Quantum Thermodynamics of Nonequilibrium Processes in Lattice Gauge Theories

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A key objective in nuclear and high-energy physics is to describe nonequilibrium dynamics of matter, e.g., in the early Universe and in particle colliders, starting from the standard model of particle physics. Classical computing methods, via the framework of lattice gauge theory, have experienced limited success in this mission. Quantum simulation of lattice gauge theories holds promise for overcoming computational limitations. Because of local constraints (Gauss's laws), lattice gauge theories have an intricate Hilbert-space structure. This structure complicates the definition of thermodynamic properties of systems coupled to reservoirs during equilibrium and nonequilibrium processes. We show how to define thermodynamic quantities such as work and heat using strong-coupling thermodynamics, a framework that has recently burgeoned within the field of quantum thermodynamics. Our definitions suit instantaneous quenches, simple nonequilibrium processes undertaken in quantum simulators. To illustrate our framework, we compute the work and heat exchanged during a quench in a \mathbb{Z}_2 lattice gauge theory coupled to matter in 1 + 1 dimensions. The thermodynamic quantities, as functions of the quench parameter, evidence a phase transition. For general thermal states, we derive a simple relation between a quantum many-body system's entanglement Hamiltonian, measurable with quantum-information-processing tools, and the Hamiltonian of mean force, used to define strong-coupling thermodynamic quantities.

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Introduction—An overarching goal in nuclear and high-energy physics is to simulate strongly interacting matter, starting from gauge theories. Key focuses include nonequilibrium phenomena described by quantum chromodynamics (QCD), the theory of the strong force. Nonequilibrium phenomena arise in ultrarelativistic particle collisions [1,2] and in the early Universe [3,4]. Theoretical studies [5–9] of in- and out-of-equilibrium phases of QCD, and of its thermalization mechanisms, are often restricted to extreme parameter regimes to facilitate perturbation theory. Alternatively, studies feature simple (often low-dimensional) models to capture qualitative features of QCD.

Studying QCD and other strongly interacting gauge theories requires nonperturbative tools, as enabled by

lattice gauge theory (LGT) [10-14]. Within the pathintegral formulation of LGTs, Monte Carlo simulations can be feasible if Euclidean (imaginary) time replaces Minkowski (real) time. The scheme permits parallels with statistical mechanics: Euclidean time stands in for inverse temperature, and vacuum expectation values serve as thermal averages. LGT has enabled thermodynamic studies of the OCD equation of state at small chemical potentials [15–26]. Nonetheless, the sampling weight in Monte Carlo computations can become nonreal, requiring infeasibly many samples [26-30]. These limitations do not inhibit Hamiltonian-based approaches, such as tensor-network methods [31–33] and quantum simulation [34–39]. These approaches, hence, suit thermodynamic studies of gauge theories, in and out of equilibrium. Still, we need a modern description of LGTs in the language of quantum thermodynamics.

The field of quantum thermodynamics extends conventional thermodynamics to small and quantum systems that exchange heat and work [40–42]. A typical setup features a subsystem of interest (the "system") interacting with a "reservoir" of inaccessible degrees of freedom (d.o.f.)

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[43,44]. The coupling is often weak because a system and reservoir typically interact only at their shared boundary. This boundary is of lower dimensionality than the system, whose volume is proportional to its internal energy. Hence, the interaction energy is much smaller than the system's and reservoir's internal energies. Yet quantum systems and reservoirs can be small while behaving thermodynamically [45–47]; their interactions need not be negligible.

Hence, the subfield of strong-coupling (quantum) thermodynamics has burgeoned recently [48–57]. Strong coupling blurs the system-reservoir boundary, complicating the definition of the system's internal energy, work, and heat. Nonetheless, definitions have been developed and obey thermodynamic laws [52,54,55,58–60].

These considerations raise the question of whether *weak-coupling thermodynamics can describe LGTs*. Local constraints, or Gauss's laws, form the defining feature of (lattice) gauge theories: the charge at a site balances the electric-field flux emanating from the site. Only a subspace of the gauge theory's Hilbert space satisfies Gauss's laws and consists of physical states. This restriction complicates the partitioning of the system into subsystems: the values of the fields on one side of any partition depend on the values on the other side. Yet a partitioning is used to define quantities such as the bipartite entanglement entropy [61–68]. The system-reservoir partitioning in LGTs, we posit, can resemble that in strong-coupling thermodynamics to define thermodynamic properties of LGTs.

We answer the following questions: What are the work and heat exchanged during instantaneous quenches [69] (simple nonequilibrium processes created in quantum simulations) [70,71]? Can these quantities signal phase transitions [72]? Can such quantities be measured efficiently with quantum-information-processing tools?

We describe how to compute internal-energy changes. We further show how to define work and heat consistently with the first and second laws of thermodynamics [58]. A simple model illustrates this framework: a \mathbb{Z}_2 LGT coupled to hardcore bosonic matter in 1 + 1 dimensions (D). We observe that thermodynamic quantities, as functions of chemical potential, signal an apparent phase transition. Furthermore, we bridge the fields of quantum information theory and strong-coupling quantum thermodynamics: we show that the entanglement Hamiltonian [81,82], which can often be efficiently measured experimentally [83–86], is related to the Hamiltonian of mean force [52], which underpins strong-coupling quantum thermodynamics.

Review of strong-coupling quantum thermodynamics— Consider a system S and a reservoir R. The composite $S \cup R$ evolves under the Hamiltonian

$$H_{S\cup R} \coloneqq H_S + H_R + V_{S\cup R}.$$
 (1)

 H_S and H_R denote the system and reservoir Hamiltonians, respectively; $V_{S \cup R}$ denotes the interaction. During a thermodynamic process, S can absorb heat Q and work

W. (*Heat*, *work*, and *internal energy* refer to averages throughout this Letter.)

In weak-coupling quantum thermodynamics, $V_{S\cup R}$ contributes negligibly to the total internal energy, $U_{S\cup R} := \langle H_{S\cup R} \rangle$. Hence, the system's internal energy is $U_S := \langle H_S \rangle$ [59]. One can measure U_S by accessing only system d.o.f. In contrast, when $\langle V_{S\cup R} \rangle$ is comparable to $\langle H_S \rangle$, one must use strong-coupling thermodynamics.

How much $V_{S\cup R}$ contributes to U_S is ambiguous. To resolve the ambiguity, one can define the global Gibbs state with respect to an inverse temperature β : $\pi_{S\cup R} := e^{-\beta H_{S\cup R}}/Z_{S\cup R}$. The partition function is $Z_{S\cup R} := \text{Tr}(e^{-\beta H_{S\cup R}})$. Throughout this Letter, we denote thermal states by π and general density matrices by ρ . Tr_X denotes the partial trace over X. Consider tracing out the reservoir from $\pi_{S\cup R}$. The system's reduced density matrix is $\pi_S := \text{Tr}_R(\pi_{S\cup R}) \equiv e^{-\beta H_S^*}/Z_S^*$. This is a thermal state with respect to an effective Hamiltonian, a "Hamiltonian of mean force" [52],

$$H_{S}^{*} \coloneqq -\frac{1}{\beta} \ln\left(\frac{\operatorname{Tr}_{R}(e^{-\beta H_{S\cup R}})}{Z_{R}}\right),$$
(2)

wherein $Z_R := \operatorname{Tr}_R(e^{-\beta H_R})$ and $Z_S^* := \operatorname{Tr}_S(e^{-\beta H_S^*}) = Z_{S \cup R}/Z_R$. Equation (2) underlies an intuitive definition for the system's free energy [52,87,88],

$$F_S \coloneqq -\frac{1}{\beta} \ln(Z_S^*). \tag{3}$$

It is natural to equate $\langle H_S^* \rangle$ with U_S [51,58,59,87]. Consequently, once H_S^* has been determined by tracing over the reservoir d.o.f. [Eq. (2)], one need not access reservoir d.o.f. further to compute U_S . Furthermore, if S := $-\text{Tr}_S(\pi_S \ln \pi_S)$ denotes the thermal von Neumann entropy, then the equality $F_S = U_S - \frac{S}{\beta}$ holds in equilibrium [89].

Any change in U_S comes from work and heat, by the first law of thermodynamics: $\Delta U_S = W + Q$. By the second law, $\Delta F_S \leq W$, or $Q \leq \Delta S/\beta$. Here, ΔU_S , ΔF_S , and ΔS denote, respectively, net changes in the system's internal energy, free energy, and entropy. Intuition guides the separation of ΔU_S into W and Q: work comes from changes in the system's Hamiltonian and heat from changes in the system's state [41]. To define work and heat, we now specify a thermodynamic process.

Instantaneous quenches—During a quench, the Hamiltonian changes rapidly. Quenches generate nonequilibrium conditions and are studied in diverse quantum-simulation experiments [86,90–100]. Figure 1 depicts the quench studied here. The system-reservoir composite begins in a Gibbs state: $\rho_{SUR}^i := \rho_{SUR}(t = 0^-) = \pi_{SUR}^i := e^{-\beta H_{SUR}^i}/\text{Tr}(e^{-\beta H_{SUR}^i})$, wherein the initial composite Hamiltonian $H_{SUR}^i := H_{SUR}(t = 0^-)$. Equation (1), with a time-dependent $H_S(t)$, specifies H_{SUR} . At time t = 0, $H_S(t)$ is instantaneously quenched from $H_S(t = 0^-) := H_S^i$ to $H_S(t = 0^+) := H_S^f$. The system-reservoir composite



FIG. 1. Overview of relevant quench protocol. The system starts in a global Gibbs state. At t = 0, the system Hamiltonian H_s is quenched instantaneously. Under the new total Hamiltonian, the system-reservoir composite equilibrates to a global Gibbs state with the initial state's temperature.

equilibrates to a Gibbs state under the final total Hamiltonian $H_{S\cup R}(t=0^+) := H_{S\cup R}^{f}$. The initial and final Gibbs states share the temperature β^{-1} by assumption. Justifications include the possibility that $S \cup R$ couples weakly to a larger reservoir, at a temperature β^{-1} , in the distant past and future [58].

Practical work and heat definitions depend on system d.o.f. alone. We present such definitions, for the quenches just described, in Ref. [58]; see also Refs. [49,52,87]. The system's internal energy is

$$U_S(t) \coloneqq \langle H_S^*(t) \rangle = \operatorname{Tr}[\rho_S(t)H_S^*(t)], \qquad (4)$$

for arbitrary states $\rho_S(t) \coloneqq \operatorname{Tr}_R[\rho_{S\cup R}(t)]$. H_S^* becomes time-dependent under the replacement $\operatorname{Tr}_R(e^{-\beta H_{S\cup R}}) \mapsto$ $\operatorname{Tr}_R(e^{-\beta H_{S\cup R}(t)})$ in Eq. (2). During the quench, ΔU_S equals the work absorbed by *S*:

$$W \coloneqq \operatorname{Tr}_{S}[\rho_{S}^{i}H_{S}^{*}(t=0^{+})] - \operatorname{Tr}_{S}[\rho_{S}^{i}H_{S}^{*}(t=0^{-})].$$
(5)

During the equilibration, ΔU_S equals the heat absorbed by S:

$$Q \coloneqq \operatorname{Tr}_{S}[\rho_{S}^{\mathrm{f}}H_{S}^{*}(t=0^{+})] - \operatorname{Tr}_{S}[\rho_{S}^{\mathrm{i}}H_{S}^{*}(t=0^{+})]. \quad (6)$$

These definitions are intuitive and obey the first and second laws of thermodynamics [58]. Upon identifying a Hamiltonian of the form in Eq. (1), one calculates work and heat by measuring $\langle H_S^* \rangle$. We show next how to measure this quantity.

Measuring thermodynamic quantities in quantum simulations—Here, we derive a relation between strongcoupling-thermodynamics quantities and a quantity called the "entanglement Hamiltonian." Every density matrix ρ can be expressed as $\rho = \sum_k p_k |k\rangle \langle k|$. The $|k\rangle$ denote eigenstates and the $p_k \in [0, 1]$, probabilities. Define $\lambda_k := -\ln(p_k) \ge 0$, such that $\rho = \sum_k e^{-\lambda_k} |k\rangle \langle k|$. This expansion has the form of a thermal state at unit temperature (with the normalization factor, or partition function, absorbed into the $e^{-\lambda_k}$). For $\rho = \rho_S := \text{Tr}_R(\rho_{S \cup R})$, this Hamiltonian is the "(bipartite) entanglement Hamiltonian" [81,82],

$$H_S^{\text{ent}} \coloneqq -\ln(\rho_S). \tag{7}$$

This operator contains more information than the bipartite entanglement entropy. It has spawned numerous studies in quantum information theory and many-body physics. Parametrized *Ansätze* for entanglement Hamiltonians [82], with random-measurement protocols [101–104], enable tomography of ground and nonequilibrium states [83–85,105,106], including of LGTs [86,107,108].

To leverage such tomography tools, we prove a relation between H_S^{ent} and H_S^* for thermal states. We rewrite the Hamiltonian of mean force as

$$H_{S}^{*} = -\frac{1}{\beta} \ln \left(\frac{\operatorname{Tr}_{R}(e^{-\beta H_{S \cup R}})}{\operatorname{Tr}_{R}(e^{-\beta H_{R}})} \right)$$
(8a)

$$=-\frac{1}{\beta}\ln{\left(\rho_{S}\frac{Z_{S\cup R}}{Z_{R}}\right)}. \tag{8b}$$

The system's reduced state is $\rho_S = \pi_S := \text{Tr}_R(e^{-\beta H_{S \cup R}})/Z_{S \cup R}$. Using Eqs. (7) and (3) yields the relation between the entanglement Hamiltonian and the Hamiltonian of mean force:

$$H_S^* = \frac{1}{\beta} H_S^{\text{ent}} + F_S. \tag{9}$$

 \mathbb{I}_S denotes the identity operator defined on *S*.

One can measure the first term in Eq. (9) using the aforementioned tomography tools (if the *Ansätze* model H_S^{ent} accurately). To measure F_S , one must measure $Z_{S\cup R}$ and Z_R [109–112], necessitating access to the reservoir



FIG. 2. (a) Partitioning of d.o.f. into system (S) and reservoir (R) d.o.f. Partitioning of total Hamiltonian's (b) hopping terms, (c) electric-field terms, and (d) mass and chemical-potential terms into $H_S(t)$ (teal), H_R (light red), and $V_{S\cup R}$ (purple). Matter (gauge-field) d.o.f. reside on lattice sites (links). The last link wraps around to indicate the lattice's periodicity.

d.o.f. To avoid measuring the second term in Eq. (9), we study the average dissipated work, $W_{\text{diss}} \coloneqq W - \Delta F_S$, a measure of entropy production [113,114]. For our quench protocol,

$$W_{\rm diss} = \frac{1}{\beta} \operatorname{Tr}_{S} \{ \rho_{S}^{\rm i} [H_{S}^{\rm ent}(t=0^{+}) - H_{S}^{\rm ent}(t=0^{-})] \}.$$
(10)

Hence, one can infer W_{diss} upon measuring the entanglement Hamiltonian alone.

Lattice gauge theories and strong-coupling quantum thermodynamics—We use the Hamiltonian formulation of LGTs [12], which suits quantum simulation. As matter and gauge fields undergo local symmetry-group transformations, the observables remain invariant. The symmetry restricts the states to a "physical subspace": for each site n, a "Gauss-law" operator G_n acts on n and commutes with the Hamiltonian. The full Hilbert space (spanned by eigenbases of electric and matter fields) decomposes into G_n eigenspaces, for each n. The eigenspace labeled by some eigenvalue g, and shared by all the G_n , is the physical subspace [115]. That is, for any physical state $|\Psi_{phys}\rangle$,

$$G_n |\Psi_{\rm phys}\rangle = g |\Psi_{\rm phys}\rangle, \quad \forall \ n.$$
 (11)

In electrodynamics, $G_n = \nabla \cdot E_n - \rho_n$. Here, E_n denotes the electric field, and ρ_n denotes the (dynamical) electriccharge density, both at site *n*. Gauss's law follows from setting g = 0 ($g \neq 0$) in Eq. (11) in the absence (presence) of a background static electric charge.

One may impose Gauss's laws by manually removing the unphysical states from the full Hilbert space [116,117]. Alternatively, the Hamiltonian $H_{S\cup R}$ may be replaced with $H_{S\cup R} + \sum_n f(G_n)$. $f(G_n)$ denotes a function of Gauss-law operators. Chosen properly, it penalizes transitions to unphysical states [118–125]. Consider partitioning a lattice into a system *S* and a reservoir *R*. Some Gauss-law penalty terms act on both *S* and *R*: Gauss-law operators are multibody operators consisting of gauge and matter fields. Such penalty terms, thus, contribute to the $V_{S\cup R}$ in Eq. (1). Their contribution must be large to constrain the state to the physical subspace. Therefore, one cannot generally neglect the internal energy's dependence on $V_{S\cup R}$ when computing thermodynamic quantities [see Supplemental Material (SM) [126]]. Consequently, LGTs can be described within the framework of strong-coupling thermodynamics.

Example of \mathbb{Z}_2 LGT coupled to matter in (1+1)D— Consider a \mathbb{Z}_2 gauge field (hardcore bosons) coupled to matter fields (chosen to be hardcore bosons). The initial state evolves under the Hamiltonian

$$H = H_{\rm h} + H_{\rm e} + H_{\rm m} + H_{\mu} + H_{c}$$

$$\equiv -J \sum_{n=0}^{N-1} (\sigma_{n}^{+} \tilde{\sigma}_{n}^{z} \sigma_{n+1}^{-} + \text{H.c.}) - \epsilon \sum_{n=0}^{N-1} \tilde{\sigma}_{n}^{x}$$

$$+ m \sum_{n=0}^{N-1} (-1)^{n} \sigma_{n}^{+} \sigma_{n}^{-} - \sum_{n=0}^{N-1} \mu_{n} \sigma_{n}^{+} \sigma_{n}^{-} + c \sum_{n=0}^{N-1} \mathbb{I}_{n}, \quad (12)$$

on a one-dimensional *N*-site spatial lattice with periodic boundary conditions ($\sigma_N = \sigma_0$). H_h , H_e , H_m , and H_μ represent the matter-hopping, electric-field, matter-mass, and matter-chemical-potential terms, respectively. A constant H_c is added such that $H_S(t)$, H_R , and $H_{S\cup R}(t)$ have only non-negative eigenvalues. *J*, ϵ , *m*, and μ_n denote the hopping strength, electric-field strength, matter mass, and site-*n* chemical potential, respectively. Pauli operator σ_n acts on the Hilbert space of the site-*n* matter field. Pauli operator $\tilde{\sigma}_n$ acts on the Hilbert space of the gauge field rightward of *n*. Specifically, $\tilde{\sigma}_n^x$ ($\tilde{\sigma}_n^z$) denotes the electricfield (gauge-link) operator.

The \mathbb{Z}_2 gauge transformation is generated by the Gausslaw operator [128]

$$G_n = \tilde{\sigma}_n^x \tilde{\sigma}_{n-1}^x \exp\left(i\pi \left[\sigma_n^+ \sigma_n^- + \frac{(-1)^n - 1}{2}\right]\right). \quad (13)$$

The physical states obey Eq. (11) with g = 1. One can realize the gauge-invariant dynamics by adding $\sum_n f(G_n) = \kappa \sum_n (1 - G_n)$ to *H*, then taking the limit $\kappa \to \infty$ [129].

The lattice can be partitioned into a system *S* and a reservoir *R*, as in Fig. 2(a). Also, the Hamiltonian (12) decomposes as in Eq. (1). Some hopping terms act only on sites in *S* (*R*) and so belong in H_S (H_R). Other terms



FIG. 3. Thermodynamic quantities as functions of the final chemical potential, $\mu_{\rm f}$, during the instantaneous quench from $\mu_{\rm i} = 0$ with N = 6, $N_S = 4$, t = -1/2, $\epsilon = 1/2$, m = 1/2, $\mu_{\rm i} = 0$, and $\beta = 10$. (a) Dissipated work $W_{\rm diss}$ (solid, black) and chiral condensate Σ (dot-dashed, teal). (b) Work W (solid, black) and change ΔF_S in the system's free energy (dotted, black). (c) Normalized heat βQ (solid, black) and change ΔS in the system's entropy (dotted, black). We also plot $\mu_{\rm f}^{\rm c}$, the $\mu_{\rm f}$ value where Σ' is maximized (dashed, gray).

describe hopping between a site in *S* and a site in *R*. These interaction terms belong in $V_{S\cup R}$; see Fig. 2(b). The electric-field Hamiltonian can be partitioned as follows; see Fig. 2(c). Terms acting on links in *S* belong in $H_S(t)$. Terms acting on links in *R*, but touching the *S*-*R* boundary, belong in $V_{S\cup R}$ due to Gauss's laws. Terms acting on links elsewhere in *R* belong in H_R . Terms in H_m and H_μ belong in $H_S(t)$ and H_R , depending on whether they act on a site in *S* or *R*; see Fig. 2(d). Finally, if penalty terms enforcing Gauss's law act at the boundary, they belong in $V_{S\cup R}$. Otherwise, they belong in H_S or H_R .

We set reservoir's chemical potential to zero and quench the chemical potential from $\mu_n = \mu_i = 0$ to $\mu_n = \mu_f > 0$ at all sites *n* in the system. We further define the "chiral condensate" [130]

$$\Sigma \coloneqq \frac{1}{N_S} \sum_{n=0}^{N_S - 1} (-1)^n \langle \sigma_n^+ \sigma_n^- \rangle.$$
(14)

 N_S denotes the system size. The expectation value is in the final thermal state, whose $\mu_n = \mu_f$ at all sites *n* in *S*. If $\mu_f \gg \epsilon$, *m*, the system's state is dominated by the matter fields' all-spin-up state, yielding $\Sigma = 0$. At other μ_f values, Σ could be nonvanishing. In fact, Σ suddenly changes from finite to vanishing values as μ_f increases, evidencing a phase transition, as Fig. 3(a) shows. This apparent phase transition does not look perfectly sharp due to finite-temperature (see SM [126]) and finite-size effects [131]. The critical value $\mu_f = \mu_f^c$ denotes the transition point, where $\Sigma' := d\Sigma/d\mu_f$ is maximized.

Figure 3 displays thermodynamic quantities, W_{diss} , W, Q, ΔF_S , and ΔS , calculated as functions of μ_{f} . As μ_{f} grows, $W_{\text{diss}} \coloneqq W - \Delta F_S$ remains near zero until around the μ_{f} value where the apparent phase transition occurs. Afterward, W_{diss} increases. Hence, W_{diss} indicates the suspected phase transition clearly. Similarly, W (βQ) begins deviating from ΔF_S (ΔS) around the transition.

Strong-coupling relations are valid in this model: $|\langle V_{S\cup R} \rangle / \langle H_S \rangle|$ is non-negligible ($\gtrsim 0.1$) in the initial and final states at all the μ_f values used. Nonetheless, in the SM [126], we apply weak-coupling relations for comparison: $U_S = \langle H_S \rangle$ and $\rho_S = e^{-\beta H_S} / \text{Tr}(e^{-\beta H_S})$. We find that the thermodynamic quantities' values differ from their strong-coupling counterparts: the weak-coupling quantities change less sharply, signaling the transition less reliably.

Outlook-This work shows how strong-coupling quantum thermodynamics applies to lattice gauge theories in and out of equilibrium. The work further shows how entanglement Hamiltonians can be leveraged to measure thermodynamic quantities in quantum simulations. Our framework may be applied to explore further questions in the quantum thermodynamics of gauge theories. Examples include whether thermodynamic quantities signal topological [81,134–141] or dynamical [142] phase transitions. While quench protocols in LGTs have been implemented in experiments [86,96-98,100,119,143-153], a longer-term vision is to simulate more-general processes, including quantum-adiabatic ones, and particle collisions relevant to nuclear and high-energy physics [154-159]. Also, non-Abelian and higher-dimensional gauge theories merit studying within our framework. Developing quantumsimulation protocols for studying gauge-theory thermodynamics is an active frontier, and this work furthers this goal.

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- [130] Σ has the form that the chiral condensate would have if the gauge field were coupled to staggered fermions [11] (a Jordan-Wigner transformation maps the fermion operators to Pauli operators). Such a chiral condensate serves as an order parameter for chiral phase transitions.
- [131] We have not performed a large-system analysis to confirm if the apparent phase transition persists in the thermodynamic limit. However, large-system analyses of a similar model (with the same discrete chiral symmetry as ours) reveal two phases, confined and deconfined [132,133]. While these studies do not directly probe the spontaneous breaking of the discrete chiral symmetry, the symmetry is broken in the confined phase.
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