Letter

Wilson loops in the Hamiltonian formalism

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(Received 23 February 2022; accepted 9 May 2022; published 1 June 2022)

In a gauge theory, the gauge invariant Hilbert space is unchanged by the coupling to arbitrary local operators. In the presence of Wilson loops, though, the physical Hilbert space must be enlarged by adding test electric charges along the loop. I discuss how at nonzero temperature Polyakov loops are naturally related to the propagator of a test charge. ’t Hooft loops represent the propagation of a test magnetic charge, and so do not alter the physical Hilbert space.

DOI: 10.1103/PhysRevD.105.L111501

I. INTRODUCTION

Since the seminal work of Wegner, Wilson, and Creutz, simulations of lattice gauge theories using Monte Carlo methods on classical computers has given us invaluable information about quantum chromodynamics (QCD). For the phase diagram at a nonzero temperature T and quark chemical potential μ, at $\mu = 0$ the order parameter for chiral symmetry exhibits crossover behavior at a temperature of $T_\chi \approx 156 \pm 1.5$ MeV [1–4]. These methods have been extended to quark chemical potentials less than the temperature, $\mu \leq T_\chi$ [2,3,5–8].

This leaves many quantities of direct experimental significance which have not yet been computed. For example, the diffusion coefficient for a heavy quark has been computed in the $SU(3)/Z(3)$ gauge theory without dynamical quarks [9,10]. The computation of other transport coefficients, notably the shear and bulk viscosities with dynamical quarks in QCD, is conceivable with much larger classical computers [11].

Many other quantities, such as correlation functions in real time, and the properties of cold, dense QCD, are only possible with quantum computers. While large scale quantum computers with logical qubits lie well in the future, it is useful to consider the questions of principle which are unique to a gauge theory.

A classical computer deals with the Lagrangian. If the chemical potential vanishes, then at any temperature the action is real, and sophisticated techniques, including those for nearly massless quarks, have been developed. While in principle many states contribute to the partition function, the Metropolis algorithm automatically selects the most important. The difficulty is the sign problem: at nonzero chemical potential the action is no longer real, and standard techniques fail.

In contrast, for a quantum computer it is best to deal with the Hamiltonian. The partition function is

$$\mathcal{Z} = \sum \mathrm{e}^{-\mathcal{H}/T - \mu\mathcal{N}}, \tag{1}$$

where $\mathcal{H}$ is the Hamiltonian, $\mathcal{N}$ the quark number density, and $\sum$ is the sum over all states. Because everything is real, there is no sign problem when $\mu \neq 0$. The difficulty is that exponentially many states contribute, and even for states near the ground state, it is not obvious how to choose the most important. Strategies to solve this have been developed in condensed matter systems, and include the density matrix renormalization group, matrix product states, and projected entangled pair states [12,13].

While some generalization of these methods will be essential in QCD, the purpose of this paper is to make an elementary point about how the Hamiltonian form of a gauge theory changes in the presence of Wilson loops.

For a theory without gauge fields, the most general correlation functions are given by adding sources for arbitrary local operators to the Lagrangian. Multiple insertions of composite operators induce new counterterms to the theory, but this is standard [14–16], and going from the Lagrangian to the Hamiltonian formalism is direct.

With gauge fields, however, there are gauge invariant nonlocal operators, such as the Wilson loop,

$$\mathcal{W}_{\mathcal{C}} = \mathrm{tr}\mathcal{P}\exp\left(ig\int_{\mathcal{C}} A_\mu dx^\mu\right). \tag{2}$$

Here g is the gauge coupling, A_μ is the vector potential for the gauge field, $\mathcal{P}$ denotes path ordering along a closed curve $\mathcal{C}$, and the trace is over color.

My basic point is simple. Dynamical quarks contribute to Gauss’s law at each point in space. If the quark mass is sent to infinity, so all that remains is one test quark propagating along $\mathcal{C}$, then Gauss's law must include the contribution of that test quark [17,18]. I show in this paper how the sum over states of the test quark generates the Wilson loop, $\mathcal{W}_{\mathcal{C}}$.

I begin with the Lagrangian formalism, where the analysis is transparent, and use that to proceed to the Hamiltonian form. While I consider systems which are independent of time, with the Hamiltonian formalism it is possible to perturb a gauge theory with a gauge-invariant, time-dependent source, and then measure the evolution of Wilson loops in time. This validates computing the "holonomous" potential for the eigenvalues of the thermal Wilson line [19–39], and using it to construct effective theories for the deconfining [40,41] and chiral [42] phase transitions [16,43–67]. Incidentally, it alleviates some concerns [68–78] about holonomous potentials

A Wilson loop alters the Hilbert space because it represents the propagation of a test electric charge. In contrast, the 't Hooft loop [75–77,79–84] represents the propagation of a test magnetic charge, and so does not modify the Hilbert space. I also show how to compute 't Hooft loops in the Hamiltonian formalism.

II. LAGRANGIAN FORMALISM

Consider a quark of mass M as $M \to \infty$. Then we can neglect the spin of the quark, as spin-dependent effects are uniformly suppressed as $\sim 1/M$. Similarly, we can consider either a quark, propagating forward in time, or an antiquark, propagating backwards in time. In either case, since it is too heavy to move, the quark (or antiquark), just sits at some point in space [85]. The gauge invariant effective Lagrangian is then

$$\mathcal{L} = \psi^\dagger D_0 \psi. \tag{3}$$

I assume that ψ lies in the fundamental representation, where the covariant derivative $D_0 = \partial_0 - igA_0$. Later I generalize to arbitrary representations.

I introduce the Wilson line, running from a point x in space-time to y:

$$\mathbf{L}(y; x) = \mathcal{P} \exp\left(ig \int_x^y A_\mu(z) dz^\mu \right), \tag{4}$$

uniformly taking a straight line path between the two. Regardless of the path, the Wilson line transforms homogeneously under a gauge transformation $\mathbf{\Omega}(x)$,

$$\mathbf{L}(y; x) \to \mathbf{\Omega}^\dagger(y) \mathbf{L}(y; x) \mathbf{\Omega}(x). \tag{5}$$

Since $D_0 \mathbf{L}(\vec{x}; t', t) = 0$, the propagator for a test quark sitting at a point $\vec{x}$ is proportional to $\mathbf{L}(\vec{x}; t', t) = \mathbf{L}(\vec{x}, t'; \vec{x}, t)$, using an obvious abbreviated notation.

A test meson is constructed by putting a test quark at one point, $(\vec{x}, 0)$, and tying it with a spatial Wilson line to a test antiquark at $(\vec{0}, 0)$. A rectangular Wilson loop represents the propagation of this test meson up in time, until it is annihilated by a test antimeson.

At nonzero temperature it is possible to construct a gauge invariant operator for a single test quark. In most gauges the gauge fields can be taken to be periodic in imaginary time, $A_\mu(\vec{x}, 1/T) = +A_\mu(\vec{x}, 0)$. The Polyakov loop is the trace of the full thermal Wilson line, which runs from $\tau\colon\ 0 \to 1/T$,

$$\mathbb{P}(\vec{x}) = \mathrm{tr}\mathbf{L}(\vec{x}; 1/T, 0). \tag{6}$$

This is invariant under strictly periodic gauge transformations. In a gauge theory without dynamical quarks, though, the gauge symmetry is $SU(N)/Z(N)$, and it is also necessary to consider global $Z(N)$ transformations. These form the center of the gauge group, $\omega_j = \mathrm{e}^{2\pi i j/N}\mathbf{1}$, $j = 1 \ldots N$, where the ω_j commute with all elements of the group. Then more general gauge transformations are possible, which are periodic only up to a factor of ω_j,

$$\mathbf{\Omega}(\vec{x}, 1/T) = \omega_j \mathbf{\Omega}(\vec{x}, 0). \tag{7}$$

Since the ω_j commute with all group elements, the gauge fields remain strictly periodic. The Polyakov loop, though, transforms linearly,

$$\mathbb{P}(\vec{x}) \to \omega_j \mathbb{P}(\vec{x}). \tag{8}$$

The spatial average of the vacuum expectation value, $\int d^3x \langle \mathbb{P}(\vec{x}) \rangle$, is an order parameter for the spontaneous breaking of a global, one-form [86] $Z(N)$ symmetry [40,41]. Without dynamical quarks, this is an exact symmetry in the confined phase, which is spontaneously broken in the deconfining phase. With dynamical quarks the Polaykov loop is still a gauge invariant operator, but the global $Z(N)$ symmetry is lost.

The expectation value of the Polyakov loop is

$$\langle \mathbb{P} \rangle = \int \frac{d^3x}{V} \int \mathcal{D}A_\mu \mathrm{e}^{-\mathcal{S}(A_\mu)} \langle \mathbb{P}(\vec{x}) \rangle = \omega_j \mathrm{e}^{-\mathcal{F}_\infty/T}. \tag{9}$$

This is the path integral over the gauge field, with action $\mathcal{S}(A_\mu)$, averaged over space, with volume V. Since the Polyakov loop is proportional to the trace of the propagator of a test quark, its expectation value is equal to an overall phase factor, ω_j, which in the deconfined phase, reflects which $Z(N)$ vacuum the theory lies in. The remainder is related to the free energy of a test quark, $\mathcal{F}_\infty$ [68–77], which is then infinite in the confined phase. The complete set of Polyakov loops for a $SU(N)/Z(N)$ gauge theory are $\mathrm{tr}\mathbf{L}^j$, $j = 1 \ldots (N-1)$, and are equivalent to the $N-1$ eigenvalues of the thermal Wilson line. The holonomous potential for the eigenvalues first arises at one loop order, and has been computed to two loop order [19–39].

At nonzero temperature, the potential between a test quark and antiquark is given by the two point function of Polyakov loops,

$$e^{-\mathcal{V}_\infty(\vec{x}-\vec{y})/T} = \langle \mathbb{P}^\dagger(\vec{y})\mathbb{P}(\vec{x})\rangle - |\langle \mathbb{P}\rangle|^2. \tag{10}$$

Another gauge invariant quantity is the thermal Wilson loop,

$$\mathcal{W}_T = \mathrm{tr}\mathbf{L}(\vec{x};1/T,0)\mathbf{L}(\vec{y},\vec{x};1/T)\mathbf{L}(\vec{y};0,1/T)\mathbf{L}(\vec{x},\vec{y};0). \tag{11}$$

Because of the spatial Wilson lines from $\vec{x}$ to $\vec{y}$ at $\tau = 0$ and $1/T$, contributions which do not appear in $\mathcal{V}_\infty(\vec{x})$ enter [87].

III. HAMILTONIAN FORMALISM

It is necessary to transform to a $A_0 = 0$ gauge. I ignore technicalities, such as fixing the residual degrees of freedom for the A_i fields [17,88–90], as these do not affect my analysis. Under a gauge transformation,

$$A_\mu(\vec{x},\tau) \to \frac{1}{-ig}\Omega^\dagger(\vec{x},\tau)D_\mu\Omega(\vec{x},\tau). \tag{12}$$

The gauge transformation which implements $A_0 = 0$ gauge is just $\Omega(\vec{x},\tau) = \mathbf{L}(\vec{x};\tau,0)$. Since in general $\Omega(\vec{x},1/T) \neq \Omega(\vec{x},0)$, when $A_0(\vec{x},\tau) = 0$ the $A_i(\vec{x},\tau)$ are no longer periodic in τ.

In the Hamiltonian formalism, the basic variables are the spatial gauge fields, $\vec{A}$, whose conjugate momenta are the color electric fields, $\vec{E} = \partial_0\vec{A}$. For a quark field ψ the conjugate momentum is $\bar{\psi}$ [17,88–90]. The Hamiltonian density is

$$\mathcal{H}(\vec{x}) = \mathrm{tr}(\vec{E}^2(\vec{x}) + \vec{B}^2(\vec{x})); \tag{13}$$

as the test quark only enters into the Lagrangian as $\bar{\psi}\partial_0\psi$, it drops out of the Hamiltonian.

To ensure the conservation of color electric charge, however, it is still necessary to impose Gauss's law. For this it is convenient to introduce an auxiliary field, $\chi(\vec{x})$:

$$\mathcal{H}_{\mathrm{Gauss}}(\vec{x}) = i\ \mathrm{tr}(\chi(\vec{x})(\vec{D}\cdot\vec{E}(\vec{x}) - g\mathcal{Q}(\vec{x}))), \tag{14}$$

where $\mathcal{Q}^a(\vec{x}) = \psi^\dagger(\vec{x})t^a\psi(\vec{x})$ is the color charge of the test quark and the t^a are the generators in the fundamental representation, $a = 1\ldots(N^2-1)$. Since only particles without spin enter in the effective Lagrangian, it is not necessary to bother with Dirac matrices. The color charge $\mathcal{Q}$ transforms homogeneously in the adjoint representation, $\mathcal{Q}(\vec{x}) \to \Omega^\dagger(\vec{x})\mathcal{Q}(\vec{x})\Omega(\vec{x})$, as does the constraint field $\chi(\vec{x})$ [91]. For a Polyakov loop, the color charge $\mathcal{Q}(\vec{x})$ is a single δ function in $\vec{x}$; for a Wilson loop, there are two δ functions, and so on for more loops.

As discussed by Gervais and Sakita [17], states for test quarks must be included in the partition function. To understand how they contribute, I ask:

How does the exponential of a trace become the trace of an exponential?

That is, how does the test charge $\mathcal{Q}$ in Eq. (14) transform into the Wilson and Polyakov loops of Eqs. (2) and (6)?

The answer is an exercise in the character for a representation of a Lie group [92–95]. This was used originally by Susskind [41,96], and is related to an analysis by Greiner and Müller [94].

A representation $\mathcal{R}$ of the $SU(N)$ group is characterized by a Young tableaux, which are $N-1$ integers, $n_1, n_2\ldots n_{N-1}$, where $n_1 \geq n_2\ldots \geq n_{N-1}$ [92–95]. For the case of $SU(2)$, there is only one row, where n_1 equals the spin, $n_1 = j = 0,1,2\ldots.$

The representations which contribute to the states of the electric field are denoted as $|\mathcal{R}(\vec{x})\rangle$, and that for the test quark as $|\tilde{\mathcal{R}}(\vec{x})\rangle$. While the test quark lies in a fixed representation at a few points in space, all representations contribute to the state space of the electric field at each point in space. For the example of $SU(2)$, all $j(\vec{x})$ contribute to the electric field at each $\vec{x}$, while only a single $\tilde{j}(\vec{x})$ contributes to that of the test quark, at the point where the Polyakov loop lies.

The expectation value of the Polyakov loop is given by

$$\begin{aligned}
\langle \mathbb{P}(\vec{y})\rangle &= \widetilde{\sum}\int \mathcal{D}\chi(\vec{x})\exp\left(-\int d^3x\mathcal{H}_0(\vec{x})/T\right),\\
\mathcal{H}_0(\vec{x}) &= \mathcal{H}(\vec{x}) + i\,\mathrm{tr}\chi(\vec{x})\vec{D}\cdot\vec{E}(\vec{x}) + \mathcal{H}_\mathcal{Q}(\vec{x}),\\
\mathcal{H}_\mathcal{Q}(\vec{x}) &= -i\,\mathrm{tr}\chi(\vec{x})\mathcal{Q}(\vec{x}).
\end{aligned} \tag{15}$$

The sum over states, $\widetilde{\sum}$, includes those for the gauge field, the $\vec{A}(\vec{x})$ and $\vec{E}(\vec{x})$, *and* the states for the test quarks, $\psi(\vec{x})$ and $\bar{\psi}(\vec{x})$. It is also necessary to include a path integral for the constraint field, $\chi(\vec{x})$. Dynamical quarks can be included directly.

I note that it is meaningful to compute the expectation value of a single Polyakov loop in a non-Abelian gauge theory, as the color charge is always screened. At low temperature this happens either because of confinement (without dynamical quarks), or the pair production of mesons (with dynamical quarks). At high temperature, there is always Debye screening [97]. Typical of a system with the spontaneous breaking of a global symmetry, the expectation value of the Polyakov loop is only well defined after introducing an appropriate [99] external source for the corresponding field, and then tuning that source to zero.

It is easy to perform the sum over states for the Polyakov loop in Eq. (15), as the only quantum number carried by the test quark is that for color electric charge. Since the color charge transforms homogeneously under gauge transformations, I can assume that it is a diagonal matrix. Then if the quark and antiquark have color 1, $\mathcal{Q}(\vec{x})^a = t^a_{11}\delta^3(\vec{x}-\vec{y})$, where $\vec{y}$ is the position of the loop, and contributes to $\mathbb{P}(\vec{x})$ as $\sim \exp(ig\chi^a t^a_{11})\delta^3(\vec{x}-\vec{y})$. If the quark and antiquark have color 2, then the contribution to $\mathbb{P}(\vec{x})$ is $\sim \exp(ig\chi^a t^a_{22})\delta^3(\vec{x}-\vec{y})$, and so on.

Thus the trace over states of the test quark is just a trace over color,

$$\langle\mathbb{P}(\vec{y})\rangle = \sum\int\mathcal{D}\chi(\vec{x})\mathrm{e}^{-\int\mathcal{H}_0/T}\mathrm{tr}\,\mathrm{e}^{ig\chi(\vec{y})}. \quad (16)$$

Having summed over the states for the test quark and antiquark, the remaining sum, $\sum$, is only for the $\vec{A}$ and $\vec{E}$, along with the path integral over the constraint field, $\chi(\vec{x})$.

From this derivation, it is apparent that $\chi(\vec{x})$ corresponds to the timelike component of the gauge potential in the Lagrangian formalism, $A_0(\vec{x})$ [17,88–90]. The transformation from $A_0 = 0$ gauge in the Lagrangian formalism is given by identifying the gauge transformation $\Omega(\vec{x}, 1/T) = \mathbf{L}(\vec{x};, 1/T, 0)$ with $\exp(ig\chi(\vec{x}))$. After averaging over the spatial volume, this agrees with Eq. (9).

For the thermal Wilson loop of Eq. (11), it is necessary to add states for both the test quark at $\vec{x}$, and the test antiquark, at $\vec{y}$. The character representation once again gives a product of exponentials, connected by spatial Wilson lines,

$$\mathcal{W}_T = \mathrm{tr}\,\mathrm{e}^{ig\chi(\vec{x})}\mathbf{L}(\vec{y};\vec{x})\mathrm{e}^{-ig\chi(\vec{y})}\mathbf{L}(\vec{x};\vec{y}). \quad (17)$$

The generalization to higher representations of the test quark is direct, while the generator is given by a bird track diagram, Eq. (4.35) of Cvitanovic [93]. The sum over all color states is given by summing over all of the legs of the bird track.

In the Lagrangian formalism, the holonomous potential for the eigenvalues of the thermal Wilson line is computed by expanding about a constant, background field $A_0 \neq 0$ [19–39]. In the Hamiltonian formalism, nontrivial holonomy is related to $\mathrm{e}^{ig\chi(\vec{x})}$, which enters as an imaginary chemical potential for the color charge.

In the gauge theory without dynamical quarks, the holonomous potential manifestly exhibits the global $Z(N)$ degeneracy for the $SU(N)/Z(N)$ theory. With dynamical quarks, however, depending upon the representation of the quarks and the color, it is possible to have metastable states with negative pressure [68–71,74]. This occurs because the zero of the potential for nontrivial holonomy has an absolute significance, as the pressure with a vanishing holonomy. However, while a bubble of such a metastable state can have negative pressure, it only lasts as long as it takes the surface of the bubble to collapse upon itself, decaying through cavitation [100,101].

IV. ’t HOOFT LOOPS

Wilson loops represent the propagation of test electric charge. ’t Hooft first constructed a dual order parameter to the Wilson loop, which represents the propagation of a test magnetic charge [79,80]. The Wilson and ’t Hooft loops satisfy a commutation law, which in vacuum excludes the simultaneous confinement of electric and magnetic charges. The commutation law follows by considering the Wilson loop as the propagator for a test electric charge: as a tiny Wilson loop encircles a ’t Hooft loop, by definition the phase of a test charge (in the fundamental representation) changes by $\mathrm{e}^{2\pi i/N}$.

At nonzero temperature in the $SU(N)/Z(N)$ gauge theory, due to the global $Z(N)$ symmetry there are N degenerate vacua in the deconfined phase. At high temperature, it is possible to consider a box which is long in one spatial direction, and to compute the interface tension between a $Z(N)$ vacuum at one end of the box, and a different $Z(N)$ vacuum at the other. This interface tension can be computed semiclassically [21–23] from the holonomous potential [24–39]. Korthals-Altes, Kovner, and Stephanov showed that the interface tension is equivalent to an area law for the spatial ’t Hooft loop [75,76]. Numerical simulations on the lattice have measured how the ’t Hooft loop changes with temperature [77,81,82]. See also Refs. [83,84].

In the Hamiltonian form, a domain wall can be constructed by using a constant χ field, corresponding to constant A_0 in the Lagrangian formalism. The simplest model to study is the Abelian theory in $1+1$ dimensions, where the object analogous to a domain wall in higher dimensions is a soliton. Since gauge fields have no physical degrees of freedom in two spacetime dimensions, it is necessary to add dynamical fermions. Adding massless fields gives the Schwinger model, but this theory behaves contrary to naive expectation, as even fractional test charges are screened by dynamical fields with integral charge [102–104].

If the dynamical fields are massive, though, then dynamical fermions with integral charge do not screen fractional test charges [102–104]. Smilga first noted the existence of thermal solitons in the massive Schwinger model [71]. In the Euclidean Lagrangian, one takes a background, classical field $A_0^{\mathrm{cl}} = 2\pi Tq/e$, where e is the Abelian coupling constant; in the Hamiltonian form, one takes a similar background for the constraint field, χ. As q is a periodic variable, a thermal soliton interpolates from $q = 0$ at $x = -\infty$ to $q = 1$ at $x = +\infty$. At high temperature, $T \gg m$, the potential for q generated at one loop order is $\sim T^2$ times a periodic function of q, Eq. (3.9) of Ref. [71]. At low temperature, the potential is Boltzmann suppressed, $\sim \mathrm{e}^{-m/T}$, and vanishes smoothly as $T \to 0$.

I suggest that such solitons are stable. At $T \neq 0$ imaginary time is topologically equivalent to a torus, S^1. As q is a periodic variable, then, mappings from space onto q are determined by the first homotopy group, $\pi_1(S^1) = Z$, which is the set of the integers.

Smilga and others argued that thermal solitons are unphysical [71–74], I suggest that they represent new, collective excitations at $T \neq 0$, which evaporate smoothly as $T \to 0$. This can be studied numerically at nonzero temperature in real time, using either tensor networks on a classical computer [105–108], or even with the noisy intermediate-scale quantum computers which are available at present. This is similar to studying the screening of background electric fields at nonzero θ [109–118].

There are many other problems which can be addressed with the formalism developed here. In particular, deep inelastic scattering is usually described by the propagation of timelike Wilson lines [18]. My approach can be adapted to the light front directly [107,108,119], especially using quantum computers [120–122].

Lastly, if thermal solitons are stable in $1+1$ dimensions, presumably thermal domain walls exist in $3+1$ dimensions. In the early Universe, they can arise from the $U(1)$ of electromagnetism, when regions which are causally disconnected from one another first come in contact. They persist until the thermal potential for the domain wall of the lightest electrically charged particle, which is the electron, is Boltzmann suppressed. As this temperature is presumably below that for nucleosynthesis, and as domain walls dominate the energy density of the universe, such thermal $U(1)$ domain walls could be of cosmological consequence.

ACKNOWLEDGMENTS

This work was inspired by a talk which Tom Cohen gave virtually at the Yukawa Institute for Theoretical Physics, during a workshop on the “QCD phase diagram and lattice QCD,” YITP-W-21-09. I thank him, M. Creutz, A. Florio, L. Glozman, C. Korthals-Altes, S. Mukherjee, P. Petreczky, O. Philipsen, E. Poppitz, A. Smilga, and I. Zahed for discussions. This research was supported by the U.S. Department of Energy under Contract No. DE-SC0012704. I was also led to consider this problem because of the support of the U.S. Department of Energy, Office of Science, National Quantum Information Science Research Centers, Co-design Center for Quantum Advantage (C^{2}QA) under Contract No. DE-SC0012704.

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