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Quantum-field transition rates at finite temperatures

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The Euclidean solutions (instantons) discovered in field theories seem to be interpretable as tunnelings between vacuums with different winding numbers. The associated transition rate for such tunnelings has been estimated. We study the effect of temperature on the transition rate between quantum-field configurations in thermodynamic equilibrium. We do this by extending the "most probable escape path" (MPEP) WKB vacuum-tunneling formalism of Bitar and Chang to finite temperatures. Our approach employs elementary results from quantum statistical mechanics. We believe the method offers an easily calculable approximation for quantum-field transition rates at finite temperatures.

I. INTRODUCTION

The discovery of finite-action solutions to the Euclidean equations of motion in field theories[1-4] has generated much interest due to the implications for non-Abelian gauge theories (e.g., the Yang-Mills gauge theory[5]). Being Euclidean solutions, the "instantons" or "pseudoparticles," as these solutions are referred to, appear to be interpretable as tunnelings among vacuums with different winding numbers[6-12] (i.e., transitions between ground-state field configurations; the phenomenon is analogous to the quantum-mechanical tunneling of a particle in a multistable potential). The instanton solution interpolates between the initial and final classically allowed field configurations.

The winding number is an integer which indexes the pseudoparticle solutions (just as eigenvalues may be said to index eigenvector solutions) and can thus be associated with the field transitions. The winding number is also referred to in the literature as the Pontryagin index, the topological number (or charge), and the degree of mapping. If the instanton solutions can be separated into homotopy (topologically distinct) classes, describing transitions between physically distinct vacuum configurations, the winding number can be used to actually label the vacuum configurations. The winding number now becomes a topological index distinguishing field configurations and leads to the so-called multiple- or θ-vacuum description of the field theory. In the event that the vacuum configuration is unique, the winding number is not a physically meaningful index for the vacuum configurations (there being only one), but of course remains a valid mathematical index for the instanton solutions.

The instantons and their relation to the multiple-vacuum description may play an important role in determining many properties of non-Abelian gauge theories (e.g., quark confinement, breakdown of axial baryon-number symmetry without the generation of a Goldstone boson, and a possible source of T violation[7-9]). If such gauge theories are a reasonable description of fundamental processes and interactions, as we presently believe, a more complete understanding of the instantons is clearly desirable.

One quantity of interest is the transition rate for instanton-mediated vacuum tunnelings. The mechanism of vacuum tunneling in Minkowski space and its relation to the instantons have been studied in some detail semiclassically,[10-12] and the transition rate for these tunnelings has been estimated.[11,12] Gervais and Sakita[10] have studied such transitions using the collective coordinate method. Bitar and Chang[11,12] have concentrated on a single collective mode and studied vacuum transitions by generalizing the "most probable escape path" (MPEP) WKB formalism of Banks, Bender, and Wu[13] to the function space in field theory. The idea behind this generalization is to reduce the infinite-dimensional field transition to an approximate one-dimensional quantum-mechanical tunneling problem by finding the paths in the function space which have the minimum (Euclidean) action and thus maximum WKB tunneling amplitude. This approach is possible because the field transition is already described naturally by a single parameter, namely the instanton winding number.

Parametrizing the vacuum-tunneling problem in terms of a one-dimensional winding-number space enables one to treat the instanton-mediated field transition like a particle tunneling through a potential barrier. Using the instanton solutions, Bitar and Chang[11,12] have shown how to construct a family of field configurations producing the maximum WKB tunneling rate (MPEP in field space) and also how to obtain the one-dimensional potential-energy barrier in winding-number space

through which the tunneling occurs.

In this paper we wish to begin a study of the effect of temperature on such quantum-field transition rates. We will do this by generalizing the zero-temperature MPEP formalism of Bitar and Chang to finite temperatures for systems in thermodynamic equilibrium. The semiclassical approximations we will employ are inherently valid only in the weak-coupling limit. This is because we are considering tunneling amplitudes which in the semiclassical approximation have the form[7]

$$\exp\left[-\frac{a_0}{g^2}(1+a_1g^2+a_2g^4+\cdots)\right], \tag{1.1}$$

where g is the coupling constant, a_0/g^2 is the classical action, and the latter terms are the one-loop, two-loop, and higher corrections. Clearly, once the coupling constant becomes of order unity, there is no guarantee that the classical action term alone will dominate the amplitude. As the coupling constant increases, the higher-order fluctuations, as represented by the terms in the loop expansion, increase. Once the effective coupling is no longer small, field configurations other than those which minimize the action become important.[9] Similar considerations must be weighed regarding important additional transition modes at very high temperatures and are discussed in Sec. II. The study of such modes is an interesting but separate problem which will not be addressed in this paper.

This paper is organized as follows. In Sec. II we discuss the one-parameter WKB approximation for multidimensional quantum transition amplitudes at both zero and finite temperatures and define the field transition rate as it will be used in this paper. In Sec. III we present a semiclassical approximation for the finite-temperature field transition rate for systems in thermodynamic equilibrium. The approximation uses known results from quantum-mechanical transition-rate theory[14,15] and is essentially a statistical-mechanical extension of the zero-temperature semiclassical formalism of Bitar and Chang.[11,12] In Sec. IV we apply our method to study the temperature dependence of finite-temperature instanton-mediated field transitions in the two-dimensional nonlinear σ model.[16,17] We find that the thermodynamic equilibrium transition rate between aligned-spin configurations increases in a simple manner. This increase results from excited transition modes in the quantized degree of freedom. The vacuum-tunneling instantons are found to be the zero-temperature remnants of these modes. The energy spectrum of the excited modes is straightforward to calculate in our approximation. In Sec. V we discuss the implications of our findings in the σ model for field transitions in non-Abelian gauge theories. We also suggest further problems for study and possible applications of our finite-temperature formalism.

Because the one-dimensional WKB ansatz to the Schrödinger equation is of fundamental importance in the MPEP method, we collect certain WKB results[18] in Appendix A. In Appendix B we apply the finite-temperature formalism of Sec. III to equilibrium transitions in a one-dimensional bistable potential. This appendix is not intended solely for aficionados of diffusion processes, rather it is a useful primer to our σ-model example in Sec. IV. The effect of quantum and thermal Gaussian fluctuations on transition amplitudes is discussed in Appendix C. In that appendix we formulate the semiclassical transition amplitude approximation in the language of path integrals rather than WKB wave functionals. The two methods are entirely equivalent, of course, because each uses the first-quantized solution of the Euler-Lagrange equation of motion to extract the leading behavior of the transition amplitude, and both treat Gaussian fluctuations as small corrections. It is a matter of convenience of which to use in practice. The path-integral formulation allows one to obtain corrections to the amplitude due to fluctuations directly from the loop expansion.

II. THE WKB APPROXIMATION FOR TRANSITION AMPLITUDES IN MULTIDIMENSIONAL SYSTEMS

Semiclassical approximation methods have become recognized as very useful techniques for studying quantum systems.[19,20] Such methods attempt to follow as close as possible well-understood classical solutions adding quantum interference effects by using amplitudes rather than probabilities alone. In many systems interference seems to be the primary quantum effect, thus accounting for the success of semiclassical methods in such cases. Unfortunately, in many instances such methods are also the only practical means known of doing certain calculations.

This is particularly evident in the case of quantum-field theory whose infinite dimensionality has proven to be problematical. In studying quantum-field transitions, presently available analytic techniques suggest that we concentrate on particular modes. This is all quite analogous to the problem of studying multidimensional tunneling in ordinary quantum mechanics. In one dimension the WKB method is a relatively simple approximation for obtaining quantum-mechanical amplitudes (see Appendix A). 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 simply intractable unless one can reduce them to an approximate one-dimensional problem.

One class of reduction methods is variational in nature. In classical mechanics the principle of least action determines the classical paths of a Hamiltonian system.[21] In a tunneling region the analog of the classically allowed path is called the "most probable escape path" (MPEP). Along an MPEP the (Euclidean) action is a minimum. The idea of most probable escape paths was first introduced into the multidimensional WKB method by Banks, Bender, and Wu.[13] Gervais and Sakita have studied the extension of WKB methods to infinite-dimensional spaces using the collective coordinate method.[10] Bitar and Chang have also extended the MPEP concept into the function space in field theory by considering only a single collective mode[11] and Gaussian fluctuations away from the MPEP.[12] It is this latter approach which we will extend to finite temperatures. However, we see no immediate reason why our extension could not be used in any other semiclassical approximation, such as the collective coordinate method.

In this section we review the formulation of the (zero-temperature) multidimensional WKB method[13] as extended to field theory in Refs. 11 and 12. The reader is referred to the original papers for details. We straightforwardly generalize the method to finite-temperature field transitions by defining the field transition rate (as used in this paper) in terms of the field operator eigenstates.

In field theory each field configuration $\phi(x)$ represents a point in the infinite-dimensional field space (a function space). Given the Lagrangian density $\mathfrak{L}(\phi, \dot{\phi})$ for a theory, one wishes to determine the amplitude for a transition between eigenstates $|\phi_1\rangle$ and $|\phi_2\rangle$ of the field operator ϕ. The state vector $|\phi(x)\rangle$ describes a physical state of the system with eigenvalue (quantum-field configuration) $\phi(x)$. To reduce such an infinite-dimensional transition to an approximate one-dimensional problem, a family of intermediate field configurations $f(x, \lambda(t))$ is introduced such that $f(x, \lambda_1) = \phi_1$ and $f(x, \lambda_2) = \phi_2$, where $\lambda(t)$ is a parameter describing the field configurations within the family. The family of field configurations $f(x, \lambda(t))$ represents a path in the field space. Figure 1 illustrates such a path in the configuration space of ϕ.

At each intermediate point $f(x, \lambda)$ on this path a local orthogonal coordinate system may be established in the field space with one axis tangent to the path at $f(x, \lambda)$ and the remaining axes $\bar{n}$ orthogonal to the first. If a path can be found such that the first variations of the action in all the n_i directions vanish, then only variations along the path need be considered and the problem becomes one dimensional. This path is the classical trajectory $\phi_0(x, \lambda)$ (either the classically allowed path or the MPEP) and lies along a minimum of the classical action S_0 (either Minkowskian or Euclidean). This trajectory is necessarily a solution to the variational equation

$$\delta S_0 = 0 . \tag{2.1}$$

Effectively, the above procedure replaces the field $\phi(x, t) = \{f(x, \lambda(t)), a_1, a_2, \ldots\}$ ($\bar{a}$ along $\bar{n}$ defined above) by simply $f(x, \lambda(t))$ and suppresses all the other variables. Stated differently, in this semiclassical approximation one pair of dynamical variables $(\lambda, \dot{\lambda})$ are treated as quantum operators and the remaining variables (the a_i's) are treated as c numbers.[22]

In general, along a path $\phi(x, \lambda)$ the Lagrangian density $\mathfrak{L}(\phi, \dot{\phi})$ of the theory can be integrated over space to obtain a one-parameter Lagrangian of the form

$$L(\lambda, \dot{\lambda}) = \int \mathfrak{L}(\phi(x, \lambda), \dot{\phi}(x, \lambda)) d^3x$$
$$= \tfrac{1}{2} m(\lambda) \dot{\lambda}^2 - V(\lambda) . \tag{2.2}$$

For specificity let us consider a scalar field theory described by a Lagrangian density

$$\mathfrak{L}(\phi, \dot{\phi}) = \tfrac{1}{2}\dot{\phi}^2 - \tfrac{1}{2}(\nabla\phi)^2 - U(\phi) . \tag{2.3}$$

(The results can be generalized straightforwardly to gauge theory in the temporal gauge, $A^0 = 0$; see Ref. 11.) For this theory,

$$m(\lambda) = \int d^3x (\partial\phi/\partial\lambda)^2 \tag{2.4}$$

and

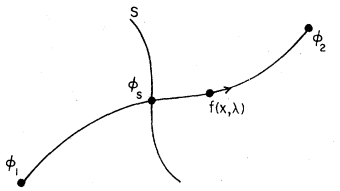

FIG. 1. A possible trajectory $f(x, \lambda(t))$ for a quantum field transition between field configurations ϕ_1 and ϕ_2 in the configuration space of the field operator ϕ. The symbol S denotes a hypersurface in the field space dividing the initial and final regions of interest for transitions. The point ϕ_S is the intersection of the path $f(x, \lambda(t))$ and the hypersurface S. If, for example, ϕ_1 and ϕ_2 were separated by a potential barrier, one might naturally choose S such that ϕ_S was the potential maximum on the path $f(x. \lambda(t))$.

$$V(\lambda)=\int d^3x[\tfrac{1}{2}(\nabla\phi)^2+U(\phi)]. \tag{2.5}$$

The corresponding Hamiltonian is

$$H(p_\lambda,\lambda)=p_\lambda^2/2m(\lambda)+V(\lambda),\quad p_\lambda=\partial L/\partial\dot{\lambda}, \tag{2.6}$$

and the action along the path $\phi(x,\lambda)$ is

$$S_0(\lambda)=\int^\lambda p(\lambda')d\lambda'=\int^\lambda\{2m(\lambda')[E-V(\lambda')]\}^{1/2}d\lambda'. \tag{2.7}$$

From Eq. (2.1) it follows that the classical trajectory $\phi_0(x,\lambda)$ can be obtained from the first-quantized solution of the Euler-Lagrange field equation (whether in a classically allowed or forbidden region) by the formal replacement of the time t (Minkowskian or Euclidean) by an arbitrary parameter $\lambda(t)$. Using Eq. (2.7), the variational principle implies from Eq. (2.1) that

$$\left(\frac{\partial}{\partial\lambda}\frac{\delta}{\delta(\partial\phi/\partial\lambda)}-\frac{\delta}{\delta\phi}\right)\{2m(\lambda)[E-V(\lambda)]\}^{1/2}=0 \tag{2.8}$$

or

$$\frac{\partial}{\partial\lambda}\left(\frac{2[E-V(\lambda)]}{m(\lambda)}\right)^{1/2}\frac{\partial\phi}{\partial\lambda}+\left(\frac{m(\lambda)}{2[E-V(\lambda)]}\right)^{1/2}\frac{\delta V}{\delta\phi}=0. \tag{2.9}$$

Now introduce a new parametrization $\tau(t)=\tau(\lambda(t))$ through

$$\frac{d\tau(\lambda)}{d\lambda}=\left(\frac{m(\lambda)}{2[E-V(\lambda)]}\right)^{1/2} \tag{2.10}$$

and note that from Eq. (2.5)

$$\delta V/\delta\phi=-\nabla^2\phi+\partial U/\partial\phi. \tag{2.11}$$

Equation (2.9) then becomes

$$\partial^2\phi/d\tau^2-\nabla^2\phi+\partial U(\phi)/\partial\phi=0, \tag{2.12}$$

which is identical in form to the Euler-Lagrange equation of motion for the field $\phi_0(x,\tau)$ with the parameter τ formally replacing the time t.

To obtain the approximate amplitude for the quantum-field transition between ϕ_1 and ϕ_2, we introduce the following semiclassical approximation. We assume that the dominant effect on the transition amplitude due to the existence of a classical trajectory $\phi_0(x,\lambda)$ connecting ϕ_1 and ϕ_2 is contained in the quantum mechanics of this degree of freedom.[10] On this assumption we then quantize the motion along this degree of freedom to obtain the one-parameter WKB wave functions (and thus the amplitudes) and their energy eigenvalues. (The effect of small Gaussian fluctuations away from the classical trajectory is discussed in Appendix C.) From Eq. (A5) in Appendix A, the first-order WKB wave functionals along the path $\phi_0(x,\lambda)$ are given by

$$\psi_E(\lambda)=\langle\phi_0(x,\lambda)\,|\,E\rangle=\left(\frac{1}{p(\lambda)}\right)^{1/2}\exp[\pm iS_0(\lambda)], \tag{2.13}$$

where $p(\lambda)$ and $S_0(\lambda)$ are defined in Eqs. (2.6) and (2.7). The infinite-dimensional quantum-field transition from ϕ_1 to ϕ_2 can thus be treated like a particle with λ-dependent mass $m(\lambda)$ moving in a potential $V(\lambda)$ from λ_1 to λ_2.

Finally, one may introduce another parametrization of the classical trajectory $\phi_0(x,\lambda)$ which yields a one-dimensional Hamiltonian with a constant mass rather than a λ-dependent one. Define a new parameter $Q(\lambda)$ and mass M by

$$\tfrac{1}{2}M\dot{Q}^2=\tfrac{1}{2}m(\lambda)\dot{\lambda}^2, \tag{2.14}$$

$$Q(\lambda)=\int_{\lambda_1}^{\lambda}[m(\lambda')]^{1/2}d\lambda'\Big/\int_{\lambda_1}^{\lambda_2}[m(\lambda')]^{1/2}d\lambda', \tag{2.15}$$

and

$$M=\left(\int_{\lambda_1}^{\lambda_2}[m(\lambda)]^{1/2}d\lambda\right)^2. \tag{2.16}$$

Along the trajectory $\phi_0(x,Q)$ the Lagrangian and action are, respectively,

$$L(Q,\dot{Q})=\tfrac{1}{2}M\dot{Q}^2-V(Q), \tag{2.17}$$

$$S_0(Q)=\int^Q p(Q')dQ'=\int^Q\{2M[E-V(Q)]\}^{1/2}. \tag{2.18}$$

Depending on the particular problem, it may be simpler to quantize the motion along the classical trajectory in terms of Q rather than λ. The first-order WKB energy eigenfunctionals along the path $\phi_0(x,Q)$ are given by

$$\psi_E(Q)=\langle\phi_0(x,Q)\,|\,E\rangle=\left(\frac{1}{p(Q)}\right)^{1/2}\exp[\pm iS_0(Q)]. \tag{2.19}$$

The transition of the system from the configuration ϕ_1 to ϕ_2 can now be treated, semiclassically, like a particle with constant mass M moving in a one-dimensional potential $V(Q)$ from Q_1 to Q_2. In general, knowledge of the transition amplitudes $\langle\phi_j\,|\,\phi_k\rangle$ and the wave functionals (or an approximation to them) $\psi(\phi)=\langle\phi\,|\,\psi\rangle$ for arbitrary states $|\psi_f\rangle$ and $|\psi_i\rangle$ is sufficient to calculate the transition amplitude $\langle\psi_f\,|\,\psi_i\rangle$. This is because any state $|\psi\rangle$ can be written as

$$|\psi\rangle=\sum_k|\phi_k\rangle\langle\phi_k\,|\,\psi\rangle=\sum_k|\phi_k\rangle\psi(\phi_k), \tag{2.20}$$

so that

$$\langle\psi_f\,|\,\psi_i\rangle=\sum_{j,k}\langle\phi_j\,|\,\phi_k\rangle\psi_f^*(\phi_j)\psi_i(\phi_k). \tag{2.21}$$

At finite temperatures we will be interested in the thermodynamic equilibrium transition rate for an equilibrium distribution of field configurations

$\phi(x, \lambda)$ [i.e., distributed in energy eigenstates $\psi_E(\phi(x, \lambda))$ weighted with Boltzmann factors $\exp(-\beta E)$] in the region $\phi(x, \lambda) \in [\phi_1, \phi_s]$ to cross some predefined hypersurface S in the field space over to a region $\phi(x, \lambda) \in [\phi_s, \phi_2]$ (Fig. 1). Consequently, this transition rate might be called more correctly a "crossing rate," that is, the number of unidirectional crossings per unit time of states through the hypersurface S. For example, if ϕ_1 and ϕ_2 were separated by a potential barrier, one might naturally choose S such that ϕ_s was the potential maximum on the path $\phi(x, \lambda)$. As defined, our transition rate is the field-theoretic analog of the equilibrium transition rate familiar from molecular chemistry for an equilibrium ensemble of particles crossing a potential barrier. The particles with positions x in coordinate space are analogous to the field configurations ϕ in field space.

The amplitude for a transition from ϕ to ϕ' is given by the density matrix in the configuration representation of the field operator ϕ as[26,31]

$$\begin{aligned}\rho(\phi', \phi) &= Z^{-1}\rho_u(\phi', \phi) \\ &= Z^{-1}\langle\phi'|e^{-\beta H}|\phi\rangle \\ &= Z^{-1}\sum_i \langle\phi'|e^{-\beta H}|E_i\rangle\langle E_i|\phi\rangle \\ &= Z^{-1}\sum_i e^{-\beta E_i}\psi_i(\phi')\psi_i^*(\phi), \end{aligned} \tag{2.22}$$

where β is the inverse temperature, Z is the partition function, and ρ_u is the unnormalized density matrix. The matrix ρ_u satisfies the equation[26]

$$-\partial\rho_u/\partial\beta = H\rho_u, \tag{2.23}$$

where the Hamiltonian H is obtained by integrating the Hamiltonian density $\mathcal{H}(\pi, \phi)$ over space. Along the classical trajectory $\phi_0(x, \lambda)$ the density matrix may be approximated by using the one-parameter WKB wave functions from Eq. (2.19) as

$$\rho(Q', Q) = Z^{-1}\sum_i e^{-\beta E_i}\psi_i(Q')\psi_i^*(Q). \tag{2.24}$$

The validity of the one-parameter approximation in Eq. (2.24) for the density matrix $\rho(Q', Q)$ depends on the dominance of the quantized modes along the classical trajectory with respect to other modes. It is quite possible that at very high temperatures other trajectories connecting ϕ and ϕ' may become important. Strictly speaking, what we have calculated in Eq. (2.24) is the contribution to $\rho(Q', Q)$ from excited modes in the degree of freedom which was most important at zero temperature. This caveat, as well as that of weak coupling (see Sec. I), are implicit in our semiclassical approximation.

We have now reduced the infinite-dimensional quantum-field transition problem to a semiclassical one-dimensional quantum-mechanical transition problem, at both zero and finite temperatures. The preceding discussion has been kept sufficiently general so as not to reduce its applicability to transition problems in arbitrary systems with many degrees of freedom. Our interest in this paper is on the effect of temperature on the "crossing rate" (as defined above) between quantum-field configurations separated by a potential barrier in field-theoretic applications.

The instantons found in field theories have been interpreted as (zero-temperature) tunnelings between classical vacuums separated by a potential barrier. At absolute zero in the absence of external sources only vacuum tunnelings will occur due to energy conservation, and so the crossing rate is simply the vacuum-tunneling rate. The WKB vacuum-tunneling amplitude for the MPEP is given by Eq. (A18) in Appendix A, where the (Euclidean) action R_0 is

$$R_0 = \int_{\lambda_1}^{\lambda_2} d\lambda\{2m(\lambda)[V(\lambda) - E]\}^{1/2}, \tag{2.25}$$

with $\phi(x, \lambda_1)$ and $\phi(x, \lambda_2)$ being the initial and final vacuum field configurations, respectively. The integral in Eq. (2.25) is along the MPEP, and R_0 is thus a minimum. It may be possible to determine, estimate, or guess a lower bound to R_0 by some heuristic argument without actually working out the integral.

If one must carry out the integration in Eq. (2.25), an explicit parametrization of the MPEP field configurations $\phi_0(x, \lambda(t))$ is required. Since the discovery of instantons and their subsequent interpretation as vacuum tunnelings in Minkowski space, it has been realized that (in the temporal gauge $A^0 = 0$) the formal replacement of the Euclidean time $\tau(=it)$ by an arbitrary parameter $\lambda(t)$ in the instanton solution yields the field configurations $\phi_0(x, \lambda(t))$ corresponding to the MPEP in function space. (See Sec. VI and Appendix B in Ref. 11, and Secs. I, III, and IV in Ref. 12; our general discussion earlier was based in part on these special zero-temperature results.) This is yet another indication that the instantons represent tunnelings in Minkowski space among vacuums with different winding numbers.

The winding number is very useful as a tunneling parameter.[11] As just noted, the MPEP for the vacuum tunneling is parametrized by a function $\lambda(t)$ in the instanton solution. This solution in turn is characterized by an integer winding number. Since the evolution of the vacuum tunneling is described by the instanton solution, one can parametrize the transition by a continuous

winding number $Q(\lambda(t))$ rather than $\lambda(t)$. This new continuous winding number is chosen to agree with the original winding number at integer values. Additionally, Q is defined as in Eq. (2.15), yielding a constant mass rather than a λ-dependent mass in the Lagrangian of Eq. (2.2). Such a reparametrization allows one to work in the very simple one-dimensional world of the winding-number space. The vacuum tunneling may then be treated like a particle of constant mass tunneling through a potential barrier in the new winding-number space. The tunneling rate of this fictitious particle is equal to the vacuum tunneling rate in the field space.

The great attraction of the MPEP method developed by Bitar and Chang[11,12] is that it reduces the infinite-dimensional vacuum tunneling described by the instanton to a one-dimensional quantum-mechanical approximation for the tunneling rate. In Sec. III we present a statistical-mechanical extension of this zero-temperature semiclassical rate formalism to finite temperatures.

III. FINITE-TEMPERATURE FIELD TRANSITION RATES

The MPEP approximation outlined briefly at the end of Sec. II offers a convenient method for approximating vacuum-to-vacuum field transition rates. The tacit assumption of course is that the transitions occur at zero temperature. At zero temperature only vacuum tunnelings can occur in the absence of external sources. At finite temperatures all field transitions between vacuum and excited configurations (consistent with energy conservation for the system plus surroundings) can occur. We wish to generalize the MPEP transition-rate approximation to finite temperatures.

In Sec. II we discussed how to reduce the field-theoretic transition problem to an approximate one-dimensional quantum-mechanical problem using semiclassical methods. The energy spectrum and one-parameter WKB wave functionals for the quantum states corresponding to the quantized motion along a classical trajectory (ignoring orthogonal modes) can be calculated from Eqs. (2.17), (2.18), and (2.19). In Eq. (2.24) we obtained a one-dimensional semiclassical approximation for the density matrix $\rho(\phi', \phi)$ along the classical trajectory connecting the quantum-field configurations ϕ and ϕ'. Equation (2.24) and the associated formalism of Sec. II allow us to study (semiclassically) transitions in the finite-temperature field theory using familiar one-dimensional quantum statistical mechanics. In this section we present a semiclassical approximation for the finite-temperature field transition rate (the "crossing rate" as defined in Sec. II) for systems in thermodynamic equilibrium.

Specifically, we want a finite-temperature approximation for the field transition rate K (number of transitions per unit time in a unit volume of space) between a specified set of initial and final quantum-field configurations $\phi(x)$ separated by an effective potential barrier. We assume that the region of space in which the transitions occur is in thermodynamic equilibrium and also that the effective potential is temperature independent. (See Appendix C for the relaxation of this latter assumption.) Recall from Sec. II that, semiclassically, a transition between vacuum field configurations at zero temperature can be treated like the tunneling of a particle through a one-dimensional potential barrier in the winding-number space. The tunneling rate of this fictitious particle is equal to the vacuum tunneling rate in the field space. This naturally suggests that, within the semiclassical approximation described in Sec. II, we may treat a finite-temperature field transition as this same particle crossing the same potential barrier but at nonzero temperature. Thus to solve the field-theoretic problem in the spirit of the zero-temperature MPEP method, we must proceed to study the statistical-mechanics problem of a particle crossing a potential barrier at finite temperature. If we can obtain an expression for the crossing rate of such a particle past a potential barrier, we will have our desired approximation for the field transition rate in the field space. This procedure is justified by the results in Sec. II and is effectively a statistical-mechanical extension of the zero-temperature semiclassical formalism of Bitar and Chang.[11,12]

A quantum-mechanically valid expression for the transition rate of a particle moving across a potential surface at finite temperatures is well known from quantum-mechanical transition-rate theory.[15] Thermodynamic rate calculations find application in molecular reaction-theory,[14,15] impurity-dislocation theory in solids,[23] cell-membrane transport theory,[24] and neutron/liquid ^{4}He scattering in phonon theory.[25,26] In the derivation presented here we follow the development given by Miller.[15]

Figure 2 is a one-dimensional schematic representation of a quantum-mechanical particle moving across the interaction region R of a potential surface $V(x)$. The "in" and "out" labels denote wave-function components. The most general form for the equilibrium transition rate through such a region (at constant particle number) is[15]

$$K = Z_I^{-1}\,\mathrm{tr}(e^{-\beta H}\mathfrak{F}\mathcal{P}), \tag{3.1}$$

where tr denotes trace, Z_I is the canonical parti-

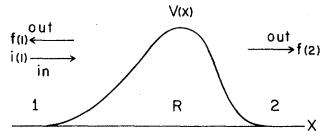

FIG. 2. One-dimensional schematic representation of a quantum-mechanical particle moving across the interaction region R of a potential surface $V(x)$. The labels "in" and "out" denote wave-function components. The labels i and f denote the initial and final states defined in Eq. (3.7).

tion function of the initial configuration, β is the inverse temperature, and H is the complete Hamiltonian (includes all interactions). The symbol $\mathcal{P}$ denotes a projection operator. In terms of momentum eigenstates for example, $\mathcal{P}$ is represented by

$$\mathcal{P}=\sum_{p_{\text{in}}}|p\rangle\langle p|\,. \tag{3.2}$$

It projects out the incoming momentum eigenstates since those states leaving the spatial interaction region R in Fig. 2 do not further contribute to the rate. The flux operator $\mathcal{F}$ (number of particles per unit time) can be formally written in multidimensional notation as

$$\mathcal{F}=\delta(f(\vec{q}))\frac{\partial f(\vec{q})}{\partial\vec{q}}\cdot\vec{v}, \tag{3.3}$$

where $f(\vec{q})=0$ defines some closed surface surrounding the interaction region R, and $\vec{v}$ is the flux velocity. Explicitly the flux has the usual form

$$\langle\mathcal{F}\rangle=\mathrm{Re}\oint d\vec{s}\cdot\Psi^*\frac{\hbar\nabla}{im}\Psi=\mathrm{Re}\int d|\vec{q}|\,\Psi^*\,\mathcal{F}\Psi\,, \tag{3.4}$$

where $d\vec{s}$ is an area element, $d|\vec{q}|$ a volume element, $\vec{q}$ a position vector, and Ψ is a wave function. Of course, the total flux is zero by probability conservation so one must use some projection operator [e.g., $\mathcal{P}$ in Eq. (3.2)] to obtain a particular flux component. Taking the real part of fluxes will be implicit henceforth. We note that $\mathcal{F}$, $\mathcal{P}$, and $e^{-\beta H}$ all commute.

Equation (3.1) for the transition rate is seen to be simply the Gibb's average of the operator $\mathcal{F}\mathcal{P}$. Since the trace is independent of representation, Eq. (3.1) may be proved using any convenient complete set of states. In particular, this expression is straightforward to obtain using S-matrix formalism.[15,18] This approach is very useful for our purposes since the one-dimensional WKB S-matrix elements are very easy to obtain, as discussed in Appendix A. We will work in one-dimensional notation for simplicity in the following.

Consider Fig. 2. From quantum mechanics we know that the transition rate from an initial state i in region 1 across a potential $V(x)$ to a final state f in region 2 is given by[18]

$$K_{fi}=\frac{2\pi}{\hbar}|T_{fi}|^2\delta(E_i-E_f)\,, \tag{3.5}$$

where the transition matrix elements are defined by

$$T_{fi}=(\psi_f, V\psi_i^{(+)})\,. \tag{3.6}$$

In Eq. (3.6), $\psi_i^{(+)}$ is an outgoing eigenstate of the full Hamiltonian H in Eq. (3.1) with energy E_i, and ψ_f is a free-momentum eigenstate with energy E_f. Assuming the initial configuration to be in thermodynamic equilibrium, the total transition rate from region 1 to 2 is obtained by a thermal average of Eq. (3.5) over the initial incoming states in region 1 [denoted by $i(1)$] and a sum over all final outgoing states in region 2 [denoted by $f(2)$] consistent with energy conservation:

$$K=Z_I^{-1}\int\sum_{f(2)}e^{-\beta E_i}K_{fi}\delta(E_i-E_f)dE_{i(1)}\,. \tag{3.7}$$

The integral form of the thermal average in Eq. (3.7) is simply a convenient device to implicitly include both bound and continuum initial states in the general case.

Equation (3.7) can be expressed in terms of S-matrix elements by recalling that, for $i\neq f$,

$$S_{fi}=(\psi_f^{(-)}, \psi_i^{(+)})=-2\pi i T_{fi}\delta(E_i-E_f)\,, \tag{3.8}$$

where $\psi_f^{(-)}$ is an incoming eigenstate of H with energy E_f. Using Eqs. (3.5) and (3.8) in Eq. (3.7), we obtain

$$K=(2\pi\hbar Z_I)^{-1}\int\sum_{f(2)}e^{-\beta E_i}(2\pi)^2|T_{fi}|^2\times[\delta(E_i-E_f)]^2dE_{i(1)} \tag{3.9}$$

$$=(2\pi\hbar Z_I)^{-1}\int e^{-\beta E_i}\sum_{f(2)}|S_{fi}|^2dE_{i(1)}\,. \tag{3.10}$$

The S-matrix elements in Eq. (3.10) can be rewritten in terms of probability fluxes by invoking the unitarity condition for a given initial state $i(1)$

$$\sum_{f(1)}|S_{fi}|^2+\sum_{f(2)}|S_{fi}|^2=1\,, \tag{3.11}$$

where $f(1)$ denotes the final states in region 1 (i.e., reflected states in Fig. 2).

The total flux in region 1 is simply

$$\langle\psi_1^{(+)}|\mathcal{F}|\psi_1^{(+)}\rangle=1\times\frac{v_i}{2\pi\hbar}-\sum_{f(1)}\left|\frac{\psi_{\text{refl}}^{(+)}}{\psi_{\text{incid}}^{(+)}}\right|^2\frac{v_f}{2\pi\hbar}$$

$$=1\times\frac{v_i}{2\pi\hbar}-\sum_{f(1)}\frac{v_i}{v_f}|S_{fi}|^2\frac{v_f}{2\pi\hbar}$$

$$=\frac{v_i}{2\pi\hbar}\left(1-\sum_{f(1)}|S_{fi}|^2\right), \tag{3.12}$$

where we have used the fact that

$$\left| \frac{\psi^{(+)}_{\text{refl}}}{\psi^{(+)}_{\text{incid}}} \right| = \left| \left(\frac{v_i}{v_f} \right)^{1/2} S_{fi} \right| . \tag{3.13}$$

[See Eqs. (A6) and (A17); also Ref. 18.] The $(2\pi\hbar)^{-1}$ factor is from our $(1-d)$ momentum eigenstate normalization $\psi \sim (2\pi\hbar)^{-1/2} \exp(ik\cdot x)$. Similarly, the flux in region 2 is

$$\begin{aligned} \langle \psi_2^{(+)} | \mathfrak{F} | \psi_2^{(+)} \rangle &= \sum_{f(2)} \left| \frac{\psi^{(+)}_{\text{trans}}}{\psi^{(+)}_{\text{incid}}} \right|^2 \frac{v_f}{2\pi\hbar} \\ &= \sum_{f(2)} \frac{v_i}{v_f} |S_{fi}|^2 \frac{v_f}{2\pi\hbar} \\ &= \frac{v_i}{2\pi\hbar} \sum_{f(2)} |S_{fi}|^2 . \end{aligned} \tag{3.14}$$

By the unitarity condition Eq. (3.11), Eq. (3.14) is equal to Eq. (3.12). Specifically we have

$$\begin{aligned} \langle \psi_1^{(+)} | \mathfrak{F} | \psi_1^{(+)} \rangle &= \langle \psi_2^{(+)} | \mathfrak{F} | \psi_2^{(+)} \rangle \\ &= \frac{v_i}{2\pi\hbar} \sum_{f(2)} |S_{fi}|^2 . \end{aligned} \tag{3.15}$$

Equation (3.15) can now be used in Eq. (3.10) to obtain

$$K = Z_I^{-1} \int e^{-\beta E_i} \langle \psi_i^{(+)} | \mathfrak{F} | \psi_i^{(+)} \rangle \frac{dE_{i(1)}}{v_i} , \tag{3.16}$$

where we have used the fact that $\psi_1^{(+)}$ is simply $\psi_i^{(+)}$ in Eq. (3.6). Equation (3.16) can be further simplified by noting that

$$E_i = p_i^2/2m , \quad dE_i = v_i dp_i . \tag{3.17}$$

Then

$$K = Z_I^{-1} \int_0^\infty e^{-\beta E_i} \langle \psi_i^{(+)} | \mathfrak{F} | \psi_i^{(+)} \rangle dp_i , \tag{3.18}$$

where we have replaced the now superfluous subscript $i(1)$ with i since the integration limits exhibit the fact that only incoming positive-momentum states contribute to K [see Eq. (3.7)].

Since $\psi_i^{(+)}$ is an energy eigenstate of H, Eq. (3.18) can be written as

$$K = Z_I^{-1} \int_0^\infty \langle \psi_i^{(+)} | e^{-\beta H} \mathfrak{F} | \psi_i^{(+)} \rangle dp_i . \tag{3.19}$$

To write Eq. (3.19) as a trace the integral must include both negative and positive momenta. [Positive- and negative-momentum states $\psi_i^{(+)}$ (plus bound states) form a complete set.] This is accomplished by using the projection operator $\mathcal{P}$ in Eq. (3.2). We then obtain Eq. (3.1),

$$\begin{aligned} K &= Z_I^{-1} \int_{-\infty}^{+\infty} \langle \psi_i^{(+)} | e^{-\beta H} \mathfrak{F}\mathcal{P} | \psi_i^{(+)} \rangle dp_i \\ &= Z_I^{-1} \operatorname{tr}(e^{-\beta H} \mathfrak{F}\mathcal{P}) . \end{aligned} \tag{3.1}$$

Being a completely general statistical-mechanics result we are manifestly guaranteed that Eq. (3.1) will reduce to the classical equilibrium rate expression at high temperature ($T \to \infty$) and the quantum-mechanical tunneling rate at low temperature ($T \to 0$).[14,15] Basically this comes about simply because the diagonal elements of the normalized statistical-mechanics density matrix $\rho = e^{-\beta H}/Z$ reduce to the classical equilibrium distribution at high temperature

$$\rho_{\text{CL}}(x) = Z^{-1} \int \frac{d^d p}{(2\pi\hbar)^d} \exp[-\beta H(p,x)] \tag{3.20}$$

and to the quantum-mechanical ground-state probability distribution at low temperature

$$\begin{aligned} \rho_{\text{QM}}(x; T=0) &= \lim_{T\to 0} \left[\sum_n e^{-\beta E_n} \psi_n(x) \psi_n^*(x)/Z \right] \\ &= |\psi_0(x)|^2 , \end{aligned} \tag{3.21}$$

where the partition function has the usual form $Z = \sum_n e^{-\beta E_n}$.[26] In Appendix B we give a simple example which illustrates this point. There we show how Eq. (3.1) provides a unified description of the equilibrium transition rate for particles in a one-dimensional bistable potential at high and low temperatures.

In Sec. IV we illustrate the use of the transition rate Eq. (3.1) in the context of field theory by studying the temperature dependence of unit winding-number field transitions (which reduce to unit winding-number vacuum tunneling instantons at zero temperature) in the O(3) two-dimensional nonlinear σ model. (We take $\hbar = c = 1$ henceforth.)

IV. AN EXAMPLE

The nonlinear σ model in two dimensions[27] (one space plus one time) exhibits many properties found in non-Abelian gauge theories in four dimensions, in particular, asymptotic freedom and Euclidean solutions (instantons) to the field equations. The σ model is a much simpler field theory, however, since its global rotational invariance is far simpler than the local invariance of a gauge theory.

The O(3) two-dimensional nonlinear σ model may be viewed as a continuum Heisenberg ferromagnet (i.e., a one-dimensional spatial string of three-dimensional classical spins with an infinitesimal lattice spacing). The Minkowski-space Lagrangian density for this field theory is

$$\mathcal{L}(x,t) = \tfrac{1}{2}(\nabla_\mu s^a)^2 , \tag{4.1a}$$

where $\bar{s}(x,t) = \bar{\sigma}(x,t)/g$ is a three-component scalar field with $\sigma^2 = \sigma_1^2 + \sigma_2^2 + \sigma_3^2 = 1$. The symbol g denotes the coupling constant. The field $\bar{s}$ can thus be parametrized by two fields $\theta(x,t)$ and $\Phi(x,t)$ according to

$$\vec{s} = (1/g)(\cos\theta,\ \sin\theta\cos\Phi,\ \sin\theta\sin\Phi)\,. \qquad (4.2)$$

The Lagrangian becomes

$$\mathcal{L}(x,t) = \frac{1}{2g^2}[(\nabla_\mu\theta)^2 + \sin^2\theta(\nabla_\mu\Phi)^2]\,. \qquad (4.1b)$$

The classical vacuum configuration is described by all spins aligned at fixed time, i.e.,

$$\vec{s}(x,t) = (1/g)(1,0,0) \text{ for all } x, \text{ fixed } t\,. \qquad (4.3)$$

Using the MPEP formalism developed in Refs. 11 and 12, Bitar *et al.*[16] have discussed the two-dimensional σ model instantons[17] as zero-temperature Minkowski-space tunnelings between two classical aligned-spin configurations which takes place through a mapping with nonvanishing winding number. Unlike gauge theories, there is no multiple- or θ-vacuum description for the two-dimensional nonlinear σ model.[16] Tunneling, however, remains an important phenomenon for understanding the quantum properties of a system even in the absence of topologically distinct vacuums. A pendulum is a simple example of this idea.[16] Here a unique classical vacuum configuration exists, but the pendulum can still wind all the way around its axis of support and return to the same ground state via quantum-mechanical tunneling. At finite temperatures the pendulum may absorb energy from the surroundings and begin oscillating about the ground state. Clearly, the probability that the pendulum will make a "winding transition" around its support axis will increase with temperature. The point is that for transitions between field configurations the initial and final configurations can be the same if the field space is multiply connected.

Pictorially, a vacuum tunneling in the σ model involves a group of spins with "size" c winding around the spatial "string" to which they are attached, returning to the (same) classical vacuum. A single such winding transition corresponds to an instanton of "size" c with unit winding number ($Q=1$). Such a transition in Euclidean space (x_1, x_2) is illustrated in Fig. 3 (taken from Ref. 16 with permission of authors). We expect the rate of such winding transitions to increase with temperature. The finite-temperature formalism presented in Sec. III can be used to study the temperature dependence of this transition rate by treating a winding transition in the σ model like a particle crossing a potential barrier. The crossing rate of this fictitious particle will be equal to the field transition rate across the corresponding potential barrier in the field space. From Eq. (3.1) it is seen that once we have the one-parameter effective Lagrangian $L(\lambda, \dot{\lambda})$ in Eq. (2.2) describing the zero-temperature vacuum tunneling,

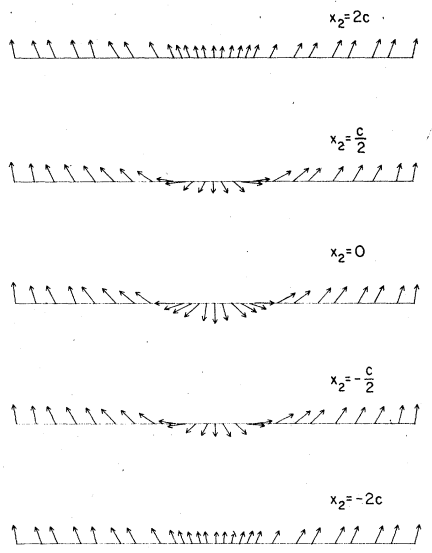

FIG. 3. The spin configuration for various values of the Euclidean time x_2 of a unit winding-number instanton (from Ref. 16).

we can proceed directly to obtain the finite-temperature transition rate. This Lagrangian for the two-dimensional nonlinear σ model was obtained in Ref. 16, and we only quote the salient results here. For simplicity we only consider unit winding-number transitions. We will calculate the rate of single winding transitions for a group of spins with size c (which reduce to pure vacuum-tunneling instantons with unit winding number and size c at zero temperature). We neglect instanton interactions and chemical potentials and work in the "dilute-gas" approximation (i.e., low instanton density, small instanton size, and weak coupling).[9]

For a unit winding-number instanton in the two-dimensional σ model the tunneling potential in terms of the tunneling parameter λ ($-\infty < \lambda < \infty$) is

$$V(\lambda) = \tfrac{1}{2}m(\lambda) = \frac{\pi c^2}{g^2}\,\frac{1}{(\lambda^2+c^2)^{3/2}}\,. \qquad (4.4)$$

The kinetic term of the one-parameter Lagrangian is $\frac{1}{2}m(\lambda)\,\dot{\lambda}^2$. In the weak-coupling limit ($g \ll 1$) the classical ground-state energy is taken as zero, and the WKB tunneling amplitude for a vacuum-to-vacuum transition is $\exp(-4\pi/g^2)$.

The kinetic term can be rewritten in terms of a λ-independent mass M by defining a new winding number [cf. Eq. (2.15)]

$$Q(\lambda) = q\int_{-\infty}^{\lambda} d\lambda'[m(\lambda')]^{1/2} \Big/ \int_{-\infty}^{\infty} d\lambda'[m(\lambda')]^{1/2}\,, \qquad (4.5)$$

where q is the original winding number ($q=1$) and $Q(\lambda=-\infty)=0$, $Q(\lambda=+\infty)=1$. The mass M for a

unit winding-number transition is [cf. Eq. (2.16)]

$$M=\left[\int_{-\infty}^{\infty} d\lambda' [m(\lambda')]^{1/2}\right]^2=\frac{2\pi\gamma^2 c}{g^2}, \tag{4.6}$$

where

$$\gamma\equiv\frac{\Gamma(\frac{1}{4})\Gamma(\frac{1}{2})}{\Gamma(\frac{3}{4})}\simeq\frac{5\pi}{3}. \tag{4.7}$$

Equation (4.5) can be inverted numerically to obtain $\lambda(Q)$ and so the potential $V(Q)$ in the winding-number space. This potential is illustrated in Fig. 4 (taken from Ref. 16 with permission of authors). The Hamiltonian in the new winding-number space is

$$H=\tfrac{1}{2}M\dot{Q}^2+V(Q). \tag{4.8}$$

This new parametrization will, of course, not change the tunneling amplitude given above. The field transition can thus be viewed as the tunneling of a particle with constant mass M through a potential barrier $V(Q)$ in the winding-number space. We remind the reader that even though the Hamiltonian in Eq. (4.8) is written in the winding-number space, it represents the physical energy associated with the unit winding-number instanton. This follows simply because Eq. (4.8) was obtained by direct integration of the original Lagrangian density terms in Eq. (4.1).

The potential $V(Q)$ is periodic in the winding-number space with period 1. This periodicity is physically understandable from Fig. 3. A single winding for a group of spins around the string corresponds to our particle in winding-number space traversing a single barrier like the one shown in Fig. 4. The group of spins can, of course, make an arbitrary number of windings either way around the string, so the potential $V(Q)$ is an infinite one-dimensional periodic potential. The potential may be very roughly approximated by

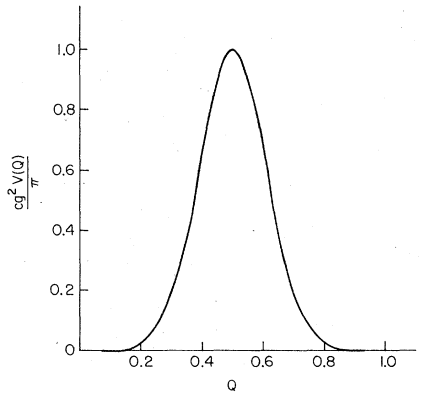

FIG. 4. The tunneling potential in the winding-number space (from Ref. 16).

$$V(Q)=\tfrac{1}{2}V_0(1-\cos 2\pi Q),\quad V_0\equiv\pi/cg^2. \tag{4.9}$$

This approximation to the potential in Fig. 4 is sufficient for purposes of illustration, but we should expect numerical deviations in our results with respect to an exact solution.

Although we have motivated this discussion using the σ model, we note that periodic winding-number potentials also occur in gauge theories with instanton solutions. For example, in the Yang-Mills gauge theory[5] with Lagrangian $\mathcal{L}=-\frac{1}{4}f^{(a)}_{\mu\nu}f^{(a)\mu\nu}$, the instanton solutions can be interpreted as tunnelings between vacuums with different winding numbers, and the tunneling potential in the winding-number space is periodic.[11] Thus the general temperature behavior of the two-dimensional σ model should tell us something of the behavior of more complicated theories. We now proceed to the finite-temperature-rate calculation.

From this point on we have a one-dimensional statistical-mechanics problem. Namely, using Eqs. (4.8), (4.9), and (3.1) we want to calculate the transition rate for a particle with mass M, initially in the neighborhood $-\frac{1}{2}\leq Q\leq\frac{1}{2}$ in Fig. 4 to make a transit over to the neighborhood $\frac{1}{2}\leq Q\leq\frac{3}{2}$. We use the conventional quantum-mechanical normalization that at zero temperature there is unit probability of finding the particle in the ground state. At finite temperature the Boltzmann factor $e^{-\beta E_n}/Z$ is the occupation probability of the nth energy level. Clearly, we still have total unit probability since $\sum_n e^{-\beta E_n}/Z=1$. We mention this only to make the point that in calculating thermodynamic quantum rates one must keep track of both quantum and thermal probabilities to obtain physically meaningful rates.

We can exploit the periodicity of $V(Q)$ to write the general rate expression Eq. (3.1) in a useful and illustrative form. Because of the periodicity we know that the energy spectrum $E_n(k)$ ($k=$ crystal momentum) consists of continuous allowed energy bands, indexed by a positive integer n, separated by forbidden gaps.[28] A typical spectrum in the direct lattice space (i.e., configuration space) is shown in Fig. 5. The energy spectrum for a one-dimensional periodic potential is determined by the transcendental equation[28]

$$\cos ka=\frac{\cos(pa+\delta)}{|t|},\quad E\equiv p^2/2M, \tag{4.10}$$

where a is the direct lattice spacing, δ is the phase shift for scattering on a single barrier in Fig. 5, and t is the transmission amplitude.

The right-hand side of the above transcendental equation is sketched in Fig. 6.[28] The physically allowed spectrum occurs for $-1\leq\cos ka\leq 1$. The

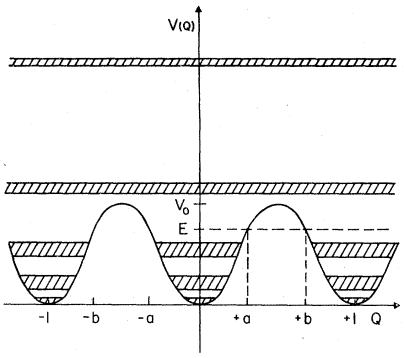

FIG. 5. A typical energy spectrum for a periodic potential of strength V_0 in the winding-number space. The points a and b are the classical turning points for a level with energy $E < V_0$. The cross-hatched regions (open regions) are the forbidden energy gaps (allowed energy bands).

cross-hatched regions (open regions) in Fig. 6 are the forbidden zones (allowed zones). For a strong (weak) potential, the energy bands (gaps) are narrow. If the reflection amplitude $|r|$ is small, the width of the nth gap is approximately[28]

$$\Delta E_{\text{gap}} \approx 2\pi n |r| / Ma^2 . \tag{4.11}$$

If the transmission amplitude $|t|$ is small, the width of a band is $O(|t|)$.

Using the Bloch wave functions $\psi_{nk}(Q)$ (Ref. 28) the normalized density matrix[26] may be written as

$$\rho = e^{-\beta H}/Z = Z^{-1} \sum_{n,k} e^{-\beta E_n(k)} |\psi_{nk}(Q)\rangle\langle\psi_{nk}(Q')| . \tag{4.12}$$

The transition rate given by Eq. (3.1) becomes

$$\begin{aligned} K &= \mathrm{tr}(\rho \mathfrak{F}\mathcal{P}) \\ &= Z_I^{-1} \mathrm{tr}\left(\sum_{n,k} e^{-\beta E_n(k)} |\psi_{nk}(Q)\rangle\langle\psi_{nk}(Q')| \mathfrak{F}\mathcal{P} \right) \\ &= Z_I^{-1} \int_{-1/2}^{1/2} \sum_{n,k} e^{-\beta E_n(k)} \langle\psi_{nk}(Q)| \mathfrak{F}\mathcal{P} |\psi_{nk}(Q)\rangle dQ , \end{aligned} \tag{4.13}$$

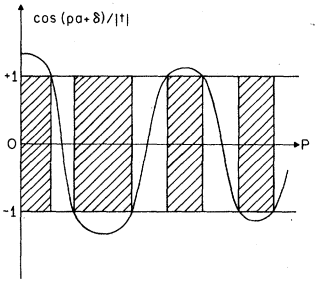

FIG. 6. The characteristic form of the function $\cos(pa+\delta)/|t|$ in Eq. (4.10). The forbidden zones (allowed zones) are cross hatched (open). Redrawn from Ref. 28.

where

$$\begin{aligned} Z_I &= \mathrm{tr}\, e^{-\beta H} \\ &= \int_{-1/2}^{1/2} \sum_{n,k} e^{-\beta E_n(k)} \langle\psi_{nk}(Q)|\psi_{nk}(Q)\rangle dQ \\ &= \sum_{n,k} e^{-\beta E_n(k)} . \end{aligned} \tag{4.14}$$

In Eqs. (4.13) and (4.14) the spatial integrations are over the direct primitive cell $-\frac{1}{2} \leq Q \leq \frac{1}{2}$ corresponding to the initial configuration for a single-barrier transit (i.e., a unit winding-number transition). Since the energy spectrum is quasicontinuous, the crystal momentum sums (n, k) in Eqs. (4.13) and (4.14) may be written as integrals[28] according to

$$K = Z_I^{-1} \sum_n \int_{\mathrm{FBZ}} \frac{dk}{2\pi} \int_{-1/2}^{1/2} dQ \langle\psi_{nk}(Q)| e^{-\beta H(k,Q)} \mathfrak{F}\mathcal{P} |\psi_{nk}(Q)\rangle \tag{4.15}$$

and

$$Z_I = \sum_n \int_{\mathrm{FBZ}} \frac{dk}{2\pi} \int_{-1/2}^{1/2} dQ \langle\psi_{nk}(Q)| e^{-\beta H(k,Q)} |\psi_{nk}(Q)\rangle . \tag{4.16}$$

In Eqs. (4.15) and (4.16) the crystal momentum integrals are over the first Brillouin zone (FBZ) for each band n consistent with the spectrum in Eq. (4.10).

Before proceeding we would like to comment on the meaning of these energy bands in the winding-number space. As we observed earlier, the Hamiltonian in the winding-number space represents a physical energy which has simply been reparametrized. At finite temperatures our system of "spins on a string" can clearly absorb energy making "winding transitions" around the string much more probable. The energy bands in the winding-number space then correspond to actual excited "spin groups" on the string in Minkowski space and are the analog of instantons at finite temperature. We may thus interpret these energy bands as excited collective transition modes in the quantized degree of freedom. This may not be the only interpretation of such a spectrum, but we think it is the simplest in the context of the σ model. We discuss the implications of this observation for gauge theories in Sec. V.

Returning to Eq. (4.15), we will calculate the transition rate in the WKB approximation. We use this approximation because of its familiarity and in order to make contact with the zero-temperature WKB vacuum-tunneling results.[11,12,16] The WKB method fails for narrowly spaced turning points and can be replaced by the "uniform approximation" of Chester *et al.*[19] This semiclassical

method is valid for arbitrarily spaced turning points. Berry and Balazs[19] have extended this approximation to study the evolution of semiclassical quantum states in phase space using the Wigner function $W(q,p)$.[26] Some results of Berry and Balazs[19] are noted in Appendix A, but they will not be employed in this paper. With our lattice spacing $a=1$, we have from Eq. (4.10)

$$\cos k = \frac{\cos(p+\delta)}{|t|}, \quad E = \frac{p^2}{2M}. \tag{4.17}$$

From Eq. (A14) in Appendix A we see that the WKB phase shift for $E < V_0$ may be taken as zero since the transmission amplitude t is real and positive relative to the initial wave-function amplitude. For $E > V_0$ the WKB phase shift $\delta(E)$ is defined by[20]

$$\Delta t(E) = 2\frac{d\delta(E)}{dE}, \tag{4.18}$$

where the classical time delay is given by

$$\Delta t(E) = \sqrt{M}\int_0^1 \{[2E]^{-1/2} - [2(E - V(Q))]^{-1/2}\} dQ. \tag{4.19}$$

Using the potential in Eq. (4.9), this integral can be written in terms of the complete elliptic integral of the first kind, $K(k)$ (Ref. 29) (k is the modulus of K, not the crystal momentum):

$$\Delta t(E) = \left(\frac{M}{2E}\right)^{1/2}\left\{1 - \frac{2}{\pi}K\left[\left(\frac{V_0}{E}\right)^{1/2}\right]\right\}. \tag{4.20}$$

The above equations contain all the information regarding the spectrum of our periodic potential in the WKB approximation. We present them for completeness although only their general features will be needed in this example.

We are going to consider the periodic potential $V(Q)$ in Eq. (4.9) in the weak coupling limit. The region $E \approx V_0$ cannot be treated in the WKB approximation. For a state with $E \approx V_0$ the WKB approximation will not be accurate, and Eq. (A18) will only give us an order-of-magnitude estimate for the transmission coefficient. This is acceptable for a first-order approximation. In the WKB approximation the rate calculation naturally separates into considering the rate contributions from energy levels below and above V_0. In an obvious notation the rate may be written as

$$K = K_< + K_>. \tag{4.21}$$

Let us first consider $K_<$. For $E < V_0$ we have $\delta = 0$, and Eq. (4.17) becomes

$$\cos k = \frac{\cos p}{|t|}. \tag{4.22}$$

The bound energy bands are then distributed about

$$p = \pm(n+\tfrac{1}{2})\pi, \quad E = p^2/2M, \quad n = 0, 1, 2, \ldots. \tag{4.23}$$

Equation (3.10) is the most convenient form for the rate contribution from these bound states. It is a matter of convenience whether to use Eq. (3.10) in the continuum form or in the discrete form as used in Appendix B for the bistable potential. The discrete form exhibits the low-temperature behavior more explicitly and is easy to use with the spectrum in Eq. (4.23). Consistent with the first-order WKB approximation we will treat the bands as single energy levels forming a spectrum

$$E_n = (n+\tfrac{1}{2})^2\pi^2/2M, \quad n = 0, 1, 2, \ldots. \tag{4.24}$$

We then write the energy integral in Eq. (3.10) as a sum over energy level differences,

$$K_< = (2\pi Z_I)^{-1}\sum_n \Delta E_n e^{-\beta E_n}|S(E_n)|^2, \tag{4.25}$$

where ΔE_n are the level spacings and $\Delta E_n/2\pi$ are simply the effective oscillation frequencies for bound particles. From Eq. (4.24) we have

$$\omega_n \equiv \Delta E_n = E_{n+1} - E_n = (\pi^2/M)(n+1), \tag{4.26}$$

and so

$$K_< = (2\pi Z_I)^{-1}\sum_n \omega_n e^{-\beta E_n}|S(E_n)|^2. \tag{4.27}$$

It remains to calculate the transmission coefficient $|S(E_n)|^2$. In the WKB approximation we must distinguish two energy regimes for such a calculation, namely $E \ll V_0$ and $E \lesssim V_0$. The WKB transmission coefficients are given in Appendix A. For the energy range $E \ll V_0$ the transmission coefficient is

$$T(E) = |S(E)|^2 \simeq \alpha^2, \tag{A19}$$

where α is given by

$$\alpha = \exp\left(-\int_a^b |p|\, dQ\right). \tag{A15}$$

The momentum $|p|$ is

$$|p| = [2M(V-E)]^{1/2} = [MV_0(1 - 2\epsilon - \cos 2\pi Q)]^{1/2}, \tag{4.28}$$

where $\epsilon \equiv E/V_0$. The classical turning points a and b are given by

$$a = 1 - b = \frac{1}{2\pi}\cos^{-1}(1-2\epsilon) \approx \epsilon^{1/2}/\pi. \tag{4.29}$$

We then have

$$\int_a^b |p|\, dQ = \int_a^b [MV_0(1 - 2\epsilon - \cos 2\pi Q)]^{1/2} dQ. \tag{4.30}$$

This integral can be written in terms of elliptic

integrals of the first and second kind, $F(\phi, k)$ and $E(\phi, k)$, as[29]

$$\int_a^b |p|\,dQ = \frac{\sqrt{MV_0}}{\pi} 2\sqrt{2}[E(\phi,k) - \epsilon F(\phi,k)]. \quad (4.31)$$

The amplitude ϕ and modulus k (not crystal momentum) are

$$\phi = \sin^{-1}\left(\frac{1-\cos(\pi - 2\pi a)}{2(1-\epsilon)}\right)^{1/2} \quad (4.32)$$

and

$$k^2 = 1 - \epsilon. \quad (4.33)$$

For $E \ll V_0$ we have $\phi \to \pi/2$, $k^2 \to 1$,

$$E(\phi, k) \approx 1 - \tfrac{1}{4}\epsilon - \tfrac{1}{4}\epsilon \ln\tfrac{1}{16}\epsilon \quad (4.34)$$

and

$$F(\phi, k) \approx -\tfrac{1}{2}\ln\tfrac{1}{16}\epsilon. \quad (4.35)$$

We then obtain

$$\int_a^b |p|\,dQ = \frac{4\gamma}{g^2}(1 - \tfrac{1}{4}\epsilon + \tfrac{1}{4}\epsilon \ln\tfrac{1}{16}\epsilon), \quad (4.36)$$

where we have used Eqs. (4.6) and (4.9) for M and V_0 [γ is defined in Eq. (4.7)].

When we exponentiate Eq. (4.36) to obtain the WKB amplitude the logarithmic term gives a slowly varying function of energy which we discard. We then find

$$\alpha \simeq \exp\left[\frac{-4\pi}{g^2}\frac{5}{3}\left(1 - \frac{cg^2E}{4\pi}\right)\right]. \quad (4.37)$$

The energy of the classical ground state is zero. Comparison of Eq. (4.37) with the WKB vacuum-tunneling amplitude in Ref. 16, namely $\exp(-4\pi/g^2)$, shows that our factor $\frac{5}{3}$ is spurious. This is due to our crude approximation of $V(Q)$ in Eq. (4.9). This factor comes from the constant γ in Eq. (4.7) and simply comes along for the ride in the mass M. We will retain this nuisance factor to keep things honest. Thus for the regime $E \ll V_0$ the transmission coefficient is

$$T(E) \simeq \exp\left[\frac{-8\pi}{g^2}\frac{5}{3}\left(1 - \frac{cg^2E}{4\pi}\right)\right]. \quad (4.38)$$

Now we have to consider the energy regime $E \lesssim V_0$. In this case the transmission coefficient is given by Eq. (A18),

$$T(E) = \frac{4}{\left(\frac{2}{\alpha} + \frac{\alpha}{2}\right)^2}. \quad (A18)$$

The calculation of α is like that done above, except that we are now considering $E \lesssim V_0$. The classical turning points are given by

$$a = 1 - b = \frac{1}{2\pi}\cos^{-1}(1 - 2\epsilon) \approx \tfrac{1}{2} - \frac{\sqrt{1-\epsilon}}{\pi}. \quad (4.39)$$

Equations (4.30) through (4.33) all follow through. For $E \lesssim V_0$ we have $\phi \to \pi/2$, $k^2 \to 0$,

$$E(\phi, k) \approx \frac{\pi}{2}\left(1 - \frac{k^2}{4}\right), \quad (4.40)$$

and

$$F(\phi, k) \approx \frac{\pi}{2}\left(1 + \frac{k^2}{4}\right). \quad (4.41)$$

To first order in $(1 - \epsilon)$ we obtain

$$\alpha \simeq \exp\left[\frac{-5}{3}\frac{\pi^2}{g^2}\left(1 - \frac{cg^2E}{\pi}\right)\right]. \quad (4.42)$$

(Note our spurious $\frac{5}{3}$ factor again.)

Putting Eq. (4.42) into Eq. (A18) will give a slightly unwieldy expression. One may of course retain this expression, but since we are interested in the regime $\alpha \lesssim O(1)$, we can extract the important behavior of $T(E)$ as follows. Denoting the (Euclidean) action in Eq. (4.42) by

$$R = \frac{5}{3}\frac{\pi^2}{g^2}\left(1 - \frac{cg^2E}{\pi}\right), \quad (4.43)$$

we simply write

$$\begin{aligned}\frac{2}{\alpha} + \frac{\alpha}{2} &= 2e^R + \tfrac{1}{2}e^{-R} \\ &= 2(1 + R + \cdots) + \tfrac{1}{2}(1 - R + \cdots) \\ &= \tfrac{5}{2}(1 + \tfrac{3}{5}R + \cdots) \\ &\simeq \tfrac{5}{2}\exp(\tfrac{3}{5}R). \end{aligned} \quad (4.44)$$

Then for $E \lesssim V_0$ the transmission coefficient is

$$T(E) \simeq \exp\left[\frac{-2\pi^2}{g^2}\left(1 - \frac{cg^2E}{\pi}\right)\right], \quad (4.45)$$

where we have discarded the numerical prefactor in Eq. (4.44) and in Eq. (A18).

Using Eqs. (4.38) and (4.45) the rate $K_<$ in Eq. (4.25) becomes

$$K_< = (2\pi Z_I)^{-1}\left\{\sum_{n(1)} \omega_n e^{-\beta E_n}\exp\left[\frac{-40\pi}{3g^2}\left(1 - \frac{cg^2E_n}{4\pi}\right)\right] + \sum_{n(2)} \omega_n e^{-\beta E_n}\exp\left[\frac{-2\pi^2}{g^2}\left(1 - \frac{cg^2E_n}{\pi}\right)\right]\right\}, \quad (4.46)$$

where the sum $n(1)$ is over the lower energy levels, and the sum $n(2)$ is over the upper levels. Of course, if the potential is sufficiently weak ($g \gg 1$) the $n(1)$ sum will not exist. Our interest is in the weak-coupling limit.

Next we must calculate $K_>$, the rate contribution from states above V_0. In the first-order WKB approximation we may neglect the energy gaps above V_0. This is seen by noting from Eq. (4.11) that the gap width decreases linearly with $|r|$.

In any energy range above V_0 the gaps will make up a small fraction of the total number of possible levels. Neglecting the gaps will then change the rate by some numerical factor which can be discarded in the WKB approximation. With this simplification the contribution to the rate from levels above V_0 may be approximated by a classical phase-space integral since neglecting gaps above V_0 is equivalent to assuming $|r|=0$. This is the classical reflection amplitude for a particle with $E>V_0$. The rate calculation is much like that done in Appendix B for the bistable potential, and we obtain the classical Arrhenius rate[14,23]

$$K_> = (2\pi\beta Z_I)^{-1}\exp(-\beta V_0)\,. \tag{4.47}$$

Finally, we need to calculate the partition function Z_I. From Eq. (4.14)

$$Z_I = \sum_{n,k} e^{-\beta E_n(k)}\,. \tag{4.48}$$

This form is useful for the bound energy levels below V_0, but for the levels above V_0 a phase-space integral is more appropriate. For $E<V_0$ we have

$$Z_{I<} = 2\sum_{n(1),n(2)} e^{-\beta E_n}, \tag{4.49}$$

where the sums $n(1)$ and $n(2)$ are defined in Eq. (4.46). For $E>V_0$,

$$Z_{I>} = 2\int_{p(Q)}^{\infty}\frac{dp}{2\pi}\int_{-1/2}^{1/2} dQ \times\exp\left[-\beta\left(\frac{p^2}{2M}+\frac{V_0}{2}(1-\cos 2\pi Q)\right)\right], \tag{4.50}$$

where

$$p(Q) = \{2M[V_0 - V(Q)]\}^{1/2} = [MV_0(1+\cos 2\pi Q)]^{1/2}\,. \tag{4.51}$$

[Note p is the usual kinetic momentum and not that in Eq. (4.17).] The factors of 2 in Eqs. (4.49) and (4.50) take into account the fact that positive- and negative-momentum states are degenerate in energy. We may rewrite Eq. (4.50) as

$$Z_{I>} = \frac{1}{\pi}\int_{-1/2}^{1/2} dQ\, e^{-\beta V(Q)}\left(\int_0^{\infty} dp\, e^{-\beta p^2/2M} - \int_0^{p(Q)} dp\, e^{-\beta p^2/2M}\right). \tag{4.52}$$

The momentum integrals are found to be

$$\int_0^{\infty} dp\, e^{-\beta p^2/2M} = \left(\frac{\pi M}{2\beta}\right)^{1/2} \tag{4.53}$$

and

$$\int_0^{p(Q)} dp\, e^{-\beta p^2/2M} = \left(\frac{\pi M}{2\beta}\right)^{1/2}\operatorname{erf}\left[\left(\frac{\beta}{2M}\right)^{1/2} p(Q)\right], \tag{4.54}$$

where the error function is defined by

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x \exp(-t^2)dt\,. \tag{4.55}$$

Furthermore,

$$\int_{-1/2}^{1/2} dQ\exp\left[\frac{-\beta V_0}{2}(1-\cos 2\pi Q)\right] = I_0\left(\frac{\beta V_0}{2}\right)e^{-\beta V_0/2}, \tag{4.56}$$

where $I_0(x)$ is the modified Bessel function of order zero[29]

$$I_0(x) = \sum_{k=0}^{\infty}\frac{(x/2)^{2k}}{(k!)^2}\,. \tag{4.57}$$

Using these results Eq. (4.52) becomes

$$Z_{I>} = \left(\frac{M}{2\pi\beta}\right)^{1/2} e^{-\beta V_0/2}\left\{I_0\left(\frac{\beta V_0}{2}\right) - \int_{-1/2}^{1/2} dQ\, e^{(\beta V_0/2)\cos 2\pi Q}\operatorname{erf}\left[\left(\frac{\beta}{2M}\right)^{1/2} p(Q)\right]\right\}\,. \tag{4.58}$$

[The partition function in Eq. (4.58) may not appear dimensionless. This illusion is the result of our lattice spacing being $a=1$.]

Putting Eqs. (4.46), (4.47), (4.49), and (4.58) together, we obtain for the transition rate in the WKB approximation

$$K = (2\pi Z_I)^{-1}\left\{\sum_{n(1)}\omega_n e^{-\beta E_n}\exp\left[\frac{-40\pi}{3g^2}\left(1-\frac{E_n}{4V_0}\right)\right] + \sum_{n(2)}\omega_n e^{-\beta E_n}\exp\left[\frac{-2\pi^2}{g^2}\left(1-\frac{E_n}{V_0}\right)\right] + \beta^{-1}\exp(-\beta V_0)\right\}, \tag{4.59}$$

with

$$Z_I = 2\sum_{n(1),n(2)} e^{-\beta E_n} + \left(\frac{M}{2\pi\beta}\right)^{1/2} e^{-\beta V_0/2}\left\{I_0\left(\frac{\beta V_0}{2}\right) - \int_{-1/2}^{1/2} dQ\, e^{(\beta V_0/2)\cos 2\pi Q}\operatorname{erf}\left[\left(\frac{\beta}{2M}\right)^{1/2} p(Q)\right]\right\}, \tag{4.60}$$

where $p(Q)$ is given in Eq. (4.51). The low- and high-temperature limits are simple to extract, being

$$K(T\to 0)=\frac{\omega_0}{4\pi}\exp\left[-\frac{5}{3}\frac{8\pi}{g^2}\left(1-\frac{E_0}{4V_0}\right)\right] \tag{4.61}$$

and

$$K(T\to\infty)=(2\pi M\beta)^{-1/2}\exp(-\tfrac{1}{2}\beta V_0)\,. \tag{4.62}$$

The behavior of the rate in Eq. (4.59) as a function of temperature will become more evident if we consider a temperature just slightly above absolute zero. Only the first two energy levels (i.e., bands) in Eq. (4.59) will contribute significantly to the rate, and we may write

$$K(T\gtrsim 0)\sim\frac{\omega}{2\pi}\exp\left[\frac{-40\pi}{3g^2}\left(1-\frac{E_0}{4V_0}\right)\right]\left[\frac{1+\exp\left(\frac{10\pi\Delta E_0}{3g^2V_0}-\beta\Delta E_0\right)}{1+\exp(-\beta\Delta E_0)}\right]$$

$$\approx\frac{\omega}{2\pi}\exp\left[\frac{-40\pi}{3g^2}\left(1-\frac{E_0}{4V_0}\right)\right]\left\{1+\left[\exp\left(\frac{10\pi\Delta E_0}{3g^2V_0}\right)-1\right]e^{-\beta\Delta E_0}\right\} \tag{4.63}$$

where ω is some convenient frequency factor to give us the correct units and $\Delta E_0=E_1-E_0$. It is useful to graph $\ln(2\pi K/\omega)$ as a function of β. From Eqs. (4.63) and (4.62) we have

$$\ln(2\pi K/\omega)\underset{T\to 0}{\sim}-\frac{40\pi}{3g^2}\left(1-\frac{E_0}{4V_0}\right)+\left[\exp\left(\frac{10\pi\Delta E_0}{3g^2V_0}\right)-1\right]e^{-\beta\Delta E_0} \tag{4.64}$$

and

$$\ln(2\pi K/\omega)\underset{T\to\infty}{\sim}-\beta V_0/2\,. \tag{4.65}$$

[For convenience we have taken $\omega/2\pi=(2\pi M\beta)^{-1/2}$ in Eqs. (4.62) and (4.65).] The behavior of Eqs. (4.64) and (4.65) is sketched in Fig. 7. The exponential term in Eq. (4.64) is seen to initiate the characteristic knee behavior in the rate curve, well known from molecular reaction theory.[14,23] Clearly, as the temperature is raised additional energy levels will begin contributing (dashed curves marked with ΔE_n labels in Fig. 7). The effect of the levels above the ground state is thus to turn the rate curve upward with the thermodynamic sum of their rate contributions producing the classical Arrhenius rate at high temperatures. The temperature $\beta^{-1}=V_0$ separates the classical and quantum regimes.

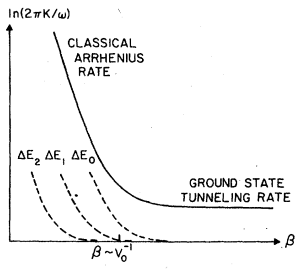

FIG. 7. The behavior of the transition rate as a function of temperature. The rate contribution of energy levels above the ground state are shown as dashed curves marked with ΔE_n labels. The temperature $\beta^{-1}=V_0$ separates the classical and quantum regimes.

Let us rephrase the results of the preceding statistical-mechanics exercise in terms of our σ-model field theory. Thinking again in terms of the "string of spins" in Fig. 3, we recall that at zero temperature the spins are all aligned in the vacuum configuration. As one raises the temperature above absolute zero the spins will absorb energy and begin swinging to and fro about the string. As shown by the above example, the probability of an excited spin group of "size" c making one winding transition around the string increases with temperature. The more energy an excited spin group has, the more likely it is to either tunnel through the "winding barrier," jump over the barrier or perform some combination thereof. Further, we have seen that the zero-temperature instantons are apparently the zero-temperature remnants of a quasicontinuous spectrum of excited field transition modes in the quantized degree of freedom. These modes correspond to the excited spin groups in Minkowski space.

V. DISCUSSION

In this paper we have presented a finite-temperature generalization of the semiclassical (weak-coupling) MPEP approximation for quantum-field transition rates in thermodynamic equilibrium. Although we have applied our finite-temperature formalism to the instantons in field theory, the semiclassical approximation methods developed in Secs. II and III are applicable to transitions in arbitrary quantum-mechanical systems with any number of degrees of freedom.

The underlying assumption of our semiclassical approximation is that the most important effect

on the transition amplitude due to the existence of a classical trajectory for the transition is contained in the quantum mechanics of this degree of freedom. The motion along the classical trajectory is then quantized to obtain the one-parameter WKB wave functionals (and so the amplitudes) and their energy spectrum. Using this information in Eq. (3.1) then yields the finite-temperature (equilibrium) transition rate across the potential-energy barrier separating the initial and final field configurations of interest. As discussed in Appendix C, the contribution of small combined quantum and thermal Gaussian fluctuations to the transition amplitude can formally be absorbed into the tunneling potential yielding an effective temperature-dependent potential. This contribution due to Gaussian fluctuations has the familiar form of a functional determinant and must be approximated in general.[30]

Although our transition rate approximation may appear rather crude at this stage, it does serve its intended purpose. Namely, we now have a simple means of extracting the general temperature behavior of field transition rates in terms of the parameters of a given field theory. In particular, Fig. 7 for the σ model has given us our first hint of the temperature dependence of the field transition rate in gauge theories. Moreover, the behavior is reasonably easy to understand in terms of excited transition modes in the quantized degree of freedom. The excitation spectrum of these modes is straightforward to calculate using conventional quantum-mechanical methods for one-dimensional periodic potentials. The suggestion here is that the statistical-mechanical extension of present semiclassical techniques used in quantum field theory may prove to be useful in understanding finite-temperature phenomena as well.

Clearly, there are many interesting subjects for further investigation, as suggested by our initial effort. In applying our method to the instantons in the σ model, we neglected any effects of instanton interactions by studying a single isolated field transition in the "dilute-gas" approximation.[9] The inclusion of such interactions would be desirable. We concentrated on instanton effects because the pseudoparticles seem to determine many properties of the vacuum at zero temperature. The study of other modes (e.g., merons) at finite temperatures should prove to be equally interesting. Further, at very high temperatures, modes other than those along the classical trajectories we have considered will probably become important. To be precise, what we have calculated is the contribution to the transition rate from the quantized modes in the degrees of freedom which predominate at zero temperature. The consideration of strongly coupled systems and systems not in equilibrium remains challenging.

Our example of finite-temperature transitions in the nonlinear σ model indicates that a rich structure of phenomena may exist in the analogous gauge theories above absolute zero. We have seen that in the σ model there appears to exist a quasicontinuous spectrum of excited transitions modes which reduce to the vacuum-tunneling instantons at zero temperature. Pictorially these modes seem to be interpretable as "excited spin groups" swinging on their one dimensional "string" in Minkowski space. What would such modes correspond to in a gauge theory? If we were considering a gauge theory, one might entertain the idea that such a spectrum could be due to specious degrees of freedom introduced by the choice of gauge. Indeed, we know that $\mathrm{tr}e^{-\beta H}$ is not the physical partition function Z in all gauges, but instead must be computed in a "physical gauge" (i.e., one with the correct number of degrees of freedom).[31] As mentioned in Sec. IV, both instanton solutions and a periodic winding-number potential also occur in the Yang-Mills gauge theory and are in fact just as evident in the Lorentz gauge ($\partial_\mu A^\mu = 0$) as in the temporal gauge ($A^0 = 0$; a so-called "physical gauge").[11] Wadia and Yoneya have shown that the instanton tunneling theory can be developed in any gauge.[32] The reason for this is that the effective Lagrangian L, the action and the winding number are all gauge-invariant quantities. Thus we expect the same type of quasicontinuous excitation spectrum to occur in gauge theories as in our two-dimensional σ-model example. We do not believe the phenomenon would be a gauge artifact.

These quasicontinuous spectra would then seem to represent true excited energy modes. While this paper was in final preparation we were made aware of the work of Harrington and Shepard.[33] These authors constructed finite-temperature periodic solutions (in $\beta\hbar$) of the SU(2) Yang-Mills field equations in Euclidean space which have finite action and can be separated into distinct homotopy classes. These results are most interesting and the relation of this work to our own is being assessed.

Finally, there may be many applications of such a transition-rate approximation as ours, albeit improved perhaps. Two interesting cases are suggested. Various authors have considered the restoration of broken symmetries at finite temperatures and have estimated the critical restoration temperature.[30] The restoration rate is just as important as the critical temperature, and our method might be useful in this regard. A closely

related problem is that of proton creation and decay rates at ultrahigh temperatures during the initial stages of the "big bang"[34] (a vacuum fluctuation par excellence?). An estimate of such rates at finite temperatures might put constraints on the possible parameter choices for unified field theories. Our rate approximation is directly applicable to the instanton mediated baryon/lepton nonconservation mechanism ($p+n\rightarrow e^{+}+\bar{\nu}_{\mu}$) of 't Hooft,[7] for example.

Notes added in proof. After this paper was accepted for publication, discussions between the author and S.-J. Chang clarified the relation of the present work with that of Harrington and Shepard.[33]

Utilizing the formal mathematical similarity of the zero-temperature Euclidean field theory and the "imaginary time" formulation of finite-temperature field theory, Harrington and Shepard constructed finite-temperature instanton solutions ("calorons") from the zero-temperature instantons. This was done by replacing the zero-temperature boundary conditions at Euclidean times $\tau=\pm\infty$ by the usual finite-temperature periodic boundary conditions on the fields at $\tau=0,\beta$. The calorons represent the dominant finite-temperature paths contributing to the statistical density matrix, and thus to the partition function. They are distinct from the zero-temperature MPEP studied in the present paper except at zero temperature where the caloron reduces to the instanton.

To understand this distinction better, consider a quantum-mechanical system in n dimensions $[X\equiv(X_1,X_2,\ldots,X_n)]$. All of the equilibrium thermodynamic information about the system is contained in the statistical density matrix $\rho(X,X')$. 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

$$\rho(X)=\sum_n e^{-\beta E_n}|\psi_n(X)|^2, \tag{5.1}$$

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. However, this semiclassical evaluation of $\rho(X)$ can be further simplified by replacing the discrete levels E_n by an energy continuum E. We assume this to be a valid approximation in the following.

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 most probable escape path (MPEP). For the MPEP starting at the turning point $X(E)$ and going to a point X in the tunneling region the distribution function is (omitting normalization and phase-space factors)

$$\rho_E(X)=\exp\left[-\beta E-2\int_{X(E)}^{X} dl_{\mathrm{MPEP}}[2m(V-E)]^{1/2}\right], \tag{5.2}$$

where the line integral is along the MPEP. The energy E in Eq. (5.2) can be varied to find the "most probable energy," that is, the energy that maximizes the distribution function.

The MPEP $X(\tau)$ with fixed end points X and $X(E)$ is determined by the variational equation

$$\delta\int_{X(E)}^{X} dl[2m(V-E)]^{1/2}=0, \tag{5.3}$$

where τ is a path parameter and l is the length along the path. The MPEP is then a solution of the Euclidean equations of motion:

$$m\frac{d^2X_i}{d\tau^2}=+\frac{\partial V(X)}{\partial X_i}, \quad i=(1,2,\ldots,n). \tag{5.4}$$

The variation of Eq. (5.2) with respect to E determines the energy and the associated turning point which maximize $\rho_E(X)$. The relevant variational equation is

$$\delta\left[\beta E+2\int_{X(E)}^{X} dl_{\mathrm{MPEP}}[2m(V-E)]^{1/2}\right]=0$$

or

$$\beta-\int_{X(E)}^{X} dl_{\mathrm{MPEP}}\left(\frac{2m}{V-E}\right)^{1/2}+2[2m(V-E)]^{1/2}\frac{\partial X}{\partial E}\bigg|_{X}$$
$$-2[2m(V-E)]^{1/2}\frac{\partial X(E)}{\partial E}\bigg|_{X(E)}=0. \tag{5.5}$$

Since the end point X has no dependence on the energy, $\partial X/\partial E=0$. At the turning point $X(E)$, $V-E=0$. Equation (5.5) then becomes

$$\beta=\int_{X(E)}^{X} dl_{\mathrm{MPEP}}\left(\frac{2m}{V-E}\right)^{1/2}. \tag{5.6}$$

Equations (5.4) and (5.6) together determine the MPEP and the turning point for a given β and X. Substituting the MPEP and turning point into Eq. (5.2) yields the dominant finite-temperature distribution function $\rho_E(X)$.

Equation (5.6) allows us to relate the above finite-temperature MPEP formalism to the "imaginary time" formulation of equilibrium thermodynamics. In the latter, one considers the particle of mass m

to be moving in the "inverted potential" $V_I = -V(X)$. The MPEP then becomes a classically allowed path with

$$V - E = E_I - V_I = \tfrac{1}{2}mv^2 , \tag{5.7}$$

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. (5.4) so that we have

$$\beta = \int_{X(E)}^{X} dl_{\mathrm{MPEP}} \left(\frac{2m}{V-E}\right)^{1/2} = 2\int_{X(E)}^{X} \frac{dl}{v} = \oint \frac{dl}{v} . \tag{5.8}$$

Thus the total "time" needed for the particle to travel from X to $X(E)$ and back to X is β, and the Euclidean solution $X(\tau)$ is periodic in τ with period β. This solution is nothing but the caloron of Harrington and Shepard, however, arrived at not by simple mathematical analogy with Euclidean field theory but instead by using the simple physical picture of finite-temperature MPEP's.

Our interest in this paper was to elucidate some effects of temperature on the rate of field transitions along the zero-temperature MPEP alone. Consequently we did not allow for explicit variation of the MPEP itself as a function of temperature. This is what characterizes the caloron and distinguishes it from the zero-temperature path we considered. Removing this constraint on our path is equivalent to changing the boundary conditions for the zero-temperature MPEP at $\tau = \pm\infty$ to the periodic boundary conditions for the caloron at $\tau = 0, \beta$. However, we have included all energy levels in our one degree of freedom at a given temperature rather than only the most probable energy as in the caloron solution. This has allowed us to see the interaction of quantum and thermal contributions to transitions across a given potential barrier as a function of temperature. The excited transition modes we found in our quantized degree of freedom are separate from the caloron modes at finite temperature. They involve different paths in the field space except at zero temperature where the instantons are recovered.

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APPENDIX A: TUNNELING IN MINKOWSKI SPACE

In one dimension the WKB ansatz to the Schrödinger equation[18]

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V\right)\psi = E\psi \tag{A1}$$

is

$$\psi(x) = \exp[iS(x)/\hbar], \quad S = S_0 + \hbar S_1 + \cdots . \tag{A2}$$

Substituting Eq. (A2) into Eq. (A1) and equating terms with equal powers of $\hbar$, one obtains the set of coupled differential equations

$$\frac{1}{2m}(\nabla S_0)^2 + V = E , \tag{A3}$$

$$-i\nabla^2 S_0 + 2\nabla S_0 \cdot \nabla S_1 = 0, \ldots . \tag{A4}$$

(We set $\hbar = 1$ henceforth.) The solution for $E > V(x)$ to first order is

$$\psi(x) = \left(\frac{1}{p(x)}\right)^{1/2} \exp[\pm i S_0(x)], \tag{A5}$$

$$S_0(x) = \int^x p(x')dx' , \tag{A6}$$

$$p(x) = [2m(E-V)]^{1/2} . \tag{A7}$$

In Eq. (A6), S_0 is the classical action and Eq. (A3) is recognized as the Hamilton-Jacobi equation.[21] In a tunneling region S_0 is imaginary. Setting $S = iR$ with R real, the tunneling solution to first order is

$$\psi(x) = \left(\frac{1}{|p(x)|}\right)^{1/2} \exp(\pm R_0) , \tag{A8}$$

$$R_0(x) = \int^x |p(x')|dx' , \tag{A9}$$

$$|p(x)| = [2m(V-E)]^{1/2} . \tag{A10}$$

Consider a one-dimensional potential of the form in Fig. 8 with a and b the classical turning points and $E < V(x)$. The "left" and "right" states

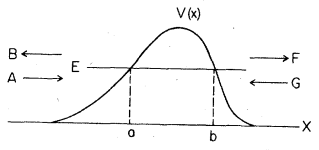

FIG. 8. One-dimensional potential barrier. The points a and b are the classical turning points for a particle with energy E. The amplitudes A and G correspond to "in" states; B and F to "out" states.

are related through a matrix M by

$$\psi_L = M\psi_R \text{ or } \begin{pmatrix} A \\ B \end{pmatrix} = M \begin{pmatrix} F \\ G \end{pmatrix}. \tag{A11}$$

Alternately the "in" and "out" states can be related by the S matrix

$$\psi_{\text{out}} = S\psi_{\text{in}} \text{ or } \begin{pmatrix} B \\ F \end{pmatrix} = S \begin{pmatrix} A \\ G \end{pmatrix}. \tag{A12}$$

The matrices M and S are related by

$$M = \begin{pmatrix} \dfrac{1}{S_{12}} & \dfrac{S_{11}^*}{S_{12}^*} \\ \dfrac{S_{11}}{S_{12}} & \dfrac{1}{S_{12}^*} \end{pmatrix}. \tag{A13}$$

Using the WKB connection formulas, one can obtain[18]

$$M = \frac{1}{2} \begin{pmatrix} \dfrac{2}{\alpha} + \dfrac{\alpha}{2} & i\left(\dfrac{2}{\alpha} - \dfrac{\alpha}{2}\right) \\ -i\left(\dfrac{2}{\alpha} - \dfrac{\alpha}{2}\right) & \dfrac{2}{\alpha} + \dfrac{\alpha}{2} \end{pmatrix}, \tag{A14}$$

where

$$\alpha = \exp\left(-\int_a^b |p(x)|\,dx\right). \tag{A15}$$

Assuming no right incoming states in Fig. 8 ($G = 0$), the transmission coefficient is

$$T(E) = \frac{|\psi_{\text{trans}}|^2 v_{\text{trans}}}{|\psi_{\text{incid}}|^2 v_{\text{incid}}} = \left| \frac{\psi_T \sqrt{p_t}}{\psi_I \sqrt{p_i}} \right|^2. \tag{A16}$$

From Eq. (A5) we find

$$T(E) = \left| \frac{\psi_T \sqrt{p_t}}{\psi_I \sqrt{p_i}} \right|^2 = \left| \frac{F}{A} \right|^2. \tag{A17}$$

Using Eqs. (A11), (A13), and (A14), $T(E)$ can be cast into additional guises,

$$T(E) = \left| \frac{1}{M_{11}} \right|^2 = |S_{12}|^2 = \frac{4}{\left(\dfrac{2}{\alpha} + \dfrac{\alpha}{2}\right)^2}. \tag{A18}$$

For a strong potential $\alpha \ll 1$ and $T(E)$ becomes

$$T(E) \simeq \alpha^2. \tag{A19}$$

We will need the general form Eq. (A18) for $T(E)$ since we will not be solely interested in states with energies much less than the potential height. The WKB approximation is inaccurate near a potential maximum with narrowly spaced classical turning points. Even in such cases Eq. (A18) still exhibits the correct qualitative tunneling features, but its numerical predictions cannot actually be trusted. Instead, the more general semiclassical "uniform approximation" of Chester *et al.*[19] is preferable since it is valid for arbitrary separations of turning points. Berry and Balazs[19] have used this method to study the evolution of semiclassical quantum states in phase space. From the Wigner function $W(q, p)$,[26] these authors find for the one-dimensional semiclassical probability density

$$|\langle q|\psi\rangle|^2 = \int dp\, W(q,p) = \frac{2\omega}{|\dot{q}(q)|} \left| \frac{3}{2\hbar} \int_q^{q_t} dq' p(q') \right|^{1/3} \times \text{Ai}^2\left(\mp \left| \frac{3}{2\hbar} \int_q^{q_t} dq' p(q') \right|^{2/3} \right), \tag{A20}$$

where $\text{Ai}(z)$ is the Airy function,[29] ω is the classical oscillation frequency for the phase-space motion, and q_t is the classical turning point. The upper (lower) sign in the argument of $\text{Ai}(z)$ in Eq. (A20) is appropriate in a classically allowed (forbidden) region. In such an allowed (forbidden) region $\text{Ai}(z)$ is oscillatory (exponentially damped). Equation (A20) reduces to the familiar WKB result for $|z| \to \infty$.

APPENDIX B: THERMODYNAMIC TRANSITIONS IN A BISTABLE POTENTIAL

Consider the bistable potential in Fig. 9. We assume that there is an ensemble of particles, each of mass m, in thermodynamic equilibrium in the potential $V(x)$. Using Eq. (3.1) we will calculate the rate at which particles cross from the metastable well to the stable well in the low- and high-temperature limits. Of course, in thermodynamic equilibrium there are equal fluxes of particles from one well to the other. This is why the projection operator is needed in Eq. (3.1). Here we are calculating thermodynamic equilibrium transition rates only. Such equilibrium transitions are physically related to, but logically distinct from nonequilibrium diffusion transitions in which particles are initially in some nonequili-

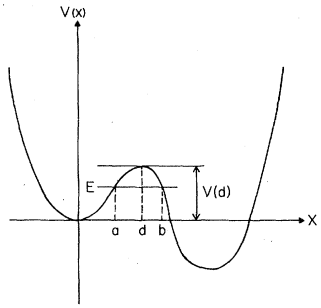

FIG. 9. One-dimensional bistable potential. The points a and b are the classical turning points for a particle with energy E.

brium distribution in the potential. In the case of equilibrium transitions the probability density ρ is stationary ($\partial\rho/\partial t = -\nabla\cdot J = 0$). For nonequilibrium transitions this is not so, and time-dependent perturbation theory, nonequilibrium thermodynamics, linear response theory, Fokker-Planck equations, and other methods must be used to calculate rates. (See for example van Kampen under Ref. 14; also Ref. 35.)

At low temperatures Eq. (3.10) for the rate is easiest to use. The energy integral becomes a sum over energy level differences of the bistable well spectrum starting at the metastable ground state with energy E_0. Because of the energy conserving δ function in the S-matrix element, there is one "final" state in the stable well for each "initial" state in the metastable well in such a one-dimensional system. This is merely a counting mnemonic telling us how to count states in Eq. (3.10) since a particle can take any "energy path" in getting from the metastable well to the stable well. The Boltzmann factors properly account for the relative probabilities of various such paths. Then according to Eq. (3.10) the rate is

$$K = Z_I^{-1} \sum_n \frac{\Delta E_n}{2\pi\hbar} e^{-\beta E_n} |S(E_n)|^2 . \tag{B1}$$

The quantities $\Delta E_n/2\pi\hbar$ are recognized as the effective oscillation frequencies of particles in the metastable well ($\Delta E_n \equiv E_{n+1} - E_n$) and are the expected kinematic factors.

At any temperature T the sum in Eq. (B1) must include energy levels up to at least $E_i \approx O(10\beta^{-1})$ for accuracy (the same applies to $Z_I = \sum_i e^{-\beta E_i}$). As $T \to 0$, $Z_I \to e^{-\beta E_0}$ and the rate reduces to the temperature-independent quantum tunneling rate for the metastable ground state

$$K_{\rm QM} = \frac{\omega_0}{2\pi} |S(E_0)|^2 , \tag{B2}$$

where $|S(E_0)|^2$ is the transmission coefficient of this state [see Eq. (A18) in Appendix A].

The classical high temperature limit for the transition rate is obtained by the usual replacement of the trace in Eq. (3.1) by a phase-space integral

$$K_{\rm CL} = (2\pi\hbar Z_I)^{-1} \int_{-\infty}^{\infty} dp \int_{-\infty}^{d} dx \exp(-\beta H) \mathfrak{F}\mathcal{P} . \tag{B3}$$

In the one-dimensional classical limit

$$\mathfrak{F}\mathcal{P} = \delta(x-a)(p/m)\mathcal{T}(p,x)\theta(p) , \tag{B4}$$

where a is the classical turning point in Fig. 9, $\mathcal{T}(p,x)$ is the classical transmission coefficient given by

$$\mathcal{T}(p,x) = \begin{cases} 1 \text{ if } \dfrac{p^2}{2m} > V(d) - V(x) \\ 0 \text{ if } \dfrac{p^2}{2m} < V(d) - V(x) \end{cases} , \tag{B5}$$

and $\theta(p)$ is the momentum step function. Doing the spatial integration in Eq. (B3) trivially we obtain

$$K_{\rm CL} = (2\pi\hbar Z_I)^{-1} \int_0^{\infty} dp \frac{p}{m} \exp[-\beta H(p,a)] \mathcal{T}(p,a) . \tag{B6}$$

The partition function is given by

$$Z_I = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp \int_{-\infty}^{d} dx \exp\left[-\beta\left(\frac{p^2}{2m} + V(x)\right)\right] \tag{B7}$$

$$= \left(\frac{m}{2\pi\hbar^2\beta}\right)^{1/2} \int_{-\infty}^{d} dx \exp[-\beta V(x)] . \tag{B8}$$

A common assumption is that the integral in Eq. (B8) is dominated by the region of a local potential minimum, in this case near the origin in Fig. 9. One then expands $V(x)$ up to quadratic terms, extends the limit $x = d$ to infinity, and does the resulting Gaussian integration. Such a cavalier approach is not always valid for some potentials, and one should be wary.

With this caveat we will proceed in a cavalier fashion anyway. In the neighborhood of the origin in Fig. 9 the potential may be approximated by

$$V(x) \simeq \tfrac{1}{2} m\omega^2 x^2 , \tag{B9}$$

where

$$\omega^2 = \frac{1}{m} \frac{d^2V}{dx^2}\bigg|_{x=0} . \tag{B10}$$

Using Eq. (B9) in Eq. (B8), extending the limit $x = d$ to infinity, and doing the Gaussian integration we obtain

$$Z_I \simeq \left(\frac{m}{2\pi\hbar^2\beta}\right)^{1/2} \left(\frac{2\pi}{\beta m\omega^2}\right)^{1/2} = (\beta\hbar\omega)^{-1} . \tag{B11}$$

Then

$$K_{\rm CL} = \frac{\beta\omega}{2\pi m} \int_0^{\infty} p \exp\left[-\beta\left(\frac{p^2}{2m} + V(a)\right)\right] \mathcal{T}(p,a) dp \tag{B12}$$

$$= \frac{\beta\omega}{2\pi m} \int_0^{\infty} p \exp\left[-\beta\left(\frac{p^2}{2m} - V(d) + V(a) + V(d)\right)\right] \times \mathcal{T}(p,a) dp \tag{B13}$$

$$= \frac{\beta\omega}{2\pi m} \exp[-\beta V(d)] \int_0^{\infty} p \exp\left(\frac{-\beta p^2}{2m}\right) dp \tag{B14}$$

$$= \frac{\omega}{2\pi} \exp[-\beta V(d)] , \tag{B15}$$

where we have used Eq. (B5) in going from Eq. (B13) to Eq. (B14). To remove the parameter $\omega/2\pi$ one commonly uses $(2\pi\hbar\beta)^{-1}$ assuming that this will be a reasonable approximation to the frequency of collisions with the barrier at high temperatures. Equation (B15) is the familiar classical Arrhenius rate for escape over a barrier.[14,15,23]

The combined temperature behavior of Eqs. (B1) and (B15) is like that shown in Fig. 7 which is derived for unit winding-number transitions in the nonlinear σ-model example of Sec. IV. The similarity is due to the fact that only a single barrier transit is being considered. Much of the structure of the rate behavior is due to the statistical mechanics and not the detailed dynamics.

APPENDIX C: PATH INTEGRAL FORMULATION OF TRANSITION AMPLITUDES

In this appendix we briefly review the path-integral formulation of quantum-field transition amplitudes at finite temperatures. The material here is taken from Refs. 30 and 31, to which the interested reader is referred for details. One advantage of the path-integral formulation is that a simple loop expansion of the action yields the contribution to the transition amplitude due to (small) combined quantum and thermal Gaussian fluctuations away from the classical trajectory $\phi_0(x, \lambda)$.

The differential equations satisfied by the finite-temperature Green's functions are identical to those of the zero-temperature theory. (For a review and references to the original literature, see Baym and Kadanoff under Ref. 25.) The difference lies in the boundary conditions. Whereas the familiar causal boundary conditions at $t=\pm\infty$ are appropriate at zero temperature (since we are only interested in S-matrix elements), periodic boundary conditions for imaginary time ($-\beta\hbar\leq\tau\leq\hbar\beta$) are relevant at finite temperature. The diagrammatic expansion gives a series solution of these differential equations, with each term in the series composed of free two-point functions and vertices. The identity of the differential equations implies that the diagrammatic analysis is the same at finite temperature as at zero temperature. The only difference lies in the type of two-point function used.

The Feynman path integral provides an indefinite integral representation of the differential equations of field theory. However, the path integral does not contain a complete specification of the boundary conditions. Consequently, we may use the same path-integral representation in both cases, supplemented with appropriate boundary conditions. Since all zero-temperature results follow from the finite-temperature results as $\beta\to\infty$, we will suppress space-time variables except for the temporal integral limits 0 and β and for important definitions. We will only consider field transitions in the absence of external sources.

Consider a quantum field theory described by a Hamiltonian density $\mathcal{H}(\pi, \phi)$. The Feynman path integral in Hamiltonian form gives the transition amplitude for going from the field operator eigenstate $|\phi_1\rangle$ at $t=t_1$ to $|\phi_2\rangle$ at $t=t_2$ as ($\hbar=c=1$)

$$\langle\phi_2|e^{-iH(t_2-t_1)}|\phi_1\rangle = N\int d\pi\int_1^2 d\phi\,\exp\left(i\int_{t_1}^{t_2}dt\int d^3x[\pi\dot{\phi}-\mathcal{H}(\pi,\phi)]\right), \tag{C1}$$

where the integral over fields ϕ runs over all possible configurations that start at ϕ_1 at $t=t_1$ and go to ϕ_2 at $t=t_2$. The momentum integral over π is unrestricted (note that $\dot{\phi}=\partial\phi/\partial t$). The symbol N represents a normalization factor.

To obtain the amplitude at finite temperature, simply let $i(t_2-t_1)=\beta$, where β is the inverse temperature, and make the change of variable $it=\tau$ (note that $\dot{\phi}=i\partial\phi/\partial\tau$). Then we have

$$\rho_u(\phi_2,\phi_1)=\langle\phi_2|e^{-\beta H}|\phi_1\rangle = N\int d\pi\int_1^2 d\phi\,\exp\left(\int_0^\beta d\tau\times\int d^3x[i\pi\dot{\phi}-\mathcal{H}(\pi,\phi)]\right), \tag{C2}$$

where $\dot{\phi}$ now means $\partial\phi/\partial\tau$. Equation (C2) is the path integral form of the unnormalized density matrix in Eq. (2.22). To obtain the partition function Z, let the ϕ integral go over all periodic paths $\phi(\tau=0)=\phi(\tau=\beta)$. We then have

$$Z=\mathrm{Tr}e^{-\beta H}=\sum_\phi\langle\phi|e^{-\beta H}|\phi\rangle = N\int d\pi\oint d\phi\,\exp\left(\int_0^\beta d\tau\int d^3x[i\pi\dot{\phi}-\mathcal{H}(\pi,\phi)]\right). \tag{C3}$$

In the usual case where $\mathcal{H}$ is no more than quadratic in π, we can do the momentum integration immediately. This replaces π in the integrand by its value at the stationary point of the integrand, given by

$$i\dot{\phi}=\partial\mathcal{H}/\partial\pi\,. \tag{C4}$$

This will be recognized as just the prescription for going from the Hamiltonian $\mathcal{H}$ to the usual effective Lagrangian $\mathcal{L}_{\mathrm{eff}}$ with all τ derivatives multiplied by i. The density matrix and partition function become

$$\rho_u(\phi_2,\phi_1)=N'(\beta)\int_1^2 d\phi\,\exp\left(\int_0^\beta d\tau\int d^3x\,\mathcal{L}_{\mathrm{eff}}(\phi,i\dot{\phi})\right) \tag{C5}$$

and

$$Z=\mathrm{Tr}e^{-\beta H}=N'(\beta)\oint d\phi\,\exp\left(\int_0^\beta d\tau\int d^3x\,\mathfrak{L}_{\mathrm{eff}}(\phi,i\dot{\phi})\right), \tag{C6}$$

where $N'(\beta)$ is a new normalization factor. The β dependence of N' comes from a careful evaluation of the π integration. At zero temperature, N' is an unimportant (infinite) constant. In quantities such as the normalized density matrix $\rho=\rho_u/Z$ and the Green's functions, $N'(\beta)$ divides out. We will omit $N'(\beta)$ in the following and also write $\mathfrak{L}(\phi,\dot{\phi})$ for $\mathfrak{L}_{\mathrm{eff}}(\phi,i\dot{\phi})$.

Equations (C5) and (C6) are the basic expressions needed to calculate equilibrium transition amplitudes at finite temperatures [additionally Z in Eq. (C6) gives the finite-temperature Feynman rules]. We will denote the action (either Minkowskian or Euclidean) by

$$I(\phi)=\int \mathfrak{L}(\phi,\dot{\phi})d^4x, \tag{C7}$$

where d^4x may be a Minkowskian or Euclidean volume element and the temporal integration limits are from 0 to β.

From Eq. (C5) the unnormalized amplitude for a transition from ϕ_1 to ϕ_2 is given by

$$\rho_u(\phi_2,\phi_1)=\int_1^2 d\phi\,\exp[iI(\phi)]. \tag{C8}$$

To calculate this amplitude in the semiclassical approximation, we perform a loop expansion of $I(\phi)$ about the classical trajectory ϕ_0 connecting ϕ_1 and ϕ_2. This trajectory is necessarily a solution to the variational equation

$$\delta I(\phi)/\delta\phi=0. \tag{C9}$$

We then obtain

$$I(\phi_0+\phi)=I(\phi_0)+\tfrac{1}{2}\phi i D^{-1}\phi+I(\phi_0;\phi), \tag{C10}$$

where

$$iD^{-1}=\left.\frac{\delta^2 I(\phi)}{\delta\phi^2}\right|_{\phi_0}. \tag{C11}$$

Our convention for the free spin-zero propagator is

$$D_\beta(k)=\frac{i}{k^2-m^2}, \tag{C12}$$

where

$$k^2=\begin{cases}-\dfrac{4\pi^2n^2}{\beta^2}-\bar{k}^2, & n=0,\pm1,\ldots,\quad \beta\neq\infty\\ (k^0)^2-\bar{k}^2, & \beta=\infty.\end{cases} \tag{C13}$$

[The expression for k^2 with $\beta\neq\infty$ in Eq. (C13) is in the imaginary-time formalism, which is convenient for equilibrium thermodynamics. See Dolan and Jackiw under Ref. 30 for a discussion of the real- and imaginary-time formalisms.] Note that the propagator in Eq. (C11) is translationally noninvariant.

The amplitude in Eq. (C8) can now be written as

$$\rho_u(\phi_2,\phi_1)=\exp[iI(\phi_0)]\times\int d\phi\,\exp\{i[\tfrac{1}{2}\phi iD^{-1}\phi+I(\phi_0;\phi)]\} \tag{C14}$$

$$=\exp[iI(\phi_0)]\,\mathrm{Det}^{-1/2}(iD^{-1})\rho_2, \tag{C15}$$

where

$$\rho_2=\frac{\int d\phi\,\exp\{i[\frac{1}{2}\phi iD^{-1}\phi+I(\phi_0;\phi)]\}}{\int d\phi\,\exp\{i[\frac{1}{2}\phi iD^{-1}\phi]\}}. \tag{C16}$$

In obtaining Eq. (C15) we have used the fundamental path integral

$$\int d\phi\,\exp(i\tfrac{1}{2}\phi M\phi)=(\mathrm{Det}M)^{-1/2}. \tag{C17}$$

The factor ρ_2 gives the two-loop and higher-order corrections (hence the subscript). The determinant factor in Eq. (C15) is the familiar one-loop term and yields the contribution to the transition amplitude from combined quantum and thermal Gaussian fluctuations away from the classical trajectory ϕ_0.

At zero temperature in a tunneling region, $\mathrm{Det}^{-1/2}(iD^{-1})$ in Eq. (C15) reduces to the same contribution obtained by Bitar and Chang[12] for Gaussian quantum fluctuations around an MPEP. As noted by those authors, if the Gaussian fluctuations are small, their contribution can be absorbed into the classical amplitude $\exp[iI(\phi_0)]$ by modifying the tunneling potential to a new effective potential. The same procedure applies at finite temperature and results in a temperature-dependent effective potential. Of course, the contribution is still in the form of a functional determinant and is by no means trivial to evaluate in general.

Interestingly enough, a one-loop contribution similar to that appearing in Eq. (C15) occurs in the functional evaluation of the effective potential for a finite-temperature field theory[30] (that is, the generating functional for zero-momentum single-particle irreducible Green's functions). The effective potential as used in Ref. 30 should not be confused with that in the preceding paragraph and in Ref. 12. They are different potentials because the tunneling potential involves a term $\frac{1}{2}(\nabla\phi)^2$ in Eq. (2.5) which is not present in the effective potential of the field theory. Still, because the one-loop correction is a simple Gaussian fluctuation contribution (always giving a functional determinant) and not typical of the more complicated higher-order terms, the one-loop correction to the tunneling potential and to the

effective potential for the field theory are formally the same. In the lowest-order approximation for this one-loop term, Dolan and Jackiw[30] take the classical field ϕ_0 as constant, making the propagator in Eq. (C11) translationally invariant and diagonal in the momentum representation. The computation of the one-loop correction is then straightforward. Thus, using this technique of Dolan and Jackiw, one can at least determine the leading effect of combined quantum and thermal fluctuations on the tunneling potential.

Finally, using Eqs. (C5) and (C6), the expectation value of any operator $A(\phi, \dot{\phi})$ can be written in path-integral form as

$$\langle A\rangle = \frac{N'(\beta)}{Z} \oint d\phi\, A(\phi, \dot{\phi}) \exp\left[\int_0^\beta d\tau \int d^3x \mathcal{L}(\phi, \dot{\phi})\right]. \tag{C18}$$

In particular, the transition rate (or "crossing rate") from a set of initial states ϕ_i to a set of final states ϕ_f, separated by a hypersurface S in the field space (Fig. 1), is given by the expectation value of the operator $\mathfrak{F}\mathcal{P}$, where $\mathfrak{F}$ is the flux operator, and $\mathcal{P}$ is a projection operator. Let a path connecting a state ϕ_i and ϕ_f be denoted by $\phi(x, \lambda)$, with $\phi(x, s)$ being a state on the hypersurface S. Such a surface in the field space can in general be parametrized by a functional $f(\phi)$, with the fields $\phi(x, s)$ on S satisfying the equation

$$f(\phi) = 0\,. \tag{C19}$$

In analogy with Eq. (3.3), the flux operator in the configuration space of ϕ can then be written as

$$\mathfrak{F} = \delta[f(\phi)]\frac{\delta f(\phi)}{\delta\phi}\frac{\hbar}{i}\frac{\delta}{\delta\phi}\,. \tag{C20}$$

The projection operator $\mathcal{P}$ projects out those states at the hypersurface S which have evolved from the initial states ϕ_i and can be written as

$$\mathcal{P} = \sum_i |\phi_i(x, s)\rangle\langle\phi_i(x, s)|\,. \tag{C21}$$

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