

Functional density matrix formulation of quantum statisticsA. Bessa,^{1,2,*} C. A. A. de Carvalho,^{3,†} and E. S. Fraga^{3,‡}¹*Escola de Ciências e Tecnologia, Universidade Federal do Rio Grande do Norte, Caixa Postal 1524, 59072-970 Natal, RN, Brazil*²*Instituto de Física, Universidade de São Paulo, Caixa Postal 66318, 05315-970 São Paulo, SP, Brazil*³*Instituto de Física, Universidade Federal do Rio de Janeiro, Caixa Postal 68528, 21941-972 Rio de Janeiro, RJ, Brazil*

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We present a unified formulation for quantum statistical physics based on the representation of the density matrix as a functional integral. For quantum statistical (thermal) field theory, the stochastic variable of the statistical theory is a boundary field configuration. We explore the properties of an effective theory for such boundary configurations and apply it to the computation of the partition function of an interacting one-dimensional quantum-mechanical system at finite temperature. Plots of free energy and specific heat show excellent agreement with more involved semiclassical results. The method of calculation provides an alternative to the usual sum over periodic trajectories: it sums over paths with coincident end points and includes nonvanishing boundary terms. An appropriately modified expansion into modified Matsubara modes is presented.

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I. INTRODUCTION

Quantum statistical physics provides the conceptual and computational framework for the treatment of interacting many-body systems in thermal equilibrium with a heat bath. It describes a great variety of systems and phenomena over a wide range of scales, thus covering practically all areas of physics, from cosmology to particle physics, with an extensive number of examples in condensed matter.

Its broad spectrum of applications includes special-relativistic systems. For those, the quantum statistical treatment is known as finite-temperature field theory [1], which is synonymous to quantum statistical field theory. In fact, just as quantum statistical mechanics adds stochastic probabilities to the quantum probabilities of quantum mechanics, finite-temperature field theory does likewise with respect to quantum-field theory, the natural combination of special relativity, and quantum mechanics.

Quantum statistical physics can be formulated in the language of Euclidean (imaginary-time) functional integrals, quite natural for finite-temperature field theories but also applicable in nonrelativistic contexts since quantum mechanics can be viewed as a field theory in zero spatial dimensions. Functional integrals thus furnish a powerful unifying formalism to compute correlations.

Indeed, the formalism expresses the partition function of a given system as a generating functional of euclidean Green's functions (correlations), similarly to zero-temperature field theory, but with the time direction made compact, and specific boundary conditions that constrain the domain of field configurations in the functional integral.

In order to best exploit the unifying aspect of the formalism, we propose to view the partition function as an integral of the diagonal density matrix element of the theory. The

integral is performed over the stochastic variable which characterizes the Schrödinger representation of the matrix element (position representation for quantum mechanics, field representation for second-quantized quantum mechanics or field theory). The density matrix is just the Boltzmann operator, whose Hamiltonian operator may either come from (second-quantized) quantum mechanics or from field theory.

The density matrix element may be written as a functional integral in euclidean time τ which starts from a given configuration (a point in quantum mechanics, a field configuration in field theory) at $\tau=0$ and returns to that same configuration at $\tau=\beta\hbar$. Clearly, there is a sum to be performed over configurations which coincide at the end points of the Euclidean time interval. Those boundary configurations are identified as the stochastic variable of the remaining integral.

This density matrix method for deriving an effective stochastic problem was already used in [2], where it led to the construction of dimensionally reduced effective actions. Likewise, in Ref. [3] we used the density matrix method, and a semiclassical approximation, to investigate the thermodynamics of scalar fields. In the latter reference, the boundary configuration of the field (considered as a fluctuation around a homogeneous background) played a very nontrivial role in the semiclassical formulation for the partition function of scalar fields.

Different approximation schemes can be used in order to obtain an effective theory for the stochastic field. Our prior uses of the density matrix method drew upon generalizations of a thermal semiclassical treatment previously developed and applied to quantum statistical mechanics, which produced excellent results for the ground-state energy and the specific heat of the anharmonic (quartic) oscillator [4–6]. In those prior uses, however, the connection with the stochastic variable was indirect, through classical solutions of equations of motion. In this paper, we have built a simple effective stochastic theory by expanding the action directly around the stochastic variable. Besides providing a realization of new conceptual ideas, we believe that this approach may be physically relevant to the discussion of infrared problems in several applications of quantum statistical physics.

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We perform an explicit calculation of the free energy and specific heat for the anharmonic oscillator (for references in the literature, see [7–18]) from the partition function of an interacting one-dimensional quantum-mechanical system at finite temperature from a path-integral representation for the density matrix. The method of calculation that we propose provides an alternative to the usual sum over periodic trajectories: it sums over paths with coincident end points, and includes the contribution of nonvanishing boundary terms.

The paper is organized as follows: in Sec. II, we introduce our formulation for quantum statistical field theory, in order to clarify the multiple role of our boundary fields, which are at the same time field eigenstates for the subjacent field theory problem, and stochastic variables for the ensuing statistical integral; in Sec. III, we particularize the discussion to quantum mechanics, presenting the contribution of nonperiodic trajectories in the density matrix formalism which lead us to a modified series expansion in Matsubara frequencies; besides, we review the high-temperature limit of the quantum theory as a classical effective theory for the boundary variable; in Sec. IV, using a simple effective theory for the stochastic variable, we compute several thermodynamic quantities for the quadratic and the quartic potentials, and compare the results to the semiclassical findings of [4], and to some exact results; and Sec. V contains our conclusions and outlook.

II. DENSITY MATRIX FOR SCALAR THEORIES

In statistical mechanics, the partition function for a system in contact with a thermal reservoir at temperature¹ T ($\beta=1/T$) is expressed as a sum (integral) over a stochastic variable, whose probabilistic weight is given by the density matrix.

For a system described by a (self-interacting) scalar field theory, the stochastic variable is the field eigenvalue in the functional Schrödinger picture, given by the function $\varphi_0(\mathbf{x})$, which satisfies $\hat{\varphi}|\varphi_0(\mathbf{x})\rangle = \varphi_0(\mathbf{x})|\varphi_0(\mathbf{x})\rangle$.

The partition function is then a functional integral over the field eigenvalue of the diagonal element of the density matrix functional ρ_β ,

$$Z(\beta) = \int [\mathcal{D}\varphi_0(\mathbf{x})] \rho_\beta[\varphi_0(\mathbf{x}), \varphi_0(\mathbf{x})], \quad (1)$$

$$\rho_\beta[\varphi_0(\mathbf{x}), \varphi_0(\mathbf{x})] \equiv \langle \varphi_0(\mathbf{x}) | \exp(-\beta \mathbf{H}) | \varphi_0(\mathbf{x}) \rangle. \quad (2)$$

The Hamiltonian in the preceding formula specifies the underlying dynamics. In the present case, it is the dynamics of a (self-interacting) scalar field $\varphi(t, \mathbf{x})$.

As is well known [19], ρ_β can also be expressed as a functional integral over dynamical fields $\varphi(\tau, \mathbf{x})$ defined for Euclidean time τ , subject to the boundary conditions $\varphi(0, \mathbf{x}) = \varphi(\beta, \mathbf{x}) = \varphi_0(\mathbf{x})$,

$$\rho_\beta[\varphi_0(\mathbf{x}), \varphi_0(\mathbf{x})] = \int_{\varphi(0, \mathbf{x}) = \varphi_0(\mathbf{x})}^{\varphi(\beta, \mathbf{x}) = \varphi_0(\mathbf{x})} [\mathcal{D}\varphi(\tau, \mathbf{x})] e^{-S[\varphi(\tau, \mathbf{x})]}. \quad (3)$$

The boundary conditions relate the stochastic variable of the integral in Eq. (1) to the dynamical fields that are integrated over in Eq. (3). The Hamiltonian

$$H[\Pi, \varphi] = \frac{1}{2} \Pi^2 + \frac{1}{2} (\nabla \varphi)^2 + \frac{m^2}{2} \varphi^2 + \frac{\lambda}{4!} \varphi^4, \quad (4)$$

which involves the time-dependent field $\varphi(t, \mathbf{x})$ and the conjugate momentum $\Pi(t, \mathbf{x})$, leads to the Euclidean action (we assume d spatial dimensions),

$$S[\varphi] = \int_0^\beta d\tau \int d^d \mathbf{x} \mathcal{L}[\varphi], \quad (5)$$

$$\mathcal{L}[\varphi] = \frac{1}{2} (\partial_\tau \varphi)^2 + \frac{1}{2} (\nabla \varphi)^2 + \frac{m^2}{2} \varphi^2 + \frac{\lambda}{4!} \varphi^4. \quad (6)$$

The density matrix is a functional of $\varphi_0(\mathbf{x})$ only. The remaining integral over $\varphi_0(\mathbf{x})$ which is required to obtain the partition function is unrestricted (except for the vacuum boundary conditions that must be imposed at spatial infinity).

We may write $\rho = e^{-S_d}$, S_d being a certain T -dependent dimensionally reduced action. The field $\varphi_0(\mathbf{x})$ which is the argument of S_d depends only on the d spatial coordinates; all the τ dependence of the original $d+1$ theory has been eliminated through the φ integration.

The fields $\varphi_0(\mathbf{x})$ are the natural degrees of freedom of the reduced theory. Any thermal observable can be constructed by integrating over the fields $\varphi_0(\mathbf{x})$ an appropriate functional of $\varphi_0(\mathbf{x})$ weighed with the corresponding diagonal element of the density matrix. The Euclidean time evolution can be viewed as an intermediate step which calculates the weights.

Notice that the density matrix is *not*, in general, of the form $e^{-\beta H_d}$ with H_d being independent of β as in ordinary statistical mechanics; its β dependence is far more complicated. This had already been pointed out in the analogous discussion of the transfer matrix carried out in Ref. [20]. The density matrix provides a direct but alternative way of deriving a dimensionally reduced theory.

In previous works, we calculated the density matrix element functional given by the integral in Eq. (3) either from a perturbative expansion [2] or from a semiclassical expansion [3] around the extremum of the integrand for the special case of a homogeneous (\mathbf{x} -independent) field φ_0 .

The semiclassical approximation corresponds to the usual saddle-point approximation with Gaussian fluctuations. For the general case, one has to obtain the extrema of the euclidean action in Eq. (3); in other words, classical solutions subject to the boundary conditions $\varphi(0, \mathbf{x}) = \varphi(\beta, \mathbf{x}) = \varphi_0(\mathbf{x})$. Since the density matrix can only depend on $\varphi_0(\mathbf{x})$, it should be clear that the classical solution is itself a functional of $\varphi_0(\mathbf{x})$.

Thus, the semiclassical expansion would lead to a somewhat indirect dependence of the density matrix on $\varphi_0(\mathbf{x})$. Furthermore, the general problem of finding classical solutions for arbitrary boundary conditions $\varphi_0(\mathbf{x})$ does not have a general solution. To circumvent these difficulties, in the

¹In order to simplify the notation, we will adopt natural units where $\hbar=1$, $c=1$, and $k_B=1$.

present work we have chosen to expand our dynamical fields $\varphi(\tau, \mathbf{x})$ directly around $\varphi_0(\mathbf{x})$,

$$\varphi(\tau, \mathbf{x}) = \varphi_0(\mathbf{x}) + \eta(\tau, \mathbf{x}), \quad (7)$$

instead of using the standard semiclassical expansion

$$\varphi(\tau, \mathbf{x}) = \varphi_{cl}[\varphi_0(\mathbf{x})] + \xi(\tau, \mathbf{x}). \quad (8)$$

Using $\varphi_0(\mathbf{x})$ as a background eliminates the τ dependence that would be present in the classical solution, and provides expressions that depend directly on $\varphi_0(\mathbf{x})$. On the other hand, we are forced to deal with linear terms when we resort to a quadratic approximation to the integral over $\eta(\tau, \mathbf{x})$ which would be absent in a quadratic approximation to the integral over $\xi(\tau, \mathbf{x})$. We emphasize that our alternative expansion is not a saddle-point approximation. However, when T is much bigger than any other scale of the theory, $\varphi_{cl}[\varphi_0]$ is approximately given by $\varphi_0[\mathbf{x}]$.

Dealing with a linear term is not a problem within a quadratic approximation, and can be handled by the usual shift in the integration variable. As for the validity of the expansion, it should be clear that it should be quite reliable at high temperatures, where $\eta(\tau, \mathbf{x})$ cannot differ appreciably from zero since the Euclidean time interval β is too small for deviations from the boundary values to become large. In fact, in a high-temperature regime, the classical solution is not very different from $\varphi_0(\mathbf{x})$.

For the sake of simplicity, we have chosen to test our strategy for computing the density matrix element in quantum mechanics, which can be viewed as a field theory in zero spatial dimension. By doing so, we do not have to deal with the subtleties of renormalization. We also need not worry about the infrared problems that plague various treatments of field theories at finite temperature [1,21,22]. Furthermore, we can compare the outcome our proposal with previous calculations done using ordinary perturbation theory, as well as to a semiclassical treatment of the η integral.

In the sequel, we calculate the partition function over a range of temperatures where we believe that our approximation will hold. In fact, we even estimate a lower bound on temperature above which we expect our computations to be valid and verify that this is indeed the case through numerical calculations.

Before proceeding in the calculation, we discuss some important features of the present approach: the inclusion of nonperiodic configurations and its exact high-temperature limit.

III. SPECIAL FEATURES OF THE METHOD

A. Inclusion of nonperiodic configurations

If we repeat the steps of the previous section, the partition function Z for a one-dimensional quantum-mechanical system in contact with a thermal reservoir at temperature $T=1/\beta$ will be written as

$$Z = \int dx_0 \rho_\beta(\beta; x_0, x_0), \quad (9)$$

where $\rho_\beta(\beta; x_0, x_0)$ is the diagonal element of the density matrix. Note that the role of the field $\varphi_0(\mathbf{x})$ of the previous

section is now played by a mere point x_0 , and that accordingly functional integrals become ordinary integrals.

In the path-integral formulation, the density matrix ρ_β is obtained from the imaginary-time evolution of the trajectory $x(\tau): [0, \beta] \rightarrow \mathbb{R}$ [which replaces $\varphi(\tau, \mathbf{x})$] determined by the Euclidean action S ,

$$\rho_\beta(x_0, x_0) = \int_{x(0)=x_0}^{x(\beta)=x_0} [\mathcal{D}x] e^{-S[x]}, \quad (10)$$

$$S[x] = \int_0^\beta d\tau \left\{ \frac{1}{2} m \dot{x}^2(\tau) + V[x(\tau)] \right\}, \quad (11)$$

where V is the potential, and the dot refers to differentiating in τ . As we have emphasized for $\varphi_0(\mathbf{x})$, it is natural to regard x_0 as the effective stochastic degree of freedom of the theory, and to compute the distribution of the variable x_0 by integrating over the dynamical variable $x(\tau)$, with boundary conditions determined by x_0 .

Integrating action (11) by parts, we obtain,

$$S[x] = \int_0^\beta d\tau \left\{ -\frac{1}{2} m x(\tau) \frac{d^2 x}{d\tau^2} + V[x(\tau)] \right\} + \frac{m}{2} x_0 [\dot{x}(\beta) - \dot{x}(0)]. \quad (12)$$

Among the trajectories with boundary value x_0 at $\tau=0$ and β , the one which contributes the most for the partition function is the (classical) solution of

$$m \frac{d^2 x_c}{d\tau^2} - V'(x_c) = 0, \quad (13a)$$

$$x_c(0) = x_c(\beta) = x_0. \quad (13b)$$

In the special case of the harmonic oscillator ($V(x) = m\omega^2 x^2/2$), it is a simple matter to show that

$$x_c(\tau) = x_0 \frac{\cosh[\omega(\tau - \beta/2)]}{\cosh(\omega\beta/2)}, \quad (14)$$

which is *not* a periodic function of τ . As a consequence, one is led to deal with boundary terms in the action [see Eq. (12)]. We stress that, as long as the only condition over paths in the path integral is to have coincident values at 0 and β , nonperiodicity *is* allowed.

In order to see that nonperiodic trajectories are a general feature of the present approach, let us now decompose the path x as

$$x(\tau) = x_0 + y(\tau) \quad (15)$$

where

$$y(\beta) = y(0) = 0. \quad (16)$$

Clearly, fluctuations obeying Eq. (16) can be expanded in a sine-Fourier series,

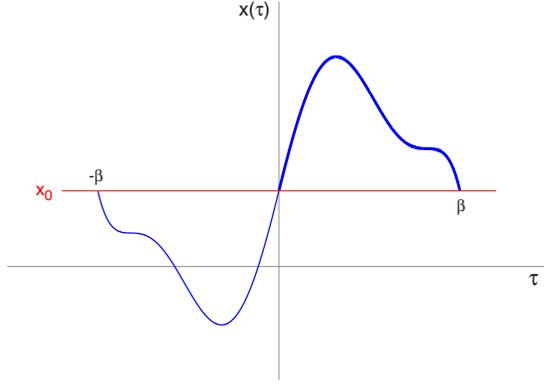


FIG. 1. (Color online) Schematic plot in $[-\beta, \beta]$ of series (18) of a configuration x defined originally in $[0, \beta]$.

$$y(\tau) \doteq \sum_{n=1}^{\infty} x_n \sin \hat{\omega}_n \tau, \quad (17)$$

where $\hat{\omega}_n = n\pi/\beta$. The notation with a dot is a reminder that the r.h.s. of Eq. (17) is a Fourier approximation of the l.h.s. The complete path is, then, given by

$$x(\tau) \doteq x_0 + \sum_{n=1}^{\infty} x_n \sin \hat{\omega}_n \tau, \quad (18)$$

which does not correspond to a periodic function in $[0, \beta]$ (see Fig. 1).

Series (18) does not impose conditions on the derivative of x . It is easy to convince oneself that evaluating the euclidean action S with the r.h.s. of Eq. (18) one obtains exactly $S[x(\tau)]$. In particular, we have for the classical solution,

$$x_c(\tau) \doteq x_0 - x_0 \sum_{n \text{ odd}} \frac{4\omega^2}{n\pi(\hat{\omega}_n^2 + \omega^2)} \sin \hat{\omega}_n \tau \quad (19)$$

so that the quantity $\dot{x}_c(\beta) - \dot{x}_c(0)$ is given by

$$\sum_{n \text{ odd}} \frac{-4x_0\omega^2\hat{\omega}_n}{n\pi(\hat{\omega}_n^2 + \omega^2)} (\cos \hat{\omega}_n\beta - 1) = \frac{2x_0\omega(\cosh \beta\omega - 1)}{\sinh \beta\omega}, \quad (20)$$

leading to the correct result. Obviously, the series defined by Eq. (18) does not correspond to the most general trajectory in Z . In particular, that series imposes a serious restriction on the second derivative of x by forcing it to vanish at 0 and β . However, at least for the calculation of usual action functionals, the boundary terms do not involve second derivatives and the aforementioned restriction is actually unimportant.

A remarkable property of decomposition (18) is that the boundary value x_0 plays the role of the zero, static component of $x(\tau)$.² Likewise, $\varphi_0(\mathbf{x})$ is the static component of

$\varphi(\tau, \mathbf{x})$ in the context of thermal field theories, which thus suggests that it plays a special role in the infrared (low-momentum) limit of the theory.

B. Exact high-temperature limit

When the typical spacing between quantum levels, $\hbar\omega$, is such that

$$\hbar\omega \ll k_B T \quad (21)$$

(or $\beta\omega \ll 1$, in natural units), we are in the classical limit of the theory. It is a known fact that the classical regime is correctly described by the effective theory for the static modes. Indeed, let us consider x_c , the solution of the equation of motion (13). In the high-temperature regime ($\beta\omega \ll 1$), thermal fluctuations dominate. In this limit, $x_c \rightarrow x_0$ and $S(x_c) \rightarrow \beta V(x_0)$, and we obtain for the partition function

$$\lim_{T \rightarrow \infty} Z = N \int dx_0 e^{-\beta V(x_0)}, \quad (22)$$

where N is a normalization factor which incorporates quantum fluctuations. A proper normalization of Z leads to $N^2 = mk_B T / (2\pi\hbar^2)$, rendering the semiclassical expression

$$\lim_{T \rightarrow \infty} Z = \int \frac{dp}{2\pi\hbar} \int dx_0 e^{-H/k_B T}, \quad (23)$$

with $H = p^2/2m + V(x_0)$, with m being the particle mass.

As discussed in [23], for $\beta\omega \ll 1$ the correlation $\langle x^2(\tau) \rangle$ follows the classical linear scaling with T . This behavior is entirely associated with the static component of x , and represents a problem for the high-temperature limit of the usual perturbative expansion. In contrast, the subtracted thermal propagator (without the contribution from the static mode) goes to zero as T increases so that one should strongly improve the convergence of the perturbation expansion by calculating diagrams with that subtracted propagator.

From the aforementioned reasons, we conclude that a separate treatment of the boundary (static) modes is convenient. The main advantage of the density matrix approach is to provide this separation in a natural fashion. In terms of y defined in Eq. (16), one can express Z conveniently as

$$Z = \int dx_0 \int_{y(0)=y(\beta)=0} [Dy] e^{-S[x_0+y]}, \quad (24)$$

and different strategies can be used to handle $S[x_0+y]$ in order to obtain an effective theory³ for x_0 ,

$$Z = \int \frac{dx_0}{\sqrt{2\pi\hbar^2/(mk_B T)}} e^{-\beta V_{\text{eff}}(x_0)}. \quad (25)$$

IV. HIGH-TEMPERATURE EXPANSION

In the last section, we have shown that the high-temperature limit of the theory is an effective theory for the

²Rigorously speaking, x_0 is not a true Fourier mode since it is not orthogonal to $\sin \hat{\omega}_n \tau$ in $[0, \beta]$ but in $[-\beta, \beta]$. With this caveat in mind, we will continue to refer to x_0 as a mode of x .

³With the normalization factor used in Eq. (25), one has the property: $V_{\text{eff}}(x_0) \rightarrow V(x_0)$ when $T \rightarrow \infty$, as follows from Eq. (23).

boundary static variable x_0 . In the sequel, we use a very simple expansion around x_0 in two cases: the harmonic potential, as a consistency check, and the single-well quartic potential, in order to verify the quality of our alternative approach when we extrapolate the high-temperature regime.

A. Quadratic case

The action in this case is given by

$$S[x] = \int_0^{\beta\hbar} d\tau \left[\frac{1}{2} m \dot{x}^2(\tau) + \frac{1}{2} m \omega^2 x^2(\tau) \right]. \quad (26)$$

Without any loss of generality, one can take $m=1$ in the previous equation by rescaling x by a factor $1/\sqrt{m}$.

Now, we use the decomposition of x given by Eq. (16) to obtain

$$\begin{aligned} S[x] &= \frac{\beta\omega^2}{2} x_0^2 + \frac{1}{2} \int d\tau d\tau' \{ y G_y^{-1} y + 2\omega^2 x_0 y \} \\ &= \frac{\beta\omega^2}{2} x_0^2 + \frac{1}{2} \int d\tau d\tau' \{ (y + \omega^2 x_0 G_y) G_y^{-1} (y + \omega^2 x_0 G_y) \} \\ &\quad - \frac{\omega^4 x_0^2}{2} \int d\tau d\tau' G_y, \end{aligned} \quad (27)$$

where G_y is the solution of

$$\left[-\frac{d^2}{d\tau^2} + \omega^2 \right] G_y(\tau, \tau') = \delta(\tau - \tau'), \quad (28a)$$

$$G_y(0, \tau') = G_y(\beta, \tau') = 0. \quad (28b)$$

A simple calculation gives

$$G_y(\tau, \tau') = \frac{\sinh[\omega(\tau_> - \beta)] \sinh(\beta\tau_<)}{\omega \sinh(\omega\beta)}, \quad (29)$$

[where $\tau_> = \max(\tau, \tau')$ and $\tau_< = \min(\tau, \tau')$], and

$$\int d\tau d\tau' G_y(\tau, \tau') = \frac{\beta}{\omega^2} - \frac{2(\cosh \beta\omega - 1)}{\omega^3 \sinh \beta\omega}. \quad (30)$$

Shifting the variable of integration to

$$\zeta(\tau) = y(\tau) + \omega^2 x_0 \int d\tau' G_y(\tau, \tau'), \quad (31)$$

which obeys $\zeta(0) = \zeta(\beta) = 0$, and performing the Gaussian integration, we obtain

$$Z = (\det G_y)^{1/2} \int dx_0 e^{-\omega(\cosh \beta\omega - 1) / \sinh \beta\omega x_0^2}. \quad (32)$$

Integrating over x_0 and taking the logarithm, one reproduces the known result for the free partition function. Therefore, for quadratic theories the present high-temperature expansion is exact.

B. Anharmonic oscillator

Let us now consider the following action:

$$S[x] = \int_0^\beta d\tau \left[\frac{1}{2} m \dot{x}^2(\tau) + \frac{1}{2} m \omega^2 x^2(\tau) + \frac{\lambda}{4} x^4(\tau) \right]. \quad (33)$$

It is convenient to define the dimensionless variables: $q = \sqrt{\lambda/(m\omega^2)} x$, $\theta = \omega\tau$, $\Theta = \omega\beta$, and $g = \lambda/(m^2\omega^3)$. The associated action for the variable q is

$$S[q] = \frac{1}{g} \int_0^\Theta d\theta \left(\frac{1}{2} \dot{q}^2(\theta) + \frac{1}{2} q^2(\theta) + \frac{1}{4} q^4(\theta) \right). \quad (34)$$

Using the decomposition $q(\theta) = q_0 + \sqrt{g} \eta(\theta)$, we write for the action

$$S[q] = S_2[q_0, \eta] + S_L[q_0, \eta], \quad (35)$$

where S_2 contains $S[q_0]$, the kinetic term, and those which are linear or quadratic in η . The remaining contributions to $S[q]$ are collected in S_L . It is a simple matter to show that

$$\begin{aligned} S_2[q_0, \eta] &= S[q_0] \\ &+ \frac{1}{2} \int_0^\Theta d\theta \left\{ \eta(\theta) \left[-\frac{d^2}{d\theta^2} + \bar{\omega}_0^2 \right] \eta(\theta) + \frac{2\alpha_0}{\sqrt{g}} \eta(\theta) \right\}, \end{aligned} \quad (36)$$

and

$$S_L[q_0, \eta] = \int_0^\Theta d\theta \left[\sqrt{g} q_0 \eta^3(\theta) + \frac{g}{4} \eta^4(\theta) \right], \quad (37)$$

where $\bar{\omega}_0^2(q_0) = 3q_0^2 + 1$ and $\alpha_0(q_0) = q_0^3 + q_0$ (here and in the sequel, the subscript is a reminder of the dependence on q_0). One obtains a quadratic approximation for the partition function by considering

$$Z_2 = \int dq_0 \int_{\eta(0)=\eta(\Theta)=0} [D\eta] e^{-S_2[q_0, \eta]}. \quad (38)$$

Proceeding as in the previous section, we perform the Gaussian integration over the variable

$$\zeta(\theta) = \eta(\theta) + \frac{\alpha_0}{\sqrt{g}} \int_0^\Theta d\theta' G_0(\theta, \theta'), \quad (39)$$

where the Green's function G_0 (again, the subscript is a reminder of the dependence of this η propagator on q_0), defined by

$$\left[-\frac{d^2}{d\theta^2} + \bar{\omega}_0^2 \right] G_0(\theta, \theta') = \delta(\theta - \theta'), \quad (40a)$$

$$G_0(0, \theta') = G_0(\Theta, \theta') = 0, \quad (40b)$$

is given by

$$G_0(\theta, \theta') = \frac{\sinh[\bar{\omega}_0(\theta_> - \Theta)] \sinh(\bar{\omega}_0\theta_<)}{\bar{\omega}_0 \sinh(\bar{\omega}_0\Theta)}, \quad (41)$$

where the q_0 dependence comes through $\bar{\omega}_0(q_0)$. The result for Z_2 is then

$$Z_2 = \int dq_0 (\det G_0)^{1/2} \exp\{-\mathcal{S}[q_0] + \Sigma_0\}, \quad (42)$$

where

$$\det G_0 = \frac{\bar{\omega}_0}{2\pi \sinh(\bar{\omega}_0 \Theta)} \quad (43)$$

and

$$\Sigma_0 = \frac{\alpha_0^2}{2g} \int_0^\Theta d\theta d\theta' G_0(\theta, \theta'). \quad (44)$$

From Eq. (42), one directly obtains an expression for $\rho_\beta(\beta; q_0, q_0)$. The positive function ρ_β is peaked at $q_0=0$ and decays to zero around $q_0=2\sqrt{g}$.

To go beyond the quadratic order in η , we use the following approximation:

$$e^{-\mathcal{S}[q_0, \eta]} \approx 1 - \int_0^\Theta d\theta \left[\sqrt{g} q_0 \eta^3(\theta) + \frac{g}{4} \eta^4(\theta) \right]. \quad (45)$$

Therefore, $Z \approx Z_2 + \delta^{(1)}Z$, where

$$\begin{aligned} \delta^{(1)}Z = & - \int dq_0 (\det G_0)^{1/2} \exp\{-\mathcal{S}[q_0] + \Sigma_0[j]\} \int_0^\Theta d\theta \\ & \times \left[\sqrt{g} q_0 \langle \eta^3(\theta) \rangle + \frac{g}{4} \langle \eta^4(\theta) \rangle \right], \end{aligned} \quad (46)$$

with

$$\langle \eta(\theta_1) \dots \eta(\theta_k) \rangle = \int_{\eta(0)=\eta(\Theta)=0} [\mathcal{D}\eta] e^{-\mathcal{S}_2[q_0, \eta]} \eta(\theta_1) \dots \eta(\theta_k). \quad (47)$$

As usual, we can introduce a linear coupling of η with an external current j :

$$\begin{aligned} Z_2[j] = & \int dq_0 \int_{\eta(0)=\eta(\Theta)=0} [\mathcal{D}\eta] \\ & \times \exp\left\{-\mathcal{S}_2[q_0, \eta] + \int d\theta j(\theta) \eta(\theta)\right\}, \end{aligned} \quad (48)$$

and obtain the correlations [Eq. (47)] as functional derivatives of $Z_2[j]$ with respect to j . With minor modifications on the recipe for Z_2 , one obtains

$$Z_2[j] = \int dq_0 (\det G_0)^{1/2} \exp\{-\mathcal{S}[q_0] + \Sigma_0[j]\}, \quad (49)$$

where

$$\Sigma_0[j] = \frac{1}{2} \int_0^\Theta d\theta d\theta' \sigma_0(\theta) G_0(\theta, \theta') \sigma_0(\theta'), \quad (50)$$

and $\sigma_0(\theta) = \alpha_0 / \sqrt{g} - j(\theta)$. Finally, we use

$$e^{-\Sigma_0[j]} \left[\frac{\delta^3}{\delta j^3(\theta)} \right]_{j=0} e^{\Sigma_0[j]} = I_0^3(\theta) + 3I_0(\theta) G_0(\theta, \theta) \quad (51)$$

and

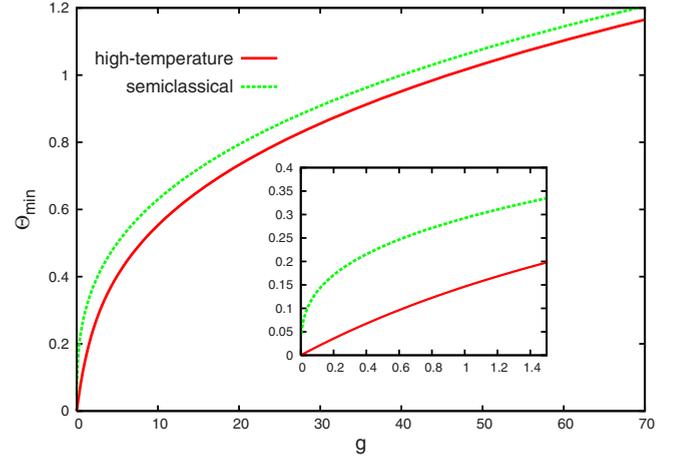


FIG. 2. (Color online) Plot of Θ_{\min} as a function of the dimensionless coupling constant g . Each approximation is applicable for temperatures larger than the associated Θ_{\min} . The inset is the same plot for smaller values of g .

$$e^{-\Sigma_0[j]} \left[\frac{\delta^4}{\delta j^4(\theta)} \right]_{j=0} e^{\Sigma_0[j]} = I_0^4(\theta) + 6I_0^2(\theta) G_0(\theta, \theta) + 3G_0^2(\theta, \theta), \quad (52)$$

where $I_0(\theta)$ plays the role of an expectation value of $\eta(\theta)$,

$$\begin{aligned} I_0(\theta) = & - \frac{\alpha_0}{\sqrt{g}} \int_0^\Theta d\theta' G_0(\theta, \theta') \\ = & \frac{\alpha_0 \cosh \bar{\omega}_0 \theta - \sinh \bar{\omega}_0 \theta \tanh \bar{\omega}_0 \Theta / 2 - 1}{\sqrt{g} \bar{\omega}_0^2}. \end{aligned} \quad (53)$$

The remaining integrations over θ can be done analytically, providing all the ingredients for the calculation of the first correction to Z_2 .

From Eq. (45), we read that corrections to the quadratic approximation become important when the expectation value of interaction (37) is about 1. As the integrand of Eq. (46) is dominated by the vicinity of $q_0=0$, where the quadratic action reaches its minimum value, one can estimate the importance of corrections using $\langle S_I(0, \eta) \rangle$. We have

$$\langle S_I(0, \eta) \rangle = \frac{3g}{4} \int_0^\Theta d\theta G_0^2(\theta, \theta) \xrightarrow{\Theta \gg 1} \frac{3g\Theta}{16}. \quad (54)$$

The temperature Θ_{\min} where $\langle S_I(0, \eta) \rangle$ goes to 1 provides a rough estimate for the validity of the quadratic approximation. Figure 2 displays Θ_{\min} as a function of the dimensionless coupling constant g for the high-temperature and the usual saddle-point approximation (see Ref. [4]). From Fig. 2, we conclude that the two methods have almost the same range of applicability. In particular, we see that Θ_{\min} is of order 1 for g as large as 50.

The results for the free energy when $g=0.4$ are displayed in two plots with different ranges of temperature: Fig. 3 shows the high-temperature region, while Fig. 4 is devoted to low temperatures, according to the criterium used in Fig. 2. The results for the specific heat are displayed in Fig. 5. In the figures, *classical* corresponds to calculation using Eq. (23),

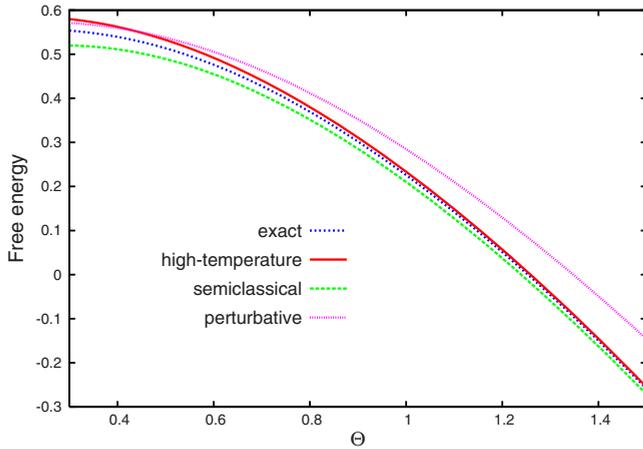


FIG. 3. (Color online) Free energy of the anharmonic oscillator as a function of the dimensionless temperature for $g=0.4$ in the high-temperature region (see text for details).

high-temperature uses Eq. (42), *improved* includes the correction corresponding to Eq. (46), *semiclassical* refers to the semiclassical result obtained in Ref. [4], *perturbative* stands for the usual first-order perturbative result, and *exact* corresponds to results from Refs. [13,14] combined with WKB estimates.

The first remarkable thing in the plots is the failure of the first-order perturbative result in the high-temperature region ($T \gg \omega$). As discussed in [23], the static component of the usual thermal propagator spoils the convergence of the perturbative series for temperatures large compared with ω . As seen in Ref. [4], the high-temperature region is well described by the semiclassical curve, and asymptotically, by the classical one. This is evident from the plots. It is interesting that, for $g=0.4$, the agreement extends to temperatures down to $\Theta \approx 1/2$, a region where the character of the system is far from classical. However, it is surprising that our simple calculation using Eq. (42) works as well as the semiclassical one in that region.

Indeed, the cited semiclassical calculation is based on a quadratic expansion around exact solutions of Eq. (13) for

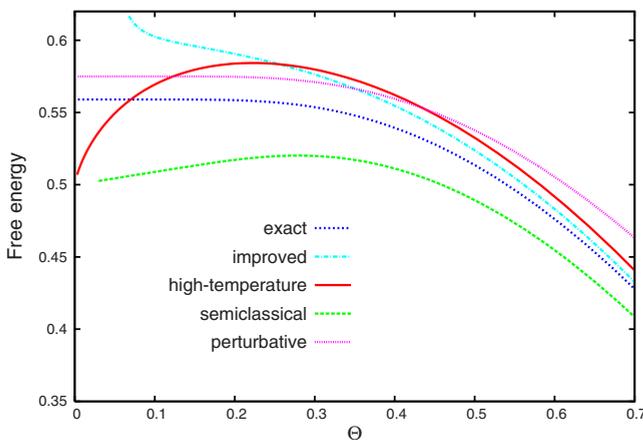


FIG. 4. (Color online) Free energy of the anharmonic oscillator as a function of the dimensionless temperature for $g=0.4$ in the low-temperature region (see text for details).

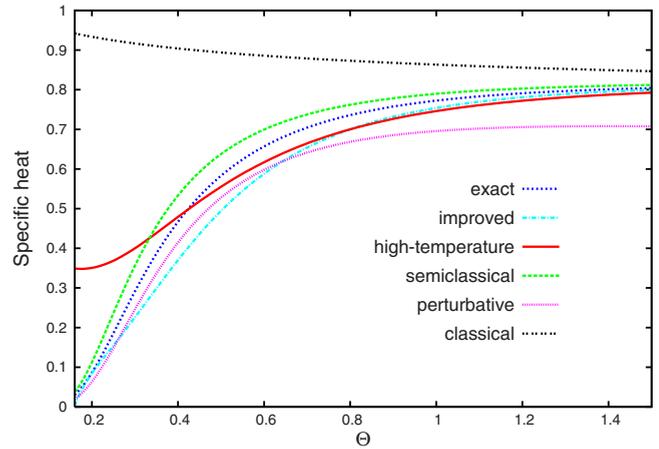


FIG. 5. (Color online) Specific heat of the anharmonic oscillator as a function of the dimensionless temperature for g (see text for details).

the quartic potential. In practice, one has to deal with rather involved Jacobi elliptic functions [4,24]. In contrast, using expansion (15) no knowledge of classical solutions is demanded. This simplification represents an economic alternative which can be crucial in contexts where exact classical solutions are not available. From the plots, one also concludes that, in the region where the approximation is supposed to be good, the improved calculation exhibits a stronger convergence, indicating that the approximation is consistent.

A detailed look at the quadratic curve in the free-energy plot (Fig. 4) reveals a nonmonotonic behavior for low temperatures: the free energy passes by a maximum and decreases toward the free value 0.5. This is a general feature regardless of the value of g , and it is a clear signal of the breakdown of the approximation below Θ_{\min} (see Fig. 2). The improved free energy diverges at Θ_{\min} because at this value the sum $Z_2 + \delta^{(1)}Z$ vanishes. The exact curve for the free energy reaches its maximum value at the ground-state energy, where it rests down to $\Theta=0$. Using the maximum value assumed by the quadratic curve as an approximate value for the ground-state energy, we obtain unexpectedly reasonable results, as shown in Table I. A path-integral general method for deriving the ground-state wave function and energy can be found in Ref. [25].

Figure 5 compares different predictions for the specific heat for $g=0.4$. Notice that all curves, except for the perturbative one, have the correct high-temperature limit. The anomalous behavior of the quadratic approximation near Θ_{\min} is even more evident in this plot. The improvement obtained in the low-temperature regime when one corrects the quadratic calculation with Eq. (46) is also clearly shown.

V. CONCLUSIONS AND OUTLOOK

The theoretical description of the thermodynamics of a given interacting many-body system kept in thermal equilibrium with a heat bath is an issue of capital importance in most realms of physics, from cosmology to condensed-matter settings.

TABLE I. Ground-state energy of the quartic oscillator for different values of the coupling λ ($m=\omega=1$). Exact data were extracted from Ref. [14], whereas E_0 (quadratic) was obtained using Eq. (42).

λ	E_0 (exact)	E_0 (quadratic)	Error (%)
0.008	0.501	0.505	0.8
0.04	0.507	0.518	2.2
0.4	0.559	0.584	4.5
1.2	0.638	0.662	3.8
2.0	0.696	0.718	3.2
4.0	0.804	0.818	1.7
8.0	0.952	0.958	0.6
200.0	2.500	2.450	2.0

A very convenient framework is provided by finite-temperature field theory, where one can use the imaginary-time formalism and make a direct connection to the powerful formulation of thermal averages in terms of functional integrals.

Rigorously speaking, the paths need not be periodic in the path-integral representation of the partition function. Indeed, the necessity of paths which are not periodic is particularly clear in the formulation of the partition function as an integral of the diagonal density matrix element of the theory.

In this paper, we have followed our alternative strategy in the case of quantum statistical mechanics, viewed not only as a toy model for the case of finite-temperature field theory, but also as a prototype for various relevant systems in statistical physics. More specifically, we have explored an alternative way of computing the partition function in the path-integral formalism that includes nonperiodic trajectories. As was shown above, one can properly incorporate the contribution of nonperiodic paths by using a modified Matsubara series expansion in which the static mode is identified with the boundary value of the path. The latter turns out to be the

stochastic variable that survives in the final effective theory which has the character of a high-temperature approximation.

We built a very simple effective theory in the nontrivial problem of the anharmonic oscillator, obtaining very precise results for practically the whole range of temperatures without any information about classical solutions. We expect that other potentials can profit from the simplicity of the present method in quantum-mechanical systems.

When more than one classical solution is present (such as in the case of double-well potentials), the method probably would still apply in the high-temperature regime down to the first bifurcation point (a discussion on caustics in the semiclassical approximation is given in [6]). However, we do not expect the method can correctly describe zero-temperature features such as tunneling driven by instantonlike solutions.

As mentioned previously, the infrared physics of bosonic theories is not accessible to plain perturbation theory, and resummation techniques are required in order to produce sensible results. In common, all such techniques render a special treatment to the static mode. Therefore, we expect that in field theory the physics of $\varphi_0(\mathbf{x})$ will play a prominent infrared role, although this is still under investigation.

In the case of finite-temperature field theory there are, of course, subtle issues of renormalization, which are absent in the quantum-mechanical setting, that will have to be addressed. Nevertheless, the results obtained in quantum statistical mechanics are encouraging, and we hope that this new perspective may shed light on the problem of infrared divergences. Results in this direction will be presented elsewhere [26].

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[1] M. Le Bellac, *Thermal Field Theory* (Cambridge University Press, London, 2000); J. I. Kapusta and C. Gale, *Finite-Temperature Field Theory: Principles and Applications* (Cambridge University Press, London, 2006); A. Das, *Finite Temperature Field Theory* (World Scientific, Singapore, 1997).

[2] C. A. A. de Carvalho, J. M. Cornwall, and A. J. da Silva, Phys. Rev. D **64**, 025021 (2001).

[3] A. Bessa, C. A. A. de Carvalho, E. S. Fraga, and F. Gelis, J. High Energy Phys. (2007) 007.

[4] C. A. A. de Carvalho, R. M. Cavalcanti, E. S. Fraga, and S. E. Jorás, Ann. Phys. **273**, 146 (1999).

[5] C. A. A. de Carvalho, R. M. Cavalcanti, E. S. Fraga, and S. E. Joras, Phys. Rev. E **61**, 6392 (2000).

[6] C. A. A. de Carvalho, R. M. Cavalcanti, E. S. Fraga, and S. E. Joras, Phys. Rev. E **65**, 056112 (2002).

[7] C. M. Bender, K. Olaussen, and P. S. Wang, Phys. Rev. D **16**, 1740 (1977).

[8] R. Balian, G. Parisi, and A. Voros, Phys. Rev. Lett. **41**, 1141 (1978).

[9] G. Parisi, *Field Theory, Disorder and Simulations* (World Scientific Publishing Company, Singapore, 1992).

[10] C. M. Bender and T. T. Wu, Phys. Rev. Lett. **21**, 406 (1968); Phys. Rev. Lett. **27**, 461 (1971).

[11] C. M. Bender and T. T. Wu, Phys. Rev. **184**, 1231 (1969).

[12] C. M. Bender and T. T. Wu, Phys. Rev. D **7**, 1620 (1973).

[13] S. N. Biswas, K. Datta, R. P. Saxena, P. K. Srivastava, and V. S. Varma, J. Math. Phys. **14**, 1190 (1973).

[14] F. T. Hioe and E. W. Montroll, J. Math. Phys. **16**, 1945 (1975).

[15] L. N. Lipatov, JETP Lett. **25**, 104 (1977) [Pis'ma Zh. Eksp. Teor. Fiz. **25**, 116 (1977)].

[16] E. Brézin, J. C. Le Guillou, and J. Zinn-Justin, Phys. Rev. D **15**, 1558 (1977).

- [17] C. Itzykson and J.-B. Zuber, *Quantum Field Theory* (McGraw-Hill, Singapore, 1985).
- [18] J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena* (Oxford University Press, Oxford, 1993).
- [19] R. P. Feynman and Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).
- [20] K. G. Wilson and J. B. Kogut, Phys. Rep. **12**, 75 (1974).
- [21] U. Kraemmer and A. Rebhan, Rep. Prog. Phys. **67**, 351 (2004).
- [22] J. O. Andersen and M. Strickland, Ann. Phys. **317**, 281 (2005).
- [23] H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets* (World Scientific, Singapore, 2004).
- [24] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1965).
- [25] G. C. Rossi and M. Testa, Ann. Phys. **148**, 144 (1983); F. Cesi, G. C. Rossi, and M. Testa, *ibid.* **206**, 318 (1991).
- [26] A. Bessa, F. T. C. Brandt, C. A. A. de Carvalho, and E. S. Fraga (unpublished).