linear gradient in $\mu$ resulting in a finite current in the steady state. We find that $S^{(2)}(t)$ is nonmonotonic in both cases, and the steady-state value is lower for the system with a finite current. In Fig. 2(h), we consider the same system, with the same initial condition of alternating filled and empty sites, but our subsystem is now composed of the $A(B)$ sublattice obtained by integrating out the $B(A)$ sublattice, as shown in Figs. 2(e) and 2(f). The evolution of Renyi entropy shows damped out-of-phase oscillation in $S^{(2)}(t)$ between the two setups, which track the oscillations in the imbalance of density on the two sublattices. The steady-state value is the same in both cases, showing that the system erases information about the initial state.

We have developed a new method for calculating Renyi entropy of bosonic many-body systems in and out of thermal equilibrium. This method has also been used to study Renyi entropy of a thermal system of interacting bosons in one and two dimensions of large sizes within a large $N$ approximation [36]. These ideas can also be extended to the case of fermionic systems with appropriate modifications[53,54].

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