Semiclassical probability distribution function for finite-temperature field theory

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We study semiclassical methods for evaluating the canonical probability distribution function $\rho(\phi)=\langle\phi|\exp(-\beta H)|\phi\rangle$ in field theory for systems in thermodynamic equilibrium. Field configurations which dominate the semiclassical distribution function are interpretable as "finite-temperature most-probable escape paths" (FTMPEP's) in field space and are related to the recently discovered caloron solutions, which are known to partially dominate the semiclassical partition function $Z=\int D\phi\,\rho(\phi)$. We present a semiclassical path-integral approximation for the distribution function and also discuss a Hartree self-consistent field approximation.

I. INTRODUCTION

Recently, new interest has developed in finite-temperature non-Abelian gauge theory (e.g., the Yang-Mills theory[1,2]). This is due in part to a better understanding of the zero-temperature semiclassical vacuum structure of such theories. The classical solutions of the Euclidean field equations, the so-called "instantons,"[3-6] are now generally considered to be interpolating field configurations for tunnelings between topologically distinct classical vacuums.[7-13] These Euclidean solutions have been shown to be the "most-probable escape paths" (MPEP's) in field space for tunnelings between vacuums,[12,13] that is, they are the paths with the largest WKB tunneling amplitude. Consequently, the instantons dominate the Euclidean vacuum-to-vacuum transition amplitude W_E (Ref. 2) in the nonzero-winding-number sectors and are distinctly nonperturbative in nature. The most general instanton solutions have been found,[14] and the first quantum, or "one-loop", correction to instanton effects in W_E has been computed.[8,15] The one-loop correction is interpretable as arising from tunneling paths in field space near the MPEP.[13]

The vacuum-to-vacuum transition amplitude W_E is the zero-temperature limit of the partition function Z. Noting the similarity between Euclidean field theory and the "imaginary-time" formulation of equilibrium thermodynamics,[16] Harrington and Shepard[17] argued for the existence of Euclidean solutions which would dominate the semiclassical Yang-Mills partition function. They later constructed such solutions, dubbed "calorons",[18] by taking the zero-temperature multi-instanton solutions,[4,5] and aligning the instantons so that they are periodic in Euclidean time τ with period $\hbar\beta$, that is,

$$A_\mu^a(x,\tau)=A_\mu^a(x,\tau+\hbar\beta)\,, \tag{1.1}$$

which is the usual periodicity condition for finite-temperature Bose fields.[16] The caloron reduces to an instanton in the zero-temperature limit. The thermodynamics of the pure Yang-Mills gas has been discussed by Harrington and Shepard,[19] while Bilic and Miller[20] have considered the thermodynamics of quantum-chromodynamic (QCD) systems. In both cases the so-called "dilute-gas approximation"[21] was employed. Batakis and Lazarides[22] have studied the mathematical structure of the gauge-theory vacuum at finite temperatures. Gross, Pisarski, and Yaffe[23] have presented a very thorough review of finite-temperature QCD and instanton effects. A summary article by Shepard[24] on the high-temperature Yang-Mills gas has also appeared.

Recently, Chang and the present author observed that such periodic Euclidean solutions are physically interpretable as "finite-temperature most-probable escape paths" (FTMPEP's).[25] The purpose of this paper is to explain this connection and use it to develop a semiclassical approximation for the canonical probability distribution function $\rho(\phi)=\langle\phi|\exp(-\beta H)|\phi\rangle$ in field theory for systems in thermodynamic equilibrium. We are interested in the distribution function because all expectation values as well as the partition function, $Z=\int D\phi\,\rho(\phi)$, can be calculated from it.

The plan of this paper is as follows. In Sec. II, after briefly reviewing the tunneling concept of MPEP's,[26] we consider finite-temperature tunneling paths in a multidimensional quantum-mechanical system and show that finite-temperature MPEP's are periodic Euclidean paths which maximize the semiclassical probability distribution function. This distinguishes FTMPEP's from calorons. The latter only partially dominate the partition function in general. We argue that FTMPEP's are necessary to fully understand the semiclassical statistical mechanics of a system. We close Sec. II by obtaining the one-loop correction to the FTMPEP distribution function.

This is done by considering tunneling paths near the FTMPEP generated by combined quantum and thermal fluctuations.

To implement the FTMPEP formalism of Sec. II efficiently, we present a Euclidean, or imaginary-time, path-integral approximation for the distribution function in Sec. III, demonstrating that it reproduces the FTMPEP distribution function of Sec. II. In Appendix A we show that this semiclassical approximation yields the exact distribution function for the simple harmonic oscillator.

In Sec. IV we generalize the path-integral method of Sec. III to field theory and obtain the semiclassical probability distribution function for a scalar field theory and for a pure Yang-Mills gauge theory. In Appendices B and C, we show that the semiclassical approximation yields the exact distribution functions and partition functions for a free scalar field theory and a pure Abelien gauge theory, respectively.

In Sec. IV we discuss an alternate method to the Euclidean loop expansion for obtaining higher-order corrections to the semiclassical distribution function. The method is a Hartree self-consistent field approximation and is essentially an improved way of obtaining the FTMPEP with corrections from neighboring paths included. We derive a Hartree equation of motion for the improved FTMPEP and a Hartree fluctuation equation. We also suggest an iterative scheme for solving these equations self-consistently.

We conclude the paper in Sec. VI with a discussion of our results and suggestions for further study and possible applications.

II. FINITE-TEMPERATURE MOST-PROBABLE ESCAPE PATHS

The idea of most-probable escape paths (MPEP (MPEP's) was first introduced into the multidimensional WKB method by Banks, Bender, and Wu.[26] In one dimension, the WKB method is a relatively simple approximation for obtaining tunneling amplitudes. In principle, the multidimensional tunneling problem can be solved in the WKB approximation by the obvious extension of the one-dimensional WKB equations to higher dimensions. In general, however, the resulting differential equations are intractable unless one can reduce them to an approximate one-dimensional problem.

In classical mechanics, the principle of least action determines the classical paths of a Hamiltonian system.[27] Banks, Bender, and Wu[26] noted that if a path in a tunneling region could be found such that the first variations of the Euclidean action vanished in all directions orthogonal to the path, then semiclassically the tunneling problem would become approximately one dimensional. If along such a path the Euclidean action is a minimum, then the amplitude of the tunneling wave function is a maximum, hence the name most-probable escape path. Tunneling occurs predominantly through small tubes around such MPEP's in multidimensional systems.

The MPEP method was later generalized by Bitar and Chang to study vacuum tunneling in gauge theory.[12,13] They showed that the instantons[3-6] are MPEP's in function space for tunnelings between topologically distinct classical vacuums, and that tunneling paths near the MPEP were responsible for the first quantum correction, calculated earlier by 't Hooft,[8] to the tunneling amplitude. Bitar and Chang also obtained explicit ground-state wave functionals in the neighborhood of an MPEP. Along an MPEP in field space, the amplitude of the tunneling wave functional is a maximum.

The MPEP concept can be further generalized to finite-temperature systems in order to calculate the semiclassical probability distribution function. Let us consider an N-dimensional quantum-mechanical system $[x \equiv (x_1, x_2, \ldots, x_N)]$ in thermodynamic equilibrium with Lagrangian

$$L = \tfrac{1}{2} m (dx/dt)^2 - V(x) . \tag{2.1}$$

All of the equilibrium thermodynamic information about the system is contained in the statistical density matrix $\rho(x, x')$.[28] The diagonal elements $\rho(x)$ provide the probability distribution function which gives the probability of finding a particle at position x. The exact form of $\rho(x)$ is

$$\rho(x) = \langle x | e^{-\beta H} | x \rangle = \sum_n e^{-\beta E_n} | \psi_n(x) |^2 , \tag{2.2}$$

where $\psi_n(x)$ and E_n are the energy eigenfunctions and eigenvalues, respectively, for the system. We can use the WKB approximation to find the wave functions $\psi_n(x)$ in the classically allowed regions $E > V$ and the tunneling regions $E < V$ and then match the solutions at the turning points. For a system with more than one degree of freedom, this will quickly develop into a complicated task. If the relevant actions in the system are large compared to $\hbar$, we may replace the discrete energy levels E_n by an energy continuum. (Strictly speaking we are considering the limit $\beta\hbar \to 0$.) This semiclassical approximation greatly simplifies the evaluation of $\rho(x)$. We will return to discuss the validity of this approximation shortly.

For the regime $E > V$, the distribution function $\rho(x)$ will be proportional to the Boltzmann factor $e^{-\beta E}$, while for $E < V$ it will be proportional to $e^{-\beta E}$ multiplied by the WKB barrier penetration factor along the MPEP at energy E. For the MPEP connecting the turning point x_E and a point

x in the tunneling region, the distribution function is (modulo normalization factors and quantum corrections)

$$\rho(x)=\exp\left\{-\beta E-\frac{2}{\hbar}\int_{\lambda(x_E)}^{\lambda(x)}d\lambda\{2m(\lambda)[V(\lambda)-E]\}_{\mathrm{CL}}^{1/2}\right\}, \tag{2.3}$$

where the integral is along the MPEP $x_{\mathrm{CL}}(\lambda)$ [CL means classical in the context of Eq. (2.8) below]. The symbol λ is a path parameter and $m(\lambda)\equiv m(dx/d\lambda)^2$. In this parametrization, the Lagrangian is

$$L=\tfrac{1}{2}m(\lambda)(d\lambda/dt)^2-V(\lambda). \tag{2.4}$$

The Boltzmann factor decreases with energy while the tunneling factor increases. The energy E in Eq. (2.3) can be varied to find the "most-probable energy," that is, the energy that maximizes the right-hand side of Eq. (2.3).

The MPEP $x_{\mathrm{CL}}(\lambda)$ with fixed end points x and x_E is determined by maximizing the WKB tunneling amplitude. The relevant variational equation is

$$\delta\left(\int_{\lambda(x_E)}^{\lambda(x)}d\lambda\{2m(\lambda)[V(\lambda)-E]\}^{1/2}\right)=0 \tag{2.5}$$

or

$$\left[\frac{2(V-E)}{m(\lambda)}\right]^{1/2}m\frac{dx_i}{d\lambda}\delta x_i\Big|_{\lambda(x_E)}^{\lambda(x)}+\int_{\lambda(x_E)}^{\lambda(x)}d\lambda\left(-\frac{d}{d\lambda}\left\{\left[\frac{2(V-E)}{m(\lambda)}\right]^{1/2}m\frac{dx_i}{d\lambda}\right\}+\left[\frac{2m(\lambda)}{V-E}\right]^{1/2}\left(\frac{1}{2}\frac{\partial V}{\partial x_i}\right)\right)\delta x_i=0. \tag{2.6}$$

The surface term vanishes since $\delta x_i(\lambda(x))=0$ and $V(\lambda(x_E))-E=0$. Making a change of parametrization from λ to τ defined by

$$\frac{d\lambda}{d\tau}=\left(\frac{2[V(\lambda)-E]}{m(\lambda)}\right)^{1/2}, \tag{2.7}$$

we obtain from Eq. (2.6) the classical Euclidean equations of motion for the MPEP, $x_{\mathrm{CL}}(\tau)$,

$$m\frac{d^2x_i}{d\tau^2}=+\frac{\partial V(x)}{\partial x_i},\quad i=1,2,\ldots,N. \tag{2.8}$$

The variation of Eq. (2.3) with respect to E determines the energy and the associated turning point which maximize $\rho(x)$. The appropriate variational equation is

$$\delta_E\left(\beta E+\frac{2}{\hbar}\int_{\lambda(x_E)}^{\lambda(x)}d\lambda\{2m(\lambda)[V(\lambda)-E]\}_{\mathrm{CL}}^{1/2}\right)=0 \tag{2.9}$$

or

$$\hbar\beta-\int_{\lambda(x_E)}^{\lambda(x)}d\lambda\left[\frac{2m(\lambda)}{V-E}\right]^{1/2}+2[2m(\lambda)(V-E)]^{1/2}\frac{\partial\lambda(x)}{\partial E}\Big|_{\lambda(x)}-2[2m(\lambda)(V-E)]^{1/2}\frac{\partial\lambda(x_E)}{\partial E}\Big|_{\lambda(x_E)}=0. \tag{2.10}$$

Since the end point x has no dependence on the energy, $\partial\lambda(x)/\partial E=0$. At the turning point x_E, $V-E=0$. Equation (2.10) then becomes

$$\hbar\beta=\int_{\lambda(x_E)}^{\lambda(x)}d\lambda\left[\frac{2m(\lambda)}{V(\lambda)-E}\right]_{\mathrm{CL}}^{1/2}. \tag{2.11}$$

Equations (2.8) and (2.11) together determine the MPEP and turning point for a given β and x. We call an MPEP satisfying these two equations for finite β a FTMPEP. Substituting the FTMPEP into Eq. (2.3) yields the semiclassical distribution function $\rho(x)$ for the system.

Equation (2.11) allows us to relate the above finite-temperature MPEP formalism to the imaginary-time formulation of equilibrium thermodynamics.[16,28-32] In the latter, one considers the particle of mass m to be moving in the "inverted potential" $V_I=-V(x)$ (Fig. 1). The MPEP $x_{\mathrm{CL}}(\tau)$ becomes a classically allowed path with

$$V-E=E_I-V_I=\tfrac{1}{2}m(dx/d\tau)^2=\tfrac{1}{2}mv^2, \tag{2.12}$$

where v is the velocity in the inverted potential system. This classically allowed path clearly obeys the same Euclidean equations of motion as in Eq. (2.8) so that we have

$$\hbar\beta=\int_{\lambda(x_E)}^{\lambda(x)}d\lambda\left[\frac{2m(\lambda)}{V(\lambda)-E}\right]_{\mathrm{CL}}^{1/2}=2\int_{x_E}^{x}\frac{dx_{\mathrm{CL}}}{v}=\oint\frac{dx_{\mathrm{CL}}}{v}. \tag{2.13}$$

Thus the total "time" needed for the particle to travel from x to x_E and back to x is $\hbar\beta$, and the Euclidean solution $x_{\mathrm{CL}}(\tau)$ is periodic in τ with period $\hbar\beta$. The FTMPEP concept has led us naturally to periodic Euclidean solutions and provides a simple physical realization of them.

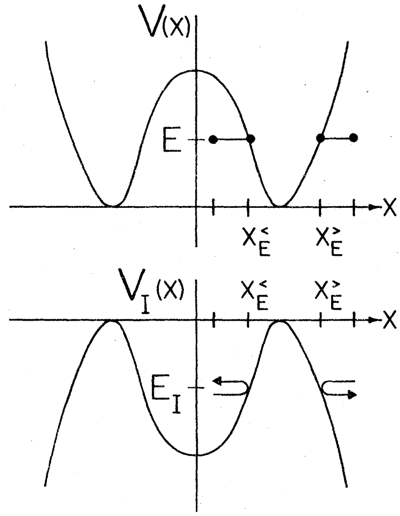

FIG. 1. Top: The dumbbells represent two possible FTMPEP's at energy E connecting the turning points $x_E^<$ and $x_E^>$ to arbitrary points x in the tunneling regions. Bottom: The hairpins represent the two classically allowed Euclidean paths at energy $E_I = -E$ in the inverted potential $V_I = -V(x)$ corresponding to the FTMPEP's in the top drawing.

Rather than giving the dominant contribution to the partition function Z alone as the calorons[18,30] do, FTMPEP's dominate the distribution function $\rho(x)$, from which all expectation values and Z itself can be calculated. In this sense, the FTMPEP is a more general concept than the caloron.

From the above discussion, it would seem that $\rho(x)$ can be calculated semiclassically for all x by considering tunneling paths alone, without any mention of classically allowed Minkowski paths. This is indeed true semiclassically, as Fig. 1 illustrates schematically in one dimension. For any given time $\hbar\beta$ and position x, there always exists a Euclidean path of some energy $E_I = -E$ such that the particle travels from x to x_E and back in time $\hbar\beta$.

This last point brings us back to the energy continuum approximation we made at the beginning of this discussion. If the energy spectrum is discrete, then for a given $\hbar\beta$ and x, the FTMPEP with energy E will generally lie between allowed levels. Tunnelings will then occur most often via the energy levels just above and just below the FTMPEP. Using the FTMPEP effectively averages the tunneling contributions from these nearby energy levels and gives us a reasonable approximation to $\rho(x)$. Consequently, our semiclassical method is expected to be useful even in those cases where the relevant actions are comparable to $\hbar$.

Regarding the relationship between calorons and FTMPEP's, it is important to realize that, in general, calorons alone are not sufficient to produce a semiclassical partition function which reduces to the complete classical partition function in the limit of vanishing $\hbar\beta$. This is because the calorons obey the free periodic boundary condition $x_{CL}(\tau) = x_{CL}(\tau + \hbar\beta)$ rather than the constrained periodic boundary conditions $x_{CL}(0) = x_{CL}(\hbar\beta) = x$ for an FTMPEP. As Dolan and Kiskis[31] noted, the former boundary condition implies, semiclassically, that $dx_{CL}(\tau)/d\tau = dx_{CL}(\tau + \hbar\beta)/d\tau$, i.e., the caloron is a closed periodic orbit in Euclidean phase space. For example, in the symmetric double-well potential in Fig. 2, such periodic orbits correspond to a particle oscillating between the turning points $\pm x_E$. As recognized earlier by Harrington,[30] the caloron solution becomes static in this model above a certain critical temperature. At this temperature, the caloron oscillation amplitude vanishes, corresponding to the particle undergoing simple harmonic motion in the bottom of the inverted potential well in Fig. 2. On the other hand, FTMPEP solutions clearly remain dynamic for all temperatures. Thus calorons only partially dominate the partition function in general. The FTMPEP solutions are necessary for a complete understanding of the semiclassical statistical mechanics of a system.

Having found the leading semiclassical contribution to the distribution function by using the FTMPEP picture, it is natural to try to calculate the one-loop correction to $\rho(x)$ by similar physical arguments. The one-loop correction is due to paths near the FTMPEP which are generated by combined quantum and thermal fluctuations. For notational convenience, we denote for any arbitrary path $x(\lambda)$ connecting x_E and x the quan-

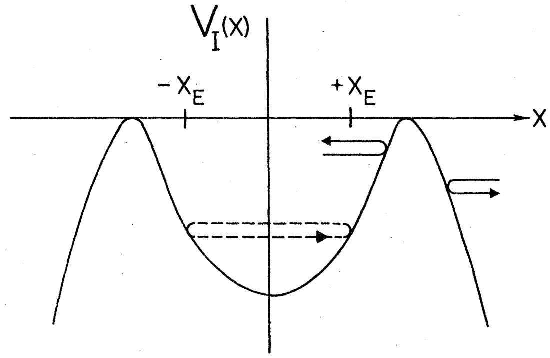

FIG. 2. The two solid hairpins represent FTMPEP's. The dashed closed loop represents a caloron and corresponds to a particle oscillating between the turning points $\pm x_E$ in the inverted-potential system.

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$$R(x)=\int_{\lambda(x_E)}^{\lambda(x)} d\lambda\{2m(\lambda)[V(\lambda)-E]\}^{1/2}, \qquad (2.14)$$

which appears in Eqs. (2.3) and (2.5). For an arbitrary variation $\eta(\lambda)\equiv x(\lambda)-x_{\rm CL}(\lambda)$ away from the FTMPEP $x_{\rm CL}(\lambda)$, $R(x)$ takes the form, to $O(\eta^2)$,

$$R(x)=R_{\rm CL}(x)+\tfrac{1}{2}\int_0^{\hbar\beta/2} d\tau\,\eta_i(\tau)\left(-\delta_{ij}m\frac{d^2}{d\tau^2}+\frac{\partial^2 V(x_{\rm CL})}{\partial x_i\partial x_j}\right)\eta_j(\tau), \qquad (2.15)$$

where the τ parametrization in Eq. (2.7) has been used.

To obtain the contribution to $\rho(x)$ from all such neighboring paths we sum over all fluctuations, $\eta(\tau)$, around $x_{\rm CL}(\tau)$ with $\eta(0)=\eta(\hbar\beta)=0$. The distribution function in Eq. (2.3) with the inclusion of the one-loop correction becomes

$$\rho(x)=\exp\left(-\beta E-\frac{2}{\hbar}\int_{\lambda(x_E)}^{\lambda(x)} d\lambda\{2m(\lambda)[V(\lambda)-E]\}_{\rm CL}{}^{1/2}\right)\oint_0^0 D\eta(\tau)\exp\left\{-\frac{1}{2\hbar}\int_0^{\hbar\beta} d\tau\,\eta_i(\tau)\left[-\delta_{ij}m\frac{d^2}{d\tau^2}+\frac{\partial^2 V(x_{\rm CL})}{\partial x_i\partial x_j}\right]\eta_j(\tau)\right\}$$

$$=\left[\det\left(-\delta_{ij}m\frac{d^2}{d\tau^2}+\frac{\partial^2 V(x_{\rm CL})}{\partial x_i\partial x_j}\right)\right]^{-1/2}\exp\left(-\beta E-\frac{2}{\hbar}\int_{\lambda(x_E)}^{\lambda(x)} d\lambda\{2m(\lambda)[V(\lambda)-E]\}_{\rm CL}{}^{1/2}\right), \qquad (2.16)$$

where the path integral is over all paths $\eta(\tau)=x(\tau)-x_{\rm CL}(\tau)$ with $\eta(0)=\eta(\hbar\beta)=0$.

The one-loop correction due to Gaussian fluctuations in Eq. (2.16) has the familiar form of a functional determinant. Within the FTMPEP framework, both the leading semiclassical contribution and the one-loop correction to the distribution function are easily understood physically, without recourse to the imaginary-time formulation of thermodynamics. The imaginary-time formulation, however, is a very convenient way of implementing the FTMPEP method. In Sec. III we present such an imaginary-time formulation via path integrals and show that it reproduces the FTMPEP result in Eq. (2.16) for $\rho(x)$.

III. PATH-INTEGRAL FORMULATION OF THE DISTRIBUTION FUNCTION

In Sec. II we saw that FTMPEP's are tunneling paths which make the dominant contribution to the semiclassical probability distribution function. Combined quantum and thermal Gaussian fluctuations around such paths produce the one-loop correction to the distribution function. In this section we show that the semiclassical path-integral expression for the distribution function is equivalent to the FTMPEP form.

Consider a system with N degrees of freedom described by a Lagrangian $L(x,\dot x)$ $[x\equiv\{x_1,x_2,\ldots,x_N\}]$. The diagonal matrix elements of the statistical density operator, $\rho=\exp(-\beta H)$, in the coordinate representation give the probability distribution function $\rho(x)$. The Feynman path-integral form for the distribution function is[28,32]

$$\rho(x)=N(\beta)\int_{x(0)=x(\hbar\beta)=x} Dx(\tau)\times\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\,L_{\rm eff}(x(\tau),\dot x(\tau))\right], \qquad (3.1)$$

where $N(\beta)$ is a β-dependent measure normalization factor independent of the potential and is easily determined later by using the known distribution function for a free particle. Of course, $N(\beta)$ also occurs in the partition function, $Z=\int\rho(x)dx$, and hence divides out in all expectation values. The effective finite-temperature Lagrangian (obtained by replacing d/dt with $id/d\tau$ in the conventional Lagrangian) is

$$L_{\rm eff}(x,\dot x)=-[\tfrac{1}{2}m\dot x_i\dot x_i+V(x)], \qquad (3.2)$$

where $\dot x=dx/d\tau$.

If the characteristic actions in the system are large with respect to $\hbar$, we can evaluate $\rho(x)$ in Eq. (3.1) semiclassically by doing the path integral within the stationary phase approximation. (As in Sec. II, we expect this to be a reasonable approximation even when this caveat is not strictly satisfied.) The path which makes the exponential argument stationary is determined by the variational equation

$$\delta\left[\int_0^{\hbar\beta} d\tau\,L_{\rm eff}(x(\tau),\dot x(\tau))\right]=0. \qquad (3.3)$$

We are then left with the Euclidean equations of motion

$$m\frac{d^2x_i(\tau)}{d\tau^2}=+\frac{\partial V(x(\tau))}{\partial x_i(\tau)},\quad i=1,\ldots,N \tag{3.4}$$

with periodic boundary conditions $x(0)=x(\hbar\beta)=x$. The solution of Eq. (3.4) is clearly the FTMPEP $x_{\rm CL}(\tau)$ obtained in Sec. II using physical arguments.

To include the contribution to $\rho(x)$ from combined quantum and thermal fluctuations around $x_{\rm CL}(\tau)$ we write a nearby path as

$$x(\tau)=x_{\rm CL}(\tau)+\eta(\tau),\quad \eta(0)=\eta(\hbar\beta)=0\,. \tag{3.5}$$

Using this in Eq. (3.2) and integrating over τ, gives to $O(\eta^2)$

$$\int_0^{\hbar\beta}d\tau\, L_{\rm eff}(x(\tau),\dot x(\tau))$$

$$=\int_0^{\hbar\beta}d\tau\, L_{\rm eff}(x_{\rm CL}(\tau),\dot x_{\rm CL}(\tau))$$

$$-\frac{1}{2}\int_0^{\hbar\beta}\eta_i\left(-\delta_{ij}m\frac{d^2}{d\tau^2}+\frac{\partial^2V(x_{\rm CL})}{\partial x_i\partial x_j}\right)\eta_j\,d\tau\,. \tag{3.6}$$

Substituting this expression into Eq. (3.1), we obtain for $\rho(x)$ in the semiclassical approximation

$$\rho(x)=N(\beta)\oint_0^0 D\eta\exp\left[\frac{-1}{2\hbar}\int_0^{\hbar\beta}d\tau\,\eta_i\left(-\delta_{ij}m\frac{d^2}{d\tau^2}+\frac{\partial^2V(x_{\rm CL})}{\partial x_i\partial x_j}\right)\eta_j\right]\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\, L_{\rm eff}(x_{\rm CL}(\tau),\dot x_{\rm CL}(\tau))\right] \tag{3.7}$$

$$=N(\beta)\left[\det\left(-\delta_{ij}\frac{d^2}{d\tau^2}+\frac{1}{m}\frac{\partial^2V(x_{\rm CL})}{\partial x_i\partial x_j}\right)\right]^{-1/2}\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\, L_{\rm eff}(x_{\rm CL},\dot x_{\rm CL})\right] \tag{3.8}$$

$$=N(\beta)\prod_n\left(\frac{1}{\omega_n}\right)\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\, L_{\rm eff}(x_{\rm CL},\dot x_{\rm CL})\right]. \tag{3.9}$$

The eigenvalues ω_n are determined from the equations

$$\left(-\delta_{ij}\frac{d^2}{d\tau^2}+\frac{1}{m}\frac{\partial^2V(x_{\rm CL})}{\partial x_i\partial x_j}\right)\eta_j^{(n)}(\tau)=\omega_n^{\,2}\eta_i^{(n)}(\tau)\,, \tag{3.10}$$

with $\eta^{(n)}(0)=\eta^{(n)}(\hbar\beta)=0$.

We can now determine the factor $N(\beta)$. The density matrix for a free particle in N dimensions is[28]

$$\rho_{\rm free}(x,x';\beta)=\left(\frac{m}{2\pi\hbar^2\beta}\right)^{N/2}\exp\left(-\frac{m}{2\pi\hbar^2\beta}\,|x-x'|^2\right), \tag{3.11}$$

where the prefactor is chosen such that

$$\rho(x,x';0)=\delta^N(x-x')\,, \tag{3.12}$$

which is the classical distribution function. For a free particle, Eq. (3.8) reduces to

$$\rho(x)=N(\beta)[\det(-\delta_{ij}d^2/d\tau^2)]^{-1/2}\,. \tag{3.13}$$

We may thus identify

$$N(\beta)=(m/2\pi\hbar^2\beta)^{N/2}[\det{}'(-\delta_{ij}d^2/d\tau^2)]^{1/2}\,. \tag{3.14}$$

In summary, we have for the semiclassical distribution function

$$\rho(x)=\left[\left(\frac{m}{2\pi\hbar^2\beta}\right)^N\frac{\det{}'(-\delta_{ij}d^2/d\tau^2)}{\det\left(-\delta_{ij}\dfrac{d^2}{d\tau^2}+\dfrac{1}{m}\dfrac{\partial^2V(x_{\rm CL})}{\partial x_i\partial x_j}\right)}\right]^{1/2}\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\, L_{\rm eff}(x_{\rm CL},\dot x_{\rm CL})\right]. \tag{3.15}$$

We have intentionally not put a prime on the determinant in the denominator of Eqs. (3.8) and (3.15). This is to remind us that there may be additional zero modes due to the symmetries of the full Lagrangian $L_{\rm eff}=-\frac{1}{2}m\dot x^2-V(x)$. Such modes give overall factors which are implicit in the unprimed determinant and product $\prod_n(1/\omega_n)$. We remark that if there is more than one path, $x_{\rm CL}(\tau)$, satisfying Eq. (3.4), then $\rho(x)$ in Eq. (3.15) becomes a sum of terms, one from each path.

Using the τ parametrization in Eq. (2.7), one sees that the exponents in Eqs. (2.16) and (3.15) are identical. Equation (3.15) thus agrees with the result found for $\rho(x)$ in Sec. II using the FTMPEP picture. The imaginary-time path-integral formulation is a useful tool for calculating $\rho(x)$ semiclassically for systems with many degrees of freedom. One can, of course, consider higher-order corrections to $\rho(x)$ by continuing the perturbation expansion beyond second order. In Appendix A we show that Eq. (3.15) gives the exact distribution function for the one-dimensional simple harmonic oscillator. This is not surprising since the Lagrangian is quadratic in x and $\dot{x}$ so there are no corrections to $\rho(x)$ beyond Gaussian fluctuations.

IV. SEMICLASSICAL EVALUATION OF THE DISTRIBUTION FUNCTION IN FIELD THEORY

In Sec. III we obtained a semiclassical path-integral approximation to the probability distribution function for a system with N degrees of freedom in thermodynamic equilibrium. Because of its generality, we can straightforwardly extend the formulation to finite-temperature field theory.

In field theory each field configuration ϕ represents a point in the infinite-dimensional function space of fields. The state vector $|\phi\rangle$ describes a physical state of the system with eigenvalue (quantum field configuration) ϕ. The probability distribution function $\rho(\phi)$ is a functional of ϕ and tells us the probability of finding the system in the field configuration ϕ in thermodynamic equilibrium. This is completely analogous to the probability interpretation of $\rho(x)$ for the finite-dimensional system discussed in Sec. II. The field configurations ϕ in field space are analogous to the particles with positions x in coordinate space.

In terms of wave functionals, the distribution function may be written as

$$\rho(\phi) = \langle\phi|e^{-\beta H}|\phi\rangle \tag{4.1a}$$

$$= \sum_i \langle\phi|e^{-\beta H}|E_i\rangle\langle E_i|\phi\rangle \tag{4.1b}$$

$$= \sum_i e^{-\beta E_i}\psi_i(\phi)\psi_i^*(\phi), \tag{4.1c}$$

where the Hamiltonian H is obtained by integrating the Hamiltonian density $\mathcal{H}(\pi,\phi)$ over space. The wave functionals $\psi_i(\phi)$ are very complicated objects, making $\rho(\phi)$ all the more so. Semiclassically, one could determine the wave functionals in the WKB approximation, but even this is a considerable undertaking. If the relevant actions in the system are large compared to $\hbar$, we can replace the discrete energy sum in Eq. (4.1) by an energy continuum, just as we did in Sec. II for the finite-dimensional case. Applying the formulation of Secs. II and III, we can then search for FTMPEP's in the field space which dominate the semiclassical distribution function $\rho(\phi)$ for a given field configuration ϕ. To illustrate the formalism, we briefly consider the distribution functions for a real scalar field theory without derivative interactions and a pure Yang-Mills gauge theory.

A. Scalar field theory

The Minkowski-space Lagrangian density for a scalar field theory is

$$\mathcal{L}(\phi(x,t),\ \partial_t\phi(x,t),\ \nabla_x\phi(x,t)) = \tfrac{1}{2}\partial_\mu\phi\partial^\mu\phi - V(\phi)$$
$$(\mu = 0,1,2,3;\ \text{metric} + - - -)\,. \tag{4.2}$$

The effective finite-temperature Lagrangian (obtained from the Minkowski-space Lagrangian by replacing $\partial/\partial t$ with $i\partial/\partial\tau$) is[32]

$$\mathcal{L}_{\rm eff}(\phi(x,\tau),\ \dot{\phi}(x,\tau),\ \nabla_x\phi(x,\tau)) = -\left[\tfrac{1}{2}\dot{\phi}^2 + \tfrac{1}{2}(\nabla_x\phi)^2 + V(\phi)\right], \tag{4.3}$$

where $\dot{\phi} = \partial\phi/\partial\tau$. Generalizing the finite-dimensional Eq. (3.1), the path-integral expression for the scalar theory distribution function is

$$\rho(\phi) = N(\beta)\int_{\phi(x,0)=\phi(x,\hbar\beta)=\phi(x)} D\phi(x,\tau)\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\int d^3x\,\mathcal{L}_{\rm eff}(\phi)\right], \tag{4.4}$$

where the path integral is over all paths in field space that begin and end at $\phi(x)$.

The path $\phi_{\rm CL}(x,\tau)$ in field space giving the dominant contribution to the semiclassical probability distribution function obeys the Euclidean equation of motion

$$\frac{\partial^2\phi(x,\tau)}{\partial\tau^2} + \nabla_x{}^2\phi(x,\tau) - \frac{\partial V(\phi(x,\tau))}{\partial\phi(x,\tau)} = 0\,, \tag{4.5}$$

with the periodic boundary conditions $\phi(x,0) = \phi(x,\hbar\beta) = \phi(x)$. With the contribution from combined quantum and thermal fluctuations, $\eta(x,\tau)$, around $\phi_{\rm CL}(x,\tau)$, we obtain for $\rho(\phi)$ in the semiclassical approximation

$$\rho(\phi) = N(\beta)\oint_0^0 D\eta\,\exp\left\{\frac{-1}{2\hbar}\int_0^{\hbar\beta}d\tau\int d^3x\,\eta\left[\frac{-\partial^2}{\partial\tau^2} - \nabla_x{}^2 + \frac{\partial^2 V(\phi_{\rm CL})}{\partial\phi^2}\right]\eta\right\}\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\int d^3x\,\mathcal{L}_{\rm eff}(\phi_{\rm CL})\right] \tag{4.6}$$

$$= N(\beta)\left[\det\left(\frac{-\partial^2}{\partial\tau^2} - \nabla_x{}^2 + \frac{\partial^2 V(\phi_{\rm Cl})}{\partial\phi^2}\right)\right]^{-1/2} \exp\left(\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \int d^3x\, \mathcal{L}_{\rm eff}(\phi_{\rm Cl})\right) \tag{4.7}$$

$$= N(\beta)\prod_n \left(\frac{1}{\omega_n}\right)\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \int d^3x\, \mathcal{L}_{\rm eff}(\phi_{\rm Cl})\right]. \tag{4.8}$$

The eigenvalues ω_n are determined from the equation

$$\left(-\frac{\partial^2}{\partial\tau^2} - \nabla_x{}^2 + \frac{\partial^2 V(\phi_{\rm Cl})}{\partial\phi^2}\right)\eta^{(n)}(x,\tau) = \omega_n{}^2\eta^{(n)}(x,\tau), \tag{4.9}$$

with $\eta^{(n)}(x,0) = \eta^{(n)}(x,\hbar\beta) = 0$.

We can now determine the normalization factor $N(\beta)$ by viewing the scalar field theory as an infinite-dimensional oscillator system. We divide space into unit cubes of side ϵ labeled by the coordinates $x = x_i$. The canonical coordinates are $q_i(\tau) \equiv \phi(x_i, \tau)$. The integrated Lagrangian density

$$L_{\rm eff} = -\int d^3x\left[\tfrac{1}{2}(\dot\phi)^2 + \tfrac{1}{2}(\nabla_x\phi)^2 + V(\phi)\right] \tag{4.10}$$

may now be replaced by the discrete sum

$$L_{\rm eff} = -\epsilon^3\sum_i\left[\frac{1}{2}\left(\frac{\partial q_i}{\partial\tau}\right)^2 + \frac{1}{2\epsilon^2}|q_{i+1} - q_i|^2 + V(q_i)\right]. \tag{4.11}$$

Generalizing the finite-dimensional discussion of Sec. III, the "free particle" $L_{\rm eff}$ corresponds to "switching off" the last two "interaction" terms in Eq. (4.11). The distribution function becomes

$$\rho_{\text{"free"}}(\phi) = N(\beta)[\det(-\partial^2/\partial\tau^2)]^{-1/2}. \tag{4.12}$$

By requiring that this reduce to $\prod_x (2\pi\hbar^2\beta)^{-1/2}$, where the infinite product is over all spatial cubes [cf. Eq. (3.11)], we may identify

$$N(\beta) = [\det(-\partial^2/\partial\tau^2)]^{1/2}\prod_x (2\pi\hbar^2\beta)^{-1/2}. \tag{4.13}$$

For our scalar field theory then, we have the semiclassical result

$$\rho(\phi) = \left[\prod_x (2\pi\hbar^2\beta)^{-1}\frac{\det\left(\frac{-\partial^2}{\partial\tau^2}\right)}{\det\left(\frac{-\partial^2}{\partial\tau^2} - \nabla_x{}^2 + \frac{\partial^2 V(\phi_{\rm Cl})}{\partial\phi^2}\right)}\right]^{1/2} \exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\int d^3x\,\mathcal{L}_{\rm eff}(\phi_{\rm Cl})\right]. \tag{4.14}$$

In Appendix B we illustrate that Eq. (4.14) gives the exact distribution function for a free scalar field theory.

B. Yang-Mills gauge theory

The Minkowski-space Lagrangian density for a pure Yang-Mills gauge theory is[2]

$$\mathcal{L}(A^a_\mu(x,t),\, \partial_t A^a_\mu(x,t),\, \nabla_x A^a_\mu(x,t)) = -\tfrac{1}{4}F^a_{\mu\nu}F^{a\mu\nu} \tag{4.15}$$

where

$$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + gf^{abc}A^b_\mu A^c_\nu, \tag{4.16}$$

g is the coupling constant, and f^{abc} are the structure constants of the gauge group. The group generators L^a obey the commutation relations

$$[L^a, L^b] = if^{abc}L^c \tag{4.17}$$

($a = 1, \ldots, n$, where n is the number of generators, which equals the number of gauge bosons). The effective finite-temperature Lagrangian (obtained from the Minkowski-space Lagrangian by replacing $\partial/\partial t$ by $i\partial/\partial\tau$) is[32]

$$\mathcal{L}_{\rm eff}(A^a_\mu(x,\tau),\, \dot A^a_\mu(x,\tau),\, \nabla_x A^a(x,\tau)) = -\tfrac{1}{4}F^a_{\mu\nu}F^{a\mu\nu}, \tag{4.18}$$

where

$$\dot A^a_\mu = \partial A^a_\mu/\partial\tau, \tag{4.19}$$

$$\partial_\mu \equiv (i\partial/\partial\tau, \partial/\partial x, \partial/\partial y, \partial/\partial z) \equiv (i\partial_\tau, \nabla_x), \tag{4.20}$$

and

$$\partial_\mu\partial^\mu = -\partial_\tau{}^2 - \nabla_x{}^2. \tag{4.21}$$

It will be convenient to use the group-space vector notation[2]

$$A_\mu \equiv (A^1_\mu, A^2_\mu, \ldots, A^n_\mu). \tag{4.22}$$

In this notation, Eq. (4.18) becomes

$$\mathcal{L}_{\rm eff}(A_\mu) = -\tfrac{1}{4}F_{\mu\nu}\cdot F^{\mu\nu}, \tag{4.23}$$

where

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + gA_\mu \times A_\nu. \tag{4.24}$$

Dots and crosses will refer to group-space vector operations, and all space-time indices will be shown explicitly.

The path-integral expression for the Yang-Mills probability distribution function is a straightforward generalization of Eq. (4.4) for the scalar field theory, along with the necessary addition of the Faddeev-Popov gauge-fixing ansatz:

$$\rho(A_\mu) = N(\beta) \int_{A_\mu(x,0)=A_\mu(x,\hbar\beta)=A_\mu(x)} DA_\mu(x,\tau) \exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \int d^3x\, \mathcal{L}_{\text{eff}}(A_\mu)\right] \det\left(\frac{\partial G^b}{\partial \omega^c}\right) \prod_{b=1}^{n} \delta(G^b), \tag{4.25}$$

where

$$DA_\mu(x,\tau) \equiv \prod_{a=1}^{n}\prod_{\mu=0}^{3} DA_\mu^a(x,\tau), \tag{4.26}$$

and the path integral is over all paths in field space that begin and end at $A_\mu(x)$. The term $\det(\partial G^b/\partial\omega^c)\prod_b \delta(G^b)$ in Eq. (4.25) is the Faddeev-Popov gauge-fixing ansatz.[2,32-35] Bernard[32] has previously discussed the application of this ansatz in calculating the gauge-invariant partition function

$$Z = N(\beta) \int_{A_\mu(x,\tau)=A_\mu(x,\tau+\hbar\beta)} DA_\mu(x,\tau) \exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \int d^3x\, \mathcal{L}_{\text{eff}}(A_\mu)\right] \det\left(\frac{\partial G^b}{\partial \omega^c}\right) \prod_{b=1}^{n} \delta(G^b). \tag{4.27}$$

The Faddeev-Popov determinant may be written as a Gaussian integral over "ghost fields" (fictitious scalar fields obeying Fermi statistics) ϕ and ϕ^*,[32,35]

$$\det\left(\frac{\partial G^b}{\partial \omega^c}\right) = \oint D\phi^*(x,\tau) D\phi(x,\tau) \times \exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \int d^3x\, \mathcal{L}_{\text{ghost}}(\phi,\phi^*)\right], \tag{4.28}$$

with

$$\phi(x,\tau) = \phi(x,\tau+\hbar\beta). \tag{4.29}$$

The only modification of Bernard's results we need to make in applying the Faddeev-Popov ansatz to $\rho(A_\mu)$ is in the gauge-fixing δ functional $\prod_b \delta(G^b)$. Bernard employs the same definition for this quantity as that used in calculating the Euclidean vacuum-to-vacuum transition amplitude W_E, namely, a product of δ functions over all space-time points $(0 \le \tau \le \hbar\beta)$. Unlike the partition function, the distribution function is obtained via the restricted path integral in Eq. (4.25) in which we do not integrate over the "starting points" $A_\mu(x)$. To make $\rho(A_\mu)$ gauge invariant by construction, we simply define the δ functional in Eq. (4.25) to be

$$\prod_{b=1}^{n} \delta(G^b) = \prod_{b=1}^{n}\prod_{x}\prod_{\tau\neq 0} \delta(G^b(A_\mu(x,\tau))). \tag{4.30}$$

The path integral in Eq. (4.25) completely integrates out the δ functional in Eq. (4.30), leaving a finite gauge-invariant result. This definition of the gauge-fixing δ functional has the desirable feature that $\rho(A_\mu)$ is interpretable as the gauge-invariant probability of finding the system in the physical field configuration A_μ.

To obtain the partition function (or any expectation value for that matter) from $\rho(A_\mu)$, a final integration over $A_\mu(x)$ is performed with the $\tau = 0$ part of the gauge-fixing δ functional:

$$Z = \int DA_\mu(x) \prod_{b=1}^{n}\prod_{x} \delta(G^b(A_\mu(x)))\rho(A_\mu). \tag{4.31}$$

Although the explicit δ functional in Eq. (4.31) might seem to complicate calculations, it does not do so in practice. One simply evaluates $\rho(A_\mu)$ in a convenient gauge, call it $\rho_G(A_\mu)$, and then integrates over the fields occurring in $\rho_G(A_\mu)$ to obtain expectation values. We are assuming that the only expectation values to be computed from $\rho(A_\mu)$ are for operators not involving the ghost fields explicitly:

$$\langle \mathcal{O}(A_\mu)\rangle = Z^{-1} \int DA_\mu(x) \prod_{b=1}^{n} \delta(G^b(A_\mu))\mathcal{O}(A_\mu)\rho(A_\mu). \tag{4.32}$$

If the operator involves the ghosts [i.e., $\mathcal{O}(A_\mu,\phi^*,\phi)$] then $\langle \mathcal{O}(A_\mu,\phi^*,\phi)\rangle$ must be calculated by removing $\det(\partial G^b/\partial\omega^c)$ in $\rho(A_\mu)$ and doing an explicit integration over ϕ^* and ϕ to obtain the expectation value:

$$\langle \mathcal{O}(A_\mu,\phi^*,\phi)\rangle = Z^{-1} \int DA_\mu(x) \prod_{b=1}^{n} \delta(G^b(A_\mu)) \oint D\phi^* D\phi \exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \int d^3x\, \mathcal{L}_{\text{ghost}}(\phi,\phi^*)\right] \times \mathcal{O}(A_\mu,\phi^*,\phi)[\det(\partial G^b/\partial\omega^c)]^{-1}\rho(A_\mu). \tag{4.33}$$

A convenient alternate notation for the Faddeev-Popov δ functional in Eq. (4.30) is

$$\prod_{b=1}^{n} \delta(G^b) = \lim_{\alpha\to 0}\left[\prod_{b=1}^{n}\prod_{x}\prod_{\tau\neq 0}(2\pi\hbar\alpha)^{-1/2}\right]\exp\left[\frac{-1}{2\alpha\hbar}\int_0^{\hbar\beta} d\tau \int d^3x\, G^2(A_\mu)\right]. \tag{4.34}$$

Absorbing the prefactor in Eq. (4.34) into $N(\beta)$, Eq. (4.25) may be written as

$$\rho(A_\mu) = N(\beta)\int_{A_\mu(x,0)=A_\mu(x,\hbar\beta)=A_\mu(x)} DA_\mu(x,\tau)\oint D\phi^*(x,\tau)D\phi(x,\tau)\exp\left\{\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\int d^3x\left[\mathcal{L}_{\rm eff}(A_\mu)-\frac{1}{2\alpha}G^2(A_\mu) + \mathcal{L}_{\rm ghost}(\phi,\phi^*)\right]\right\}, \tag{4.35}$$

where α is an arbitrary real number (which all observable expectation values are, of course, independent of). The path $A_\mu^{\rm CL}$ which dominates the semiclassical distribution function satisfies the Euclidean equation of motion

$$\partial^\mu F_{\mu\nu}(x,\tau) + gA^\mu(x,\tau)\times F_{\mu\nu}(x,\tau) = D^\mu F_{\mu\nu}(x,\tau) = 0, \tag{4.36}$$

with periodic boundary conditions $A_\mu(x,0) = A_\mu(x,\hbar\beta) = A_\mu(x)$. With the inclusion of quantum and thermal fluctuations, $\eta_\mu(x,\tau)$, around $A_\mu^{\rm CL}(x,\tau)$, we obtain for the semiclassical distribution function

$$\rho(A_\mu) = N(\beta)\oint_0^0 D\eta_\mu(x,\tau)\oint D\phi^*(x,\tau)D\phi(x,\tau) \times\exp\left\{\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\int d^3x\left[-\tfrac{1}{2}D_\mu\eta_\nu\cdot D^\mu\eta^\nu + \tfrac{1}{2}D_\mu\eta^\mu\cdot D_\nu\eta^\nu - gF_{\mu\nu}^{\rm CL}\cdot(\eta^\mu\times\eta^\nu) - \frac{1}{2\alpha}G^2(A_\mu) + \mathcal{L}_{\rm ghost}(\phi,\phi^*)\right]\right\}\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\int d^3x\,\mathcal{L}_{\rm eff}(A_\mu^{\rm CL})\right], \tag{4.37}$$

where

$$D_\mu\eta_\nu = \partial_\mu\eta_\nu + gA_\mu^{\rm CL}\times\eta_\nu\,. \tag{4.38}$$

The factor $N(\beta)$ in Eq. (4.37) can be determined in the same way as for the scalar case. We "switch off the interactions" and require that ρ reduce to

$$\rho_{\text{"free"}} = \prod_x (2\pi\hbar^2\beta)^{-p/2}, \tag{4.39}$$

where p is the number of field components which are treated as dynamically independent in the chosen gauge. For a Yang-Mills theory in the Feynman gauge ($\partial_\mu A^\mu = 0$), $p = 4n$. In the axial gauge ($A_3 = 0$), Coulomb gauge ($\nabla_i A_i = 0$), and temporal gauge ($A_0 = 0$), $p = 2n$. (Recall that for the scalar theory, $p = 1$.) In Appendix C we show that Eq. (4.37) gives the exact probability distribution function for a pure Abelian gauge theory in the Feynman gauge.

V. HARTREE SELF-CONSISTENT FIELD APPROXIMATION

As we have seen in Secs. III and IV, the Euclidean loop expansion proved to be a versatile method for implementing the FTMPEP formalism of Sec. II. Beyond the one-loop correction, however, this type of expansion becomes notoriously difficult. To extend the range of applicability of the semiclassical method, higher-order corrections are necessary. In this section we discuss a Hartree self-consistent method for including such corrections to the semiclassical distribution function. This method was first suggested in Ref. 13 for including the effect of quantum fluctuations in the (zero-temperature) vacuum tunneling amplitude. Here we straightforwardly generalize the method to finite-temperature tunneling.

Using the FTMPEP concept, we found in Sec. II that the probability distribution function could be written in the semiclassical form (modulo normalization)

$$\rho(x) = [\det(-\delta_{ij}md^2/d\tau^2 + \partial^2V(x_{\rm CL})/\partial x_i\partial x_j)]^{-1/2}\exp\left(-\beta E - \frac{2}{\hbar}\int_{\lambda(x_E)}^{\lambda(x)} d\lambda\{2m(\lambda)[V(\lambda)-E]\}_{\rm CL}{}^{1/2}\right),\quad i=1,\ldots,N \tag{5.1}$$

where the integral is along the FTMPEP $x_{\rm CL}(\lambda)$ connecting the turning point x_E and the point x in the tunneling region. The symbols λ and τ are path parameters related by

$$\frac{d\lambda}{d\tau}=\left[\frac{2[V(\lambda)-E]}{m(\lambda)}\right]^{1/2}, \quad m(\lambda)=m(\partial x/\partial\lambda)^2\,, \tag{5.2}$$

with $\lambda(x)\equiv\lambda(\tau=0)=\lambda(\tau=\hbar\beta)$ and $\lambda(x_E)\equiv\lambda(\tau=\hbar\beta/2)$. The determinant represents the contribution to $\rho(x)$ from paths near the FTMPEP,

$$[\det(-\delta_{ij}md^2/d\tau^2+\partial^2V(x_{\rm CL})/\partial x_i\partial x_j)]^{-1/2}=\oint_0^0 D\eta(\tau)\exp\left\{\frac{-1}{2\hbar}\int_0^{\hbar\beta}d\tau\,\eta_i[-\delta_{ij}md^2/d\tau^2+\partial^2V(x_{\rm CL})/\partial x_i\partial x_j]\eta_j\right\}, \tag{5.3}$$

where $\eta(\tau)\equiv x(\tau)-x_{\rm CL}(\tau)$ and $\eta(0)=\eta(\hbar\beta)=0$.

Let us define two functions, ξ_β and $f(\tau)$, by

$$\zeta_\beta\equiv\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau f(\tau)\right] \tag{5.4}$$

$$\equiv\oint_0^0 D\eta\exp\left\{\frac{-1}{2\hbar}\int_0^{\hbar\beta}d\tau\,\eta_i[-\delta_{ij}md^2/d\tau^2+\partial^2V(x_{\rm CL})/\partial x_i\partial x_j]\eta_j\right\}. \tag{5.5}$$

The distribution function may now be written as

$$\rho(x)=\exp\left(-\beta E-\frac{2}{\hbar}\int_{\lambda(x_E)}^{\lambda(x)}d\lambda\{2m(\lambda)[V(\lambda)-E]\}_{\rm CL}{}^{1/2}+\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau f(\tau)\right), \tag{5.6}$$

with the contribution of paths near the FTMPEP now appearing in the exponent as $(1/\hbar)\int_0^{\hbar\beta}d\tau f(\tau)$. Semiclassically, we assume that the third term is small compared to the second term in the exponent. Consequently, we may absorb $f(\tau)$ into $V(\lambda)$ to obtain an effective potential $U=V-f$,

$$\rho(x)=\exp\left\{-\beta E-\frac{2}{\hbar}\int_{\lambda(x_E)}^{\lambda(x)}d\lambda[2m(\lambda)(U-E)]_{\rm CL}{}^{1/2}\right\}. \tag{5.7}$$

Using the effective potential U reproduces Eq. (5.6) to $O(f^2)$:

$$\begin{aligned}\int_{\lambda(x_E)}^{\lambda(x)}d\lambda[2m(\lambda)(U-E)]^{1/2}&=\int_{\lambda(x_E)}^{\lambda(x)}d\lambda[2m(\lambda)(V-E)]^{1/2}-\int_{\lambda(x_E)}^{\lambda(x)}d\lambda\left[\frac{2m(\lambda)}{V-E}\right]^{1/2}\tfrac{1}{2}f(\tau)+O(f^2)\\&=\int_{\lambda(x_E)}^{\lambda(x)}d\lambda[2m(\lambda)(V-E)]^{1/2}-\tfrac{1}{2}\int_0^{\hbar\beta}d\tau f(\tau)+O(f^2)\,.\end{aligned} \tag{5.8}$$

The contribution of the neighboring paths is then to modify the potential V associated with the FTMPEP to the effective potential $U=V-f$. This suggests the following improved method of obtaining the FTMPEP with corrections from neighboring paths included. We choose a trial path $x(\lambda)$ and compute V, and additionally f due to neighboring paths. The FTMPEP is then determined by minimizing

$$R(x)=\int_{\lambda(x_E)}^{\lambda(x)}d\lambda[2m(\lambda)(U-E)]^{1/2} \tag{5.9}$$

in Eq. (5.7) with potential $U=V-f$. This method is closely related to the self-consistent Hartree approximation applied to the finite-temperature tunneling problem. A self-consistent method is of interest because it includes higher-order corrections which are difficult to obtain by a loop expansion.

To make the connection with the Hartree approximation, we first derive the equation for the improved FTMPEP through the variation of Eq. (5.9) with fixed end points x and x_E, giving

$$\begin{aligned}\delta\int_{\lambda(x_E)}^{\lambda(x)}d\lambda[2m(\lambda)(U-E)]^{1/2}&=\delta\left(\int_{\lambda(x_E)}^{\lambda(x)}d\lambda[2m(\lambda)(V-E)]^{1/2}-\tfrac{1}{2}\int_0^{\hbar\beta}d\tau f(\tau)\right)\\&=\int_{\lambda(x_E)}^{\lambda(x)}d\lambda\left(-\frac{d}{d\lambda}\left\{\left[\frac{2(V-E)}{m(\lambda)}\right]^{1/2}m\frac{dx_i}{d\lambda}\right\}+\left[\frac{2m(\lambda)}{V-E}\right]^{1/2}\left(\frac{1}{2}\frac{\partial V}{\partial x_i}\right)\right)\delta x_i\\&\quad-\delta\tfrac{1}{2}\int_0^{\hbar\beta}d\tau f(\tau)=0\,.\end{aligned} \tag{5.10}$$

From Eqs. (5.4) and (5.5) we have

$$\frac{\delta}{\delta x_i(\tau)}\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau f(\tau)$$

$$=\frac{\delta}{\delta x_i(\tau)}\ln\left\{\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau f(\tau)\right]\right\}$$

$$=\frac{1}{\zeta_\beta}\oint_0^0 D\eta\left(\frac{-1}{2\hbar}\eta_j\frac{\partial^3 V(x_{\mathrm{CL}})}{\partial x_i\partial x_j\partial x_k}\eta_k\right)\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau f(\tau)\right]$$

$$=\frac{-1}{2\hbar}\frac{\partial^3 V(x_{\mathrm{CL}})}{\partial x_i\partial x^2}\langle\eta^2\rangle$$

$$=\frac{-1}{2\hbar}\frac{\partial^3 V(x_{\mathrm{CL}})}{\partial x_i\partial x^2}\langle(x-x_{\mathrm{CL}})^2\rangle\,, \tag{5.11}$$

where

$$\langle(x-x_{\mathrm{CL}})^2\rangle\equiv\frac{1}{\zeta_\beta}\oint_0^0 D\eta\,\eta^2\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau f(\tau)\right]\,, \tag{5.12}$$

and we have used the fact that $\langle x-x_{\mathrm{CL}}\rangle=0$. Using Eq. (5.11) in Eq. (5.10), we obtain

$$\int_{\lambda(x_E)}^{\lambda(x)} d\lambda\left(\frac{-d}{d\lambda}\left\{\left[\frac{2(V-E)}{m(\lambda)}\right]^{1/2} m\frac{dx_i}{d\lambda}\right\}+\left[\frac{2m(\lambda)}{V-E}\right]^{1/2}\left(\frac{1}{2}\frac{\partial V}{\partial x_i}\right)\right)\delta x_i$$
$$+\frac{1}{4}\int_0^{\hbar\beta} d\tau\,\frac{\partial^3 V}{\partial x_i\partial x^2}\langle\eta^2\rangle\delta x_i=0\,. \tag{5.13}$$

Expressing this result in terms of the τ parametrization in Eq. (5.2) yields the equation of motion for the improved FTMPEP, $x_{\mathrm{CL}}(\tau)$,

$$-m\frac{d^2 x_{\mathrm{CL}i}}{d\tau^2}+\frac{\partial V(x_{\mathrm{CL}})}{\partial x_i}+\frac{1}{2}\frac{\partial^3 V(x_{\mathrm{CL}})}{\partial x_i\partial x^2}\langle(x-x_{\mathrm{CL}})^2\rangle=0\,, \tag{5.14}$$

with periodic boundary condition $x_{\mathrm{CL}}(0)=x_{\mathrm{CL}}(\hbar\beta)=x$. We can relate the last two terms in Eq. (5.14) to the expectation value of $\partial V/\partial x_i$ via

$$\left\langle\frac{\partial V(x)}{\partial x_i}\right\rangle_{x_{\mathrm{CL}}}=\left\langle\frac{\partial V(x_{\mathrm{CL}})}{\partial x_i}+\frac{\partial^2 V(x_{\mathrm{CL}})}{\partial x_i\partial x_j}(x_j-x_{\mathrm{CL}j})+\frac{1}{2}\frac{\partial^3 V(x_{\mathrm{CL}})}{\partial x_i\partial x_j\partial x_k}(x_j-x_{\mathrm{CL}j})(x_k-x_{\mathrm{CL}k})+\cdots\right\rangle$$
$$=\frac{\partial V(x_{\mathrm{CL}})}{\partial x_i}+\frac{1}{2}\frac{\partial^3 V(x_{\mathrm{CL}})}{\partial x_i\partial x^2}\langle(x-x_{\mathrm{CL}})^2\rangle\,. \tag{5.15}$$

We may thus interpret Eq. (5.14) as the expectation value of the equation of motion

$$-m\frac{d^2 x_i}{d\tau^2}+\frac{\partial V(x)}{\partial x_i}=0 \tag{5.16}$$

under the Gaussian fluctuation. It is well known that the use of Gaussian fluctuations as trial functions is equivalent to the Hartree approximation.[13,36]

To be able to solve Eq. (5.14) self-consistently, we need a Hartree equation for the fluctuation, $\eta(\tau)=x(\tau)-x_{\mathrm{CL}}(\tau)$. This can be obtained through the variation of Eq. (5.16) followed by taking its expectation value,

$$\left\langle-\delta_{ij}m\frac{d^2}{d\tau^2}+\frac{\partial^2 V(x)}{\partial x_i\partial x_j}\right\rangle_{x_{\mathrm{CL}}}=-\delta_{ij}m\frac{d^2}{d\tau^2}+\left\langle\frac{\partial^2 V(x)}{\partial x_i\partial x_j}\right\rangle_{x_{\mathrm{CL}}}$$
$$=-\delta_{ij}m\frac{d^2}{d\tau^2}+\left\langle\frac{\partial^2 V(x_{\mathrm{CL}})}{\partial x_i\partial x_j}+\frac{\partial^3 V(x_{\mathrm{CL}})}{\partial x_i\partial x_j\partial x_k}(x_k-x_{\mathrm{CL}k})+\frac{1}{2}\frac{\partial^4 V(x_{\mathrm{CL}})}{\partial x_i\partial x_j\partial x_k\partial x_l}(x_k-x_{\mathrm{CL}k})(x_l-x_{\mathrm{CL}l})+\cdots\right\rangle_{x_{\mathrm{CL}}}$$
$$=-\delta_{ij}m\frac{d^2}{d\tau^2}+\frac{\partial^2 V(x_{\mathrm{CL}})}{\partial x_i\partial x_j}+\frac{1}{2}\frac{\partial^4 V(x_{\mathrm{CL}})}{\partial x_i\partial x_j\partial x^2}\langle(x-x_{\mathrm{CL}})^2\rangle\,. \tag{5.17}$$

We then have the Hartree fluctuation equation

$$\left[-\delta_{ij}m\frac{d^2}{d\tau^2}+\frac{\partial^2 V(x_{\mathrm{CL}})}{\partial x_i\partial x_j}+\frac{1}{2}\frac{\partial^4 V(x_{\mathrm{CL}})}{\partial x_i\partial x_j\partial x^2}\langle(x-x_{\mathrm{CL}})^2\rangle\right]\eta_j(\tau)=0 \tag{5.18}$$

with $\eta_j(0)=\eta_j(\hbar\beta)=0$. From Eqs. (5.14) and (5.18), $x_{\mathrm{CL}}(\tau)$ and $\eta(\tau)$ can, in principle, be determined self-consistently.

In general, a direct self-consistent solution of Eqs. (5.14) and (5.18) is quite difficult. An iterative approach may be easier. We first determine $x_{\rm CL}^{(0)}(\tau)$ from Eq. (5.16), that is, neglecting $\langle\eta^2\rangle=\langle(x-x_{\rm CL})^2\rangle$ in Eq. (5.14). One then guesses some reasonable $\langle\eta^{(0)2}\rangle$ and substitutes it and $x_{\rm CL}^{(0)}(\tau)$ into Eq. (5.18). Equation (5.18) is now solved for $\eta^{(1)}(\tau)$. With the solution $\eta^{(1)}(\tau)$, one computes $\langle\eta^{(1)2}\rangle$ using Eq. (5.12) and substitutes this back into Eq. (5.14). Equation (5.14) is solved for $x_{\rm CL}^{(1)}(\tau)$ which, along with $\langle\eta^{(1)2}\rangle$, is set into Eq. (5.18) for the next iteration. At any stage, one can calculate $\rho(x)$ using $x_{\rm CL}^{(n)}$ and $\eta^{(n)}$ in Eq. (5.7).

The above Hartree approximation can be generalized to field theory to evaluate the probability distribution function. In Sec. IV we showed that the distribution function for a scalar field theory could be written in the semiclassical form (modulo normalization)

$$\rho(\phi)=\left\{\det\left[\frac{-\partial^2}{\partial\tau^2}-\nabla_x{}^2+\frac{\partial^2V(\phi_{\rm CL})}{\partial\phi^2}\right]\right\}^{-1/2}\times\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\int d^3x\,\mathcal{L}_{\rm eff}(\phi_{\rm CL})\right],\qquad(5.19)$$

where

$$\mathcal{L}_{\rm eff}(\phi)=-\tfrac{1}{2}\left(\frac{\partial\phi}{\partial\tau}\right)^2-\tfrac{1}{2}(\nabla_x\phi)^2-V(\phi)\,,\qquad(5.20)$$

and the τ integral is along the FTMPEP $\phi_{\rm CL}(x,\tau)$, with $\phi_{\rm CL}(x,0)=\phi_{\rm CL}(x,\hbar\beta)=\phi(x)$.

Equation (5.19) can be put into a form similar to Eq. (5.6) by introducing a new path parameter $\lambda(\tau)$ defined by

$$\frac{d\lambda}{d\tau}=\left[\frac{2(V(\lambda)-E)}{m(\lambda)}\right]^{1/2},\qquad(5.21)$$

where

$$m(\lambda)\equiv\int d^3x(\partial\phi/\partial\lambda)^2\qquad(5.22)$$

and

$$V(\lambda)\equiv\int d^3x[\tfrac{1}{2}(\nabla_x\phi)^2+V(\phi)]\,.\qquad(5.23)$$

It is simple to show that

$$\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\int d^3x\,\mathcal{L}_{\rm eff}(\phi_{\rm CL})=-\beta E-\frac{2}{\hbar}\int_{\lambda(\phi_E)}^{\lambda(\phi)}d\lambda\{2m(\lambda)[V(\lambda)-E]\}_{\rm CL}{}^{1/2},\qquad(5.24)$$

where

$$\begin{aligned}&\lambda(\phi)\equiv\lambda(\tau=0)=\lambda(\tau=\hbar\beta)\,,\\&\lambda(\phi_E)\equiv\lambda(\tau=\hbar\beta/2)\,,\\&\phi_E(x)\equiv\phi_{\rm CL}(x,\tau=\hbar\beta/2)\,.\end{aligned}\qquad(5.25)$$

Let us define two functions, ζ_β and $f(\tau)$, just as we did in the finite-dimensional case, by

$$\begin{aligned}\zeta_\beta&\equiv\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau f(\tau)\right]\\&\equiv\left[\det\left(\frac{-\partial^2}{\partial\tau^2}-\nabla_x{}^2+\frac{\partial^2V(\phi_{\rm CL})}{\partial\phi^2}\right)\right]^{-1/2}\\&=\oint_0^0 D\eta(x,\tau)\exp\left[\frac{-1}{2\hbar}\int_0^{\hbar\beta}d\tau\int d^3x\,\eta\left(\frac{-\partial^2}{\partial\tau^2}-\nabla_x{}^2+\frac{\partial^2V(\phi_{\rm CL})}{\partial\phi^2}\right)\eta\right].\end{aligned}\qquad(5.26)$$

The distribution function in Eq. (5.19) may now be written as

$$\rho(\phi)=\exp\left(-\beta E-\frac{2}{\hbar}\int_{\lambda(\phi_E)}^{\lambda(\phi)}d\lambda\{2m(\lambda)[V(\lambda)-E]\}_{\rm CL}{}^{1/2}+\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau f(\tau)\right),\qquad(5.27)$$

with the contribution of paths near the FTMPEP now appearing in the exponent as $(1/\hbar)\int_0^{\hbar\beta}d\tau f(\tau)$. Equation (5.27) is identical in form to Eq. (5.6) for the finite-dimensional system, and the Hartree analysis follows similarly. We only quote the results.

We absorb $f(\tau)$ into $V(\lambda)$ to obtain an effective potential $U=V-f$,

$$\rho(\phi)=\exp\left\{-\beta E-\frac{2}{\hbar}\int_{\lambda(\phi_E)}^{\lambda(\phi)}d\lambda[2m(\lambda)(U-E)]_{\rm CL}{}^{1/2}\right\}.\qquad(5.28)$$

The FTMPEP, $\phi_{\rm CL}(x,\tau)$, which maximizes $\rho(\phi)$ in Eq. (5.28) satisfies the Hartree equation of motion

$$\frac{-\partial^2\phi_{\rm CL}}{\partial\tau^2} - \nabla_x{}^2\phi_{\rm CL} + \left\langle\frac{\partial V}{\partial\phi}\right\rangle_{\phi_{\rm CL}} = \frac{-\partial^2\phi_{\rm CL}}{\partial\tau^2} - \nabla_x{}^2\phi_{\rm CL} + \frac{\partial V(\phi_{\rm CL})}{\partial\phi} + \frac{1}{2}\frac{\partial^3 V(\phi_{\rm CL})}{\partial\phi^3}\langle\eta^2\rangle = 0\,, \quad (5.29)$$

with periodic boundary conditions $\phi_{\rm CL}(x,0) = \phi_{\rm CL}(x,\hbar\beta) = \phi(x)$, where

$$\langle\eta^2\rangle = \langle[\phi(x,\tau)-\phi_{\rm CL}(x,\tau)]^2\rangle \equiv \frac{1}{\zeta_\beta}\oint_0^0 D\eta\,\eta^2\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau f(\tau)\right]. \quad (5.30)$$

The field $\eta(x,\tau)=\phi(x,\tau)-\phi_{\rm CL}(x,\tau)$ satisfies the Hartree fluctuation equation

$$\left[\frac{-\partial^2}{\partial\tau^2} - \nabla_x{}^2 + \frac{\partial^2 V(\phi_{\rm CL})}{\partial\phi^2} + \frac{1}{2}\frac{\partial^4 V(\phi_{\rm CL})}{\partial\phi^4}\langle\eta^2\rangle\right]\eta(x,\tau) = 0\,, \quad (5.31)$$

with $\eta(x,0)=\eta(x,\hbar\beta)=0$.

The Hartree self-consistent field approximation can also be extended to gauge theory.[13] We consider a Yang-Mills theory in the temporal gauge, $A_0=0$. In this gauge

$$\mathcal{L}_{\rm eff}(A_l) = -\tfrac{1}{2}\partial_\tau A_l\cdot\partial_\tau A_l - \tfrac{1}{4}F_{kl}\cdot F_{kl}\,, \quad (5.32)$$

where

$$F_{kl} = \partial_k A_l - \partial_l A_k + gA_k\times A_l\,.$$

The Euclidean equation of motion (4.36) for the FTMPEP, $A_l^{\rm CL}(x,\tau)$, is

$$\frac{\partial^2 A_l(x,\tau)}{\partial\tau^2} + D_k F_{kl}(x,\tau) = 0\,, \quad (5.33)$$

with periodic boundary conditions $A_l(x,0) = A_l(x,\hbar\beta) = A_l(x)$, and where D_k is the gauge-covariant derivative. The distribution function has the semiclassical form (modulo normalization)

$$\rho(A_l) = \left[\det{}'\left(-\delta_{kl}\frac{\partial^2}{\partial\tau^2} - \frac{\partial}{\partial A_k}(D_m F_{ml})_{\rm CL}\right)\right]^{-1/2} \times\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\int d^3x\,\mathcal{L}_{\rm eff}(A_l^{\rm CL})\right], \quad (5.34)$$

where the τ integral is along the FTMPEP $A_l^{\rm CL}(x,\tau)$, and the primed determinant means that the gauge-fixing and ghost terms are implicit in the integration measure.

Using the λ parametrization in Eq. (5.21), Eq. (5.34) takes the form

$$\rho(A_l) = \left[\det{}'\left(-\delta_{kl}\frac{\partial^2}{\partial\tau^2} - \frac{\partial}{\partial A_k}(D_m F_{ml})_{\rm CL}\right)\right]^{-1/2} \times\exp\left(-\beta E - \frac{2}{\hbar}\int_{\lambda(A_l^E)}^{\lambda(A_l)} d\lambda\{2m(\lambda)[V(\lambda)-E]\}_{\rm CL}{}^{1/2}\right), \quad (5.35)$$

where

$$m(\lambda) \equiv \int d^3x\,\frac{\partial A_l}{\partial\lambda}\cdot\frac{\partial A_l}{\partial\lambda}\,,$$

$$V(\lambda) \equiv \tfrac{1}{4}\int d^3x\,F_{kl}\cdot F_{kl}\,,$$

$$\lambda(A_l) \equiv \lambda(\tau=0) = \lambda(\tau=\hbar\beta)\,, \quad (5.36)$$

$$\lambda(A_l^E) \equiv \lambda(\tau=\hbar\beta/2)\,,$$

$$A_l^E(x) \equiv A_l^{\rm CL}(x,\tau=\hbar\beta/2)\,.$$

Defining two functions, ζ_β and $f(\tau)$, by

$$\zeta_\beta \equiv \exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau f(\tau)\right] \equiv \left[\det{}'\left(-\delta_{kl}\frac{\partial^2}{\partial\tau^2} - \frac{\partial}{\partial A_k}(D_m F_{ml})_{\rm CL}\right)\right]^{-1/2} = \oint_0^0 D'\eta(x,\tau)\exp\left(\frac{-1}{2\hbar}\int_0^{\hbar\beta} d\tau\int d^3x\,\eta_k\cdot\left(-\delta_{kl}\frac{\partial^2}{\partial\tau^2} - \frac{\partial}{\partial A_k}(D_m F_{ml})_{\rm CL}\right)\eta_l\right), \quad (5.37)$$

the distribution function in Eq. (5.35) becomes

$$\rho(A_l) = \exp\left(-\beta E - \frac{2}{\hbar}\int_{\lambda(A_l^E)}^{\lambda(A_l)} d\lambda\{2m(\lambda)[V(\lambda)-E]\}_{\rm CL}{}^{1/2} + \frac{1}{\hbar}\int_0^{\hbar\beta} d\tau f(\tau)\right). \quad (5.38)$$

[The prime on $D'\eta$ means the same as on det′ in Eq. (5.34).]

As before, we absorb $f(\tau)$ into $V(\lambda)$ to obtain an effective potential $U = V - f$,

$$\rho(A_i)=\exp\left\{-\beta E-\frac{2}{\hbar}\int_{\lambda(A_i^E)}^{\lambda(A_i)}d\lambda[2m(\lambda)(U-E)]_{\mathrm{CL}}{}^{1/2}\right\}. \quad (5.39)$$

The FTMPEP, $A_i^{\mathrm{CL}}(x,\tau)$, which maximizes $\rho(A_i)$ in Eq. (5.39) satisfies the Hartree equation of motion

$$\frac{\partial^2 A_i^{\mathrm{CL}}}{\partial\tau^2}+\langle D_k F_{ki}\rangle_{A_{\mathrm{CL}}} =\frac{\partial^2 A_i^{\mathrm{CL}}}{\partial\tau^2}+(D_k F_{ki})_{\mathrm{CL}} +\frac{1}{2}\frac{\partial^2}{\partial A_m \partial A_n}(D_k F_{ki})_{\mathrm{CL}}\langle\eta_m\cdot\eta_n\rangle=0\,, \quad (5.40)$$

with periodic boundary conditions $A_i^{\mathrm{CL}}(x,0)=A_i^{\mathrm{CL}}(x,\hbar\beta)=A_i(x)$, and where

$$\langle\eta_m\cdot\eta_n\rangle=\langle[A_m(x,\tau)-A_m^{\mathrm{CL}}(x,\tau)]\cdot[A_n(x,\tau)-A_n^{\mathrm{CL}}(x,\tau)]\rangle \equiv\frac{1}{\xi_\beta}\oint_0^0 D'\eta\,\eta_m\cdot\eta_n\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau f(\tau)\right]. \quad (5.41)$$

The fields $\eta_j(x,\tau)=A_j(x,\tau)-A_j^{\mathrm{CL}}(x,\tau)$ satisfy the Hartree fluctuation equations

$$\left[\delta_{ji}\frac{\partial^2}{\partial\tau^2}+\frac{\partial}{\partial A_j}(D_k F_{ki})_{\mathrm{CL}}+\frac{1}{2}\frac{\partial^3}{\partial A_j\partial A_m\partial A_n}(D_k F_{ki})_{\mathrm{CL}}\langle\eta_m\cdot\eta_n\rangle\right]\eta_j(x,\tau)=0\,, \quad (5.42)$$

with $\eta_j(x,0)=\eta_j(x,\hbar\beta)=0$. From Eqs. (5.40) and (5.42), $A_i^{\mathrm{CL}}(x,\tau)$ and $\eta_i(x,\tau)$ can be determined self-consistently.

A direct self-consistent solution is difficult, and the iterative method might be preferable. Because such an iterative calculation is self-consistent, ξ_β will contain the one-loop correction to $\rho(A_i)$ plus higher-order corrections after some number of iterations. How many iterations are necessary to achieve this depends on how good our initial guess for $\langle\eta_n^{(0)}\circ\eta_m^{(0)}\rangle$ is. Hence, we pay a price for the higher-order corrections using the Hartree approximation. In this respect, the benefit over the conventional loop expansion may be marginal. Of course, the self-consistent solution does not include all higher-order effects and could neglect some important corrections. Yet in many-body theory, the Hartree self-consistent method is known to give improved results compared to the lowest-order calculation. For example, the Hartree-Fock Hamiltonian provides, for most purposes, a better starting point for nuclear many-body calculations (Ref. 16, Chap. 15). This is because it already includes the average interaction of a particle with the particles in the nuclear core. It is an interesting but separate problem to investigate other methods for solving the above Hartree equations, but we have not pursued this avenue. At present the Hartree approximation is only potentially more feasible analytically than the loop expansion for obtaining higher-order corrections to the distribution function.

VI. DISCUSSION

In the preceding sections, we have illustrated a semiclassical path-integral approximation for calculating the canonical probability distribution function in field theory for systems in thermodynamic equilibrium. The method can be physically understood using the WKB concept of finite-temperature most-probable escape paths. The FTMPEP'S are tunneling paths which maximize the semiclassical distribution function and are generally necessary for a complete understanding of the semiclassical statistical mechanics of a system. We have also proposed an improved method for determining FTMPEP's with corrections from neighboring paths included. This Hartree self-consistent field approximation is in principle capable of taking into account higher-order corrections which are difficult to obtain by the conventional loop expansion.

Our Hartree approximation scheme for the distribution function requires further development. It would be an interesting problem to study the application of this Hartree method to finite-temperature systems. The possible returns are high because of the self-consistent calculation automatically includes some (but not necessarily all) higher-order corrections. As for the loop expansion, it would be useful to calculate the next-order correction beyond Gaussian fluctuations. This is necessary to extend the applicability of the semiclassical approximation. Finally, our results remain to be generalized to include couplings between scalar, fermion, and gauge fields. To take account of density effects, finite values of the chemical potential μ must also be included [i.e., one must calculate the grand canonical distribution function $\rho(\phi)=\langle\phi|\exp(-\beta H+\mu N)|\phi\rangle$ and the grand canonical partition function].

In Sec. II we discussed the distinction between calorons and FTMPEP's with regard to the semiclassical partition function. The question arises as to how much information in the partition function is missed by using vacuum fields and calorons alone. This question was recently addressed by Gross *et al.*[23] for a Yang-Mills gauge theory. They conclude that the classical fields dominating the functional integral expression for the partition function are vacuum fields, periodic instantons, and magnetic monopoles. The Prasad-Sommerfield monopole is a gauge transform of the $\rho T\to\infty$ limit of the periodic instanton. Also, Yang-Mills periodic instantons remain dynamic for all temperatures because unlike the symmetric double well-potential in Fig. 2, a Yang-Mills gauge theory is scale invariant.[11,19] Under what general conditions vacuum fields and calorons alone are sufficient to dominate the semiclassical partition function should be investigated further.

Even if vacuum fields and calorons alone dominate the Yang-Mills partition function in the high temperature regime, the utility of the distribution function is not reduced since it contains more thermodynamic information than the partition function. The evaluation of $\rho(A_\mu)$ in Eq. (4.37) for a non-Abelian gauge theory is, to say the least, a challenge. As the mathematical machinery to solve nonlinear partial differential equations improves, Eq. (4.37) will become more tractable. Our initial effort at least demonstrates that the problem is physically well posed and it is hoped it will generate further interest. A better understanding of finite-temperature gauge theory will certainly find application in cosmological and astrophysical problems.[37,38] Finite-temperature QCD may hold as yet unknown experimental predictions for perturbative and nonperturbative phenomena in colliding-beam experiments and heavy-ion collisions.[39,40]

Added notes. After the completion of this work, we became aware of a paper by H. Hata and T. Kugo [Phys. Rev. D 21, 3333 (1980)]. They propose a modified statistical operator $\exp(-\beta H-\pi Q_c)$ rather than the usual form $\exp(-\beta H)$ for the physical equilibrium system in gauge theory, where Q_c is the Faddeev-Popov "ghost charge." Their ghost-charge method for fixing the gauge is equivalent to the more familiar method used in the literature and in our work. The diagrammatic expansion for the partition function is discussed in their operator formalism, and Bernard's[32] path-integral rule that the Faddeev-Popov ghosts should be assigned periodic Green's functions in spite of their Fermi statistics is confirmed. The gauge independence of physical quantities is also discussed.

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APPENDIX A: PROBABILITY DISTRIBUTION FUNCTION FOR THE SIMPLE HARMONIC OSCILLATOR

We will consider a one-dimensional simple harmonic oscillator, with Lagrangian

$$L\left(x,\,\frac{dx}{dt}\right)=\tfrac{1}{2}m\left(\frac{dx}{dt}\right)^2-\tfrac{1}{2}m\omega^2x^2 \tag{A1}$$

in thermodynamic equilibrium and calculate the probability distribution function semiclassically using Eq. (3.15). The effective finite-temperature Lagrangian is

$$L_{\rm eff}\,(x(\tau),\,\dot{x}(\tau))=-\left[\tfrac{1}{2}m\dot{x}^2+\tfrac{1}{2}m\omega^2x^2\right], \tag{A2}$$

where

$$\dot{x}=dx/d\tau\;. \tag{A3}$$

First, the FTMPEP with periodic boundary conditions $x(0)=x(\hbar\beta)=x$ must be determined. The Euclidean equation of motion is

$$\frac{d^2x(\tau)}{d\tau^2}=\omega^2\,x(\tau) \tag{A4}$$

which has the general solution

$$x(\tau)=ae^{\omega\tau}+be^{-\omega\tau}\;. \tag{A5}$$

Imposing the periodic boundary conditions, one easily obtains the FTMPEP

$$x_{\rm CL}(\tau)=x\left[(1-e^{-\beta\hbar\omega})e^{\omega\tau}+(e^{\beta\hbar\omega}-1)e^{-\omega\tau}\right]/(e^{\beta\hbar\omega}-e^{-\beta\hbar\omega}). \tag{A6}$$

From this follows

$$\dot{x}_{\rm CL}(\tau)=\omega x\frac{\left[(1-e^{-\beta\hbar\omega})e^{\omega\tau}-(e^{\beta\hbar\omega}-1)e^{-\omega\tau}\right]}{(e^{\beta\hbar\omega}-e^{-\beta\hbar\omega})} \tag{A7}$$

Integrating Eq. (A2) over τ, we have

$$\int_0^{\hbar\beta}d\tau\;L_{\rm eff}(x_{\rm CL},\,\dot{x}_{\rm CL})=\frac{-m}{2}\int_0^{\hbar\beta}d\tau(\dot{x}_{\rm CL}{}^2+\omega^2x_{\rm CL})^2$$

$$=\frac{-m}{2}\,x_{\rm CL}\dot{x}_{\rm CL}\Big|_0^{\hbar\beta}\;. \tag{A8}$$

Using Eqs. (A6) and (A7), we obtain

$$x_{\rm CL}\dot{x}_{\rm CL}\Big|_0^{\hbar\beta} = 2\omega x^2 \tanh(\beta\hbar\omega/2)\ . \tag{A9}$$

Equation (A8) now becomes

$$\int_0^{\hbar\beta} d\tau\, L_{\rm eff}\,(x_{\rm CL}, \dot{x}_{\rm CL}) = -m\omega x^2 \tanh(\beta\hbar\omega/2)\ . \tag{A10}$$

By Eq. (3.15), the distribution function is then

$$\rho(x) = \left[\frac{m}{2\pi\beta\hbar^2}\,\frac{\det(-d^2/d\tau^2)}{\det(-d^2/d\tau^2+\omega^2)}\right]^{1/2} \times \exp\left[\frac{-m\omega x^2}{\hbar}\tanh(\beta\hbar\omega/2)\right]\ . \tag{A11}$$

It remains to calculate the determinants. The eigenfunctions satisfying

$$(-d^2/d\tau + \omega^2)\eta^{(n)}(\tau) = \omega_n{}^2\,\eta^{(n)}(\tau)\ , \tag{A12}$$

with the boundary conditions $\eta^{(n)}(0) = \eta^{(n)}(\hbar\beta) = 0$, are

$$\eta^{(n)}(\tau) = \sin(n\pi\tau/\hbar\beta),\quad n = 1, 2, \ldots\ . \tag{A13}$$

The determinants in Eq. (A11) are thus[28]

$$\det(-d^2/d\tau^2) = \prod_{n=1}^{\infty}(n^2\pi^2/\hbar^2\beta^2)\ , \tag{A14}$$

$$\det(-d^2/d\tau + \omega^2) = \prod_{n=1}^{\infty}\left(\frac{n^2\pi^2}{\hbar^2\beta^2} + \omega^2\right)\ . \tag{A15}$$

The ratio of determinants in Eq. (A11) is[28, 41]

$$\left[\frac{\det(-d^2/d\tau^2)}{\det(-d^2/d\tau^2+\omega^2)}\right]^{1/2} = \prod_{n=1}^{\infty}\left(1 + \frac{\hbar^2\beta^2\omega^2}{n^2\pi^2}\right)^{-1/2} = \left(\frac{\beta\hbar\omega}{\sinh(\beta\hbar\omega)}\right)^{1/2}\ . \tag{A16}$$

Substituting this into Eq. (A11) yields

$$\rho(x) = \left[\frac{m\omega}{2\pi\hbar\sinh(\beta\hbar\omega)}\right]^{1/2} \times \exp\left[\frac{-m\omega x^2}{\hbar}\tanh(\beta\hbar\omega/2)\right]\ . \tag{A17}$$

Reassuringly, this is the exact quantum-mechanical probability distribution function for a simple harmonic oscillator in thermodynamic equilibrium.[28] The partition function is then

$$Z = \int \rho(x)dx = (2\sinh\hbar\beta\omega/2)^{-1} = \exp\left[\frac{-\beta\hbar\omega}{2} - \ln(1 - e^{-\beta\hbar\omega})\right]\ , \tag{A18}$$

which is the usual result.

APPENDIX B: PROBABILITY DISTRIBUTION FUNCTION FOR A FREE SCALAR FIELD THEORY

We consider a four-dimensional free scalar field theory with Lagrangian

$$\mathcal{L}(\phi) = \tfrac{1}{2}\left[\left(\frac{\partial\phi}{\partial t}\right)^2 - (\nabla_x\phi)^2 - m^2\phi^2\right] \tag{B1}$$

in thermodynamic equilibrium and calculate the semiclassical probability distribution function using Eq. (4.14). Because $\mathcal{L}_{\rm eff}$ is quadratic in ϕ, it is convenient to Fourier transform x to k in Eq. (4.14):

$$\rho(\phi) = \left[\prod_k (2\pi\hbar^2\beta)^{-1}\,\frac{\det(-\partial^2/\partial\tau^2)}{\prod_k\det(-\partial^2/\partial\tau^2 + k^2 + m^2)}\right]^{1/2} \times \exp\left\{\frac{-1}{2\hbar}\int_0^{\hbar\beta} d\tau \int\frac{d^3k}{(2\pi)^3}\left[\left(\frac{\partial\phi_{\rm CL}(k,\tau)}{\partial\tau}\right)^2 + \omega^2(k)\,\phi_{\rm CL}^2(k,\tau)\right]\right\}, \tag{B2}$$

where $\omega^2(k) = k^2 + m^2$, $\phi_{\rm CL}(k, \tau)$ is the Fourier transform of the FTMPEP $\phi_{\rm CL}(x, \tau)$, and the product $\prod_k$ is over unit cubes in momentum space (analog of $\prod_x$). The exponential in Eq. (B2) can be written as

$$\prod_k \exp\left\{\frac{-1}{2\hbar}\int_0^{\hbar\beta} d\tau\left[\left(\frac{\partial\phi_{\rm CL}(k,\tau)}{\partial\tau}\right)^2 + \omega^2(k)\phi_{\rm CL}(k,\tau)\right]\right\} \tag{B3}$$

We have now reduced the calculation to an infinite product (one for each k) of independent, frequency-$\omega(k)$, harmonic-oscillator contributions.

For each oscillator, we can use the results of Appendix A. We then find

$$\rho(\phi) = \prod_k\left[\left(\frac{1}{2\pi\hbar}\,\frac{\omega(k)}{\sinh\beta\hbar\omega(k)}\right)^{1/2} \times \exp\left(\frac{-\omega(k)\phi^2(k)}{\hbar}\tanh[\beta\hbar\omega(k)/2]\right)\right], \tag{B4}$$

which is the exact distribution function for a spinless ideal Bose gas.[32] The field of $\phi(k)$ is the Fourier transform of $\phi(x)$. Equation (B4) can be written in continuum notation as

$$\rho(\phi)=\exp\left\{\int\frac{d^3k}{(2\pi)^3}\ln\left[\left(\frac{1}{2\pi\hbar}\frac{\omega(k)}{\sinh\beta\hbar\omega(k)}\right)^{1/2}\exp\left(\frac{-\omega(k)\phi^2(k)}{\hbar}\tanh[\beta\hbar\omega(k)/2]\right)\right]\right\}. \tag{B5}$$

The partition function is then

$$Z_\phi=\int D\phi\,\rho(\phi)=\prod_k\left(2\sinh\frac{\hbar\beta\omega(k)}{2}\right)^{-1}=\exp\left\{\int\frac{d^3k}{(2\pi)^3}\left[\frac{-\beta\hbar\omega(k)}{2}-\ln(1-e^{-\beta\hbar\omega(k)})\right]\right\}. \tag{B6}$$

This is the usual result for a spinless ideal Bose gas, with the zero-point energy of the vacuum included.

APPENDIX C: PROBABILITY DISTRIBUTION FUNCTION FOR A PURE ABELIAN GAUGE THEORY

We consider a four-dimensional pure Abelian gauge theory with Lagrangian

$$\mathcal{L}(A_\mu)=-\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu} \tag{C1}$$

in thermodynamic equilibrium and calculate the semiclassical probability distribution function in the Feynman gauge using Eq. (4.37).

In the Feynman gauge ($\partial_\mu A^\mu=0,\ \alpha=1$), Eq. (4.37) becomes

$$\rho(A_\mu)=N(\beta)\oint_0^0 D\eta_\mu(x,\tau)\oint D\phi^*(x,\tau)D\phi(x,\tau)$$
$$\times\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\int d^3x\,(\tfrac{1}{2}\eta_\mu\partial_\nu\partial^\nu\eta^\mu-\phi^*\partial_\nu\partial^\nu\phi)\right]\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\int d^3x\,\mathcal{L}_{\text{eff}}(A_\mu^{\text{CL}})\right] \tag{C2}$$
$$=N(\beta)\frac{\det M_{\text{ghost}}}{(\det M_A)^{1/2}}\exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\int d^3x\,\mathcal{L}_{\text{eff}}(A_\mu^{\text{CL}})\right], \tag{C3}$$

where

$$N(\beta)=\frac{[\det_A(-\partial^2/\partial\tau^2)]^2}{\det_{\text{ghost}}(-\partial^2/\partial\tau^2)}\prod_x(2\pi\hbar^2\beta)^{-2}, \tag{C4}$$

$$M_A\eta_\mu=\partial_\nu\partial^\nu\eta_\mu, \tag{C5}$$

with $\eta_\mu(x,0)=\eta_\mu(x,\hbar\beta)=0$,

$$M_{\text{ghost}}\phi=-\partial_\mu\partial^\mu\phi, \tag{C6}$$

with $\phi(x,\tau)=\phi(x,\tau+\hbar\beta)$, and

$$\mathcal{L}_{\text{eff}}(A_\mu^{\text{CL}}(x,\tau))=-\tfrac{1}{2}\partial_\mu A_\nu^{\text{CL}}(x,\tau)\partial^\mu A^\nu_{\text{CL}}(x,\tau), \tag{C7}$$

with $A_\mu^{\text{CL}}(x,0)=A_\mu^{\text{CL}}(x,\hbar\beta)=A_\mu(x)$.

Equation (C3) now takes the explicit form

$$\rho(A_\mu)=\frac{\det_{\text{ghost}}(\partial_\mu\partial^\mu)}{\det_{\text{ghost}}(-\partial^2/\partial\tau^2)}\times\left[\prod_x(2\pi\hbar^2\beta)^{-1/2}\frac{[\det_A(-\partial^2/\partial\tau^2)]^{1/2}}{[\det_A(\partial_\mu\partial^\mu)]^{1/2}}\right]^4\times\exp\left(\frac{-1}{2\hbar}\int_0^{\hbar\beta}d\tau\int d^3x\,\partial_\mu A_\nu^{\text{CL}}\partial^\mu A^\nu_{\text{CL}}\right). \tag{C8}$$

The exponential is the product of four terms, one for each ν. Each term is identical in form to that of the scalar field theory discussed in Appendix B. The ghost determinants are straightforward and one obtains

$$\rho(A_\mu)=Z_\phi^{-2}\prod_{\mu=0}^{3}\rho'(A_\mu), \tag{C9}$$

where $\rho'(A_\mu)$ is given by Eq. (B5) with $A_\mu(k)$ replacing $\phi(k)$. This is the exact distribution function for a massless spin-1 ideal Bose gas in the Feynman gauge.[32] The partition function is then

$$Z_A=Z_\phi^{-2}\int DA_0\,\rho'(A_0)\times\int DA_1\rho'(A_1)\int DA_2\rho'(A_2)\int DA_3\rho'(A_3)$$
$$=Z_\phi^2$$
$$=\exp\left\{2\int\frac{d^3k}{(2\pi)^3}\left[\frac{-\beta\hbar\omega(k)}{2}-\ln(1-e^{-\beta\hbar\omega(k)})\right]\right\}. \tag{C10}$$

This is the usual result for a massless vector ideal Bose gas. The two physically allowed polarization states (two degrees of freedom) are evident from the form Z_ϕ^2, which is a gauge-invariant result.

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