Zero-mode analysis of quantum statistical physics

A. Bessa\textsuperscript{1}, C. A. A. de Carvalho\textsuperscript{2} and E. S. Fraga\textsuperscript{3}

\textsuperscript{1}Instituto de Física, Universidade de São Paulo, Caixa Postal 66318, 05315-970, São Paulo, SP, Brazil
\textsuperscript{2}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. We identify the stochastic variable of the effective statistical theory that we derive as a boundary configuration and a zero mode relevant to the discussion of infrared physics. We illustrate our formulation by computing the partition function of an interacting one-dimensional quantum mechanical system at finite temperature from the path-integral representation for the density matrix. The method of calculation provides an alternative to the usual sum over periodic trajectories: it sums over paths with coincident endpoints, and includes non-vanishing boundary terms. An appropriately modified expansion into Matsubara modes provides a natural separation of the zero-mode physics. This feature may be useful in the treatment of infrared divergences that plague the perturbative approach in thermal field theory.

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 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 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 \( \tau \) 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 \( \tau = \beta h \). Clearly, there is a sum to be performed over configurations which coincide at the endpoints of the euclidean time interval. Those boundary configurations are identified as the stochastic variable of the remaining integral. Furthermore, it will be shown that they are zero modes of a modified Matsubara series. The theory of the zero modes is the effective stochastic theory obtained from the original Hamiltonian.

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 (written as a constant plus gaussian fluctuations) played a very nontrivial role in the semiclassical formulation for the partition function of scalar fields.

Our prior uses of the 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 en-
ergy 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. Now, we have opted instead for a direct connection with the stochastic variable, to be identified with a zero mode, because we believe this is physically relevant to the discussion of infrared problems in several applications of quantum statistical physics.

In the context of finite-temperature field theory, for instance, it is known that a naive implementation of perturbation theory for the calculation of Feynman diagrams is ill-defined in the presence of massless bosons. This is due to the appearance of severe infrared divergences, brought about by the vanishing bosonic Matsubara mode in thermal propagators. The divergences plague the entire series, making it essentially meaningless [1, 7, 8].

As a result, one is forced to resort to resummation techniques that reorganize the perturbative series, and resum certain classes of diagrams, in order to extract sensible results. There are several ways of performing resumations, and rewriting the degrees of freedom more efficiently in terms of quasiparticles; we refer the reader to the reviews [7, 8], and to Ref. [3], for a discussion and a list of specific references.

All such techniques are designed to partially tame the infrared divergences, creating a non-zero domain of validity for weak-coupling expansions\(^1\). Nevertheless, the zero-mode problem remains, and the region of validity of resummed perturbation treatments can not be indefinitely enlarged.

The infrared problems of finite temperature field theory resemble those encountered in the functional integral treatment of various condensed matter systems [10], where they are connected to collective excitations. This suggests that one should explore the unifying feature of the formalism, which is its statistical nature, to profit from parallel physical interpretations and insights. This is yet another reason for resorting to the density matrix formulation.

In the present article, we resume the study of quantum statistical mechanics, viewed as an exercise in zero-dimensional finite-temperature field theory. Our objective is to show that boundary configurations are the zero-mode stochastic variables of the effective statistical theory, and to compute that theory in various approximate schemes. Although we restrict our analysis to quantum mechanical examples, this should be regarded as a preliminary to the field theory case.

We compute 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 endpoints, and includes the contribution of non-vanishing boundary terms. Indeed, an appropriately modified expansion into Matsubara modes provides a natural separation of the zero-mode physics, which is connected to the infrared problems in thermal field theory and elsewhere, and relates the zero mode to the boundary value of the quantum-mechanical coordinate.

The paper is organized as follows: in Section II, we present the proposed modified series expansion in Matsubara frequencies, and make a detailed comparison of our density matrix procedure with the standard one, for clarity; in Section III, we relate the boundary value of the quantum-mechanical coordinate (the stochastic variable) to the zero mode; In Section IV, we compute several thermodynamic quantities for the quadratic and the quartic potentials, and compare our results to the semiclassical findings of [4], and to some exact results; Section V contains our conclusions and outlook.

## II. A MODIFIED SERIES EXPANSION

The partition function \( Z \) for a one-dimensional quantum-mechanical system in contact with a thermal reservoir at temperature \( T = 1/(k_B\beta) \) may be written as

\[
Z = \int dx_0 \rho (\beta; x_0, x_0) ,
\]

where \( \rho (\beta; x_0, x_0) \) is the diagonal element of the density matrix. In a path-integral formulation, the density matrix \( \rho \) is obtained from the imaginary-time evolution of the trajectory \( x: [0, \beta \hbar] \to \mathbb{R} \) determined by an euclidian action \( S \):

\[
\rho (\beta; x_0, x_0) = \int \left[ Dx \right] e^{-S[x]/\hbar} ,
\]

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

where \( V \) is the potential\(^2\). In such a formalism, 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 auxiliary variable \( x \), with boundary conditions determined by \( x_0 \). In this article, we want to show that the effective theory for the static variable \( x_0 \) not only underscores its statistical-mechanical character, but can also be identified with the theory of the zero mode of an appropriately modified Matsubara expansion.

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1 In the case of thermal QCD, for instance, the domain of validity of the naive perturbative expansion is the empty set [9].

2 In order to simplify the notation, we will adopt natural units where \( \hbar = 1 \) and \( k_B = 1 \).
We can show that the formalism requires a modified Matsubara expansion for $x$ by calculating the partition function of the harmonic oscillator in two different manners. The action $S$, in this simple case, is given by

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

(4)

Without any loss of generality, one can take $m = 1$ in the previous equation by rescaling $x$ by a factor $1/\sqrt{m}$. One may compute the partition function using the following path integral:

$$Z = \int_{x(0) = x(\beta)} [Dx] e^{-S[x]}.$$  

(5)

The condition $x(0) = x(\beta)$ is usually implemented by expanding the path $x$ in Matsubara modes:

$$x(\tau) = \sum_{n=-\infty}^\infty c_n e^{-i\omega_n \tau} \text{ with } \omega_n = \frac{2\pi n}{\beta}. \quad (6)$$

The standard procedure is, then, to integrate Eq. (4) by parts:

$$S[x] = \frac{1}{2} \int_0^\beta d\tau x(\tau) \left[ -\frac{d^2}{d\tau^2} + \omega^2 \right] x(\tau) + \frac{1}{2} \left[ x(\tau) \dot{x}(\tau) \right]_0^\beta.$$  

(7)

Using the periodicity of Eq. (6), one shows that the boundary term in (7) is zero. The remaining term can be cast in the form

$$S[x] = \frac{1}{2} \int_0^\beta d\tau d\tau' x(\tau) K(\tau, \tau') x(\tau'),$$

(8)

where the Green function $K(\tau, \tau') = \Delta_F(\tau - \tau')$ is such that

$$\Delta_F(\tau) = \frac{1}{2\omega} \left[ (1 + n(\omega)) e^{-\omega \tau} + n(\omega) e^{\omega \tau} \right],$$

(10)

where $n(\omega)$ is the Bose-Einstein distribution. Using $\Delta_F$, it is straightforward to obtain the partition function. Up to an infinite constant, one obtains the well known result for the free energy

$$-\frac{1}{\beta} \log Z = \frac{\omega}{2} + \frac{1}{\beta} \log(1 - e^{-\beta\omega}).$$

(11)

There exists, however, an alternative path-integral method to calculate the partition function of the harmonic oscillator, which has the advantage of being free of spurious divergences. We start with (1), and decompose the configuration $x$ as

$$x(\tau) = x_c(\tau) + y(\tau),$$

(12)

where $x_c$ is the solution of the following Euler-Lagrange equation:

$$\frac{d^2 x_c}{d\tau^2} - \omega^2 x_c = 0,$$

(13a)

$$x_c(0) = x_c(\beta) = x_0,$$

(13b)

which is given by

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

It is easy to show that

$$S[x] = \frac{1}{2} x_0 [\dot{x}(\beta) - \dot{x}(0)] + S[y] = \frac{x_0^2 \omega (\cosh(\beta\omega) - 1)}{\sinh(\beta\omega)} + S[y].$$

(15)

Using that $y$ vanishes at $\tau = 0, \beta$, one rewrites the action of the trajectory $y$ as

$$S[y] = \frac{1}{2} \int d\tau d\tau' y(\tau) G^{-1}_y(\tau, \tau') y(\tau').$$

(16)

where the Green function $G_y$ satisfies the following equation:

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

(17a)

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

(17b)

One can show [4] that

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

(18)

and

$$\det G_y = \frac{\omega}{2\pi \sinh(\omega\beta)}.$$  

(19)

In Eq. (18), $\tau_\tau = \max(\tau, \tau')$ and $\tau_\tau = \min(\tau, \tau')$. The path integral over $y$ produces, then,

$$Z = (\det G_y)^{1/2} \int d\tau_\tau e^{-\omega(\cosh(\beta\omega - 1)/\sinh(\beta\omega) |x_0^2)}$$

(20)

$$= (2 \cosh(\beta\omega - 2))^{-1/2}.$$  

(21)

Using $(2 \cosh(\beta\omega - 2) = [1 - \exp(-\beta\omega)]^2 \exp(\beta\omega)$, and taking the logarithm we recover Eq. (11).

Notice, however, that the two methods treat in a different way the quantity

$$\dot{x}(\beta) - \dot{x}(0).$$

(22)
Let us focus on the usual Matsubara expansion of the classical path (Eq. (14)). Being periodic, the corresponding series has a periodic derivative, so that the quantity (22) is put to zero. That was used to eliminate the boundary term in Eq. (7). However, we see from (15) that \( \dot{x}_c(\beta) - \dot{x}_c(0) \neq 0 \), otherwise one would obtain an incorrect result for \( Z \).

The second method of calculation sums over paths which have coincident endpoints, and thus includes paths that are not periodic. It is easy to realize that we introduce an error in the value of the action of any non-periodic path \( x \) by evaluating the action of the associate Matsubara series as given by Eq. (6). The reason is that the usual Matsubara expansion is not suitable to handle boundary terms involving the derivative of \( x \) at 0 and \( \beta \). We stress that, as long as the only condition over paths is the zero mode of the usual Matsubara expansion. In fact, from Eq. (6), one can notice that \( \dot{x}_c(\beta) - \dot{x}_c(0) \) is given by

\[
\sum_{n = 0}^{\infty} \frac{-4x_0 \omega_n^2}{\pi \omega_n^2 + \omega_n^2} (\cos \omega_n \beta - 1) = \frac{2x_0 \omega (\cosh \beta \omega - 1)}{\sinh \beta \omega},
\]

as implied by Eq. (15). Obviously, the series defined by Eq. (25) 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 \( \beta \). 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.

III. THE BOUNDARY VALUE AS THE ZERO MODE

The first remarkable property of the decomposition (25) is that the boundary value \( x_0 \) is the zero, static component of \( x \) which, in the context of thermal field theories, plays a special role in the infrared (low-momentum) limit of the theory. 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 zero mode\(^3\).

It is important to stress that the zero mode \( x_0 \) is not the zero mode of the usual Matsubara expansion. In fact, from Eq. (6), one can notice that \( x_0 \) involves the coefficients of all Matsubara modes:

\[
x_0 = \sum_{n = -\infty}^{\infty} c_n.
\]

The present identification of the zero mode with the boundary field in the context of quantum statistical mechanics aggregates to the zero-mode physics yet another

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\(^3\) Rigorously speaking, \( x_0 \) is not a true Fourier mode since it is not orthogonal to \( \sin \omega_n \tau \) in \([0, \beta]\), but in \([-\beta, \beta]\). With this caveat in mind, we will continue to refer to \( x_0 \) as a mode of \( x \).
important feature: the connection with the classical behavior at high temperatures. That regime is characterized by the condition
\[ \hbar \omega \ll k_B T \] (30)
(or \( \beta \omega \ll 1 \), in natural units), where \( \hbar \) is the typical spacing between quantum levels. In order to see why the static mode governs the classical limit of the partition function, let us consider \( x_c \), the solution of the equation of motion:
\[ \frac{d^2 x_c}{d\tau^2} - V'(x_c(\tau)) = 0, \]
\[ x_c(0) = x_c(\beta) = x_0. \]

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
\[ \lim_{T \rightarrow \infty} Z = N \int dx_0 \exp(-\beta V(x_0)), \]
where \( N \) is a normalization factor which incorporates quantum fluctuations. A proper normalization of \( Z \) leads to \( N^2 = m k_B T/(2\pi \hbar^2) \), rendering the semiclassical expression
\[ \lim_{T \rightarrow \infty} Z = \int \frac{dp}{2\pi \hbar} \int dx_0 \exp(-H/k_B T), \]
with \( H = \frac{p^2}{2m} + V(x_0) \), \( m \) being the particle mass.

As discussed in [11], 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.

We conclude that, either to control infrared divergences in thermal field theories or to describe the classical limit in quantum statistical mechanics, we need a separate treatment of the zero mode. The main advantage of our approach is to provide this separation in a natural fashion.

In order to explore the zero-mode physics, it is convenient to write
\[ x(\tau) = x_0 + y(\tau), \]
where \( y \) corresponds to the sinusoidal modes of Eq. (25) and has the following property:
\[ y(0) = y(\beta) = 0. \]

In terms of \( y \) one can express \( Z \) conveniently as
\[ Z = \int dx_0 \int_{y(0)=y(\beta)=0} [Dy] \exp(-S[x_0+y]), \]
and different strategies can be used to handle \( S[x_0+y] \) in order to obtain an effective theory\(^4\) for \( x_0 \):
\[ Z = \int \frac{dx_0}{\sqrt{2\pi \hbar^2/(m k_B T)}} \exp(-\beta V_{\text{eff}}(x_0)). \]

Notice that the intermediate step, including the paths \( y \), is built using quantities which vanish at the boundary of imaginary time, and the contribution from problematic static quantities is factorized in the final integration over \( x_0 \). Besides, for interacting systems, the interaction potential evaluated at \( x(\tau) = x_0 + y(\tau) \) can produce a \( y \)-dependent quadratic term for the zero mode \( x_0 \), which could prevent possible divergences in the effective theory.

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 test the quality of our alternative approach and compare it to previous descriptions.

### IV. APPLICATIONS AND COMPARISON TO PREVIOUS RESULTS

#### A. The quadratic case revisited

The action is again the one given by Eq. (4). Now, we use the decomposition of \( x \) given by Eq. (34) to obtain
\[ S[x] = \frac{\beta \omega^2}{2} x_0^2 + \frac{1}{2} \int d\tau d\tau' \left\{ y G_y^{-1} y + 2\omega^2 x_0 y \right\} \]
\[ = \frac{\beta \omega^2}{2} x_0^2 + \frac{1}{2} \int d\tau \left\{ (y + \omega^2 x_0 G_y) G_y^{-1} \times \right\} \]
\[ \left\{ y + \omega^2 x_0 G_y \right\} - \frac{\omega^4 x_0^2}{2} \int d\tau d\tau' G_y, \]
where \( G_y \) was defined in (17). A simple calculation gives
\[ \int d\tau d\tau' G_y(\tau, \tau') = \frac{\beta}{\omega^2} \left[ \frac{2}{\omega^4} \right] \frac{\sinh \beta \omega}{\sinh \beta \omega}. \]

Shifting the variable of integration to
\[ \zeta(\tau) = y(\tau) + \omega^2 x_0 \int d\tau' G_y(\tau, \tau'), \]
which obeys \( \zeta(0) = \zeta(\beta) = 0 \), and performing the gaussian integration, we obtain
\[ Z = (\det G_y)^{1/2} \int dx_0 e^{-\omega(\cosh \beta \omega - 1)/\sinh \beta \omega} x_0^2. \]

Integrating over \( x_0 \) and taking the logarithm, one reproduces Eq. (20). Notice that the propagator used in the perturbation expansion of the integral over the path \( y \) is well-behaved in the limit of small \( \omega \):
\[ |G_y(\tau, \tau')| \leq \frac{\tanh \beta \omega/2}{2\omega} \frac{\beta \omega \ll 1}{\beta/4}. \]

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\(^4\) With the normalization factor used in (37), one has the property: \( V_{\text{eff}}(x_0) \rightarrow V(x_0) \) when \( T \rightarrow \infty \), as follows from (33).
B. The anharmonic oscillator

Let us now consider the following action:

\[ S[x] = \int_0^\beta d\tau \left[ \frac{1}{2} m \dot{x}^2(\tau) + \frac{1}{2} m \omega^2 x^2(\tau) + \frac{\lambda}{4} x^4(\tau) \right] . \]  
(43)

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

\[ S[q] = \frac{1}{g} \int_0^{\Theta} d\theta \left( \frac{1}{2} q^2(\theta) + \frac{1}{2} q^2(\theta) + \frac{1}{4} q^4(\theta) \right) . \]  
(44)

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

\[ S[q] = S_2[q_0, \eta] + S_I[q_0, \eta] , \]  
(45)

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

\[ S_2[q_0, \eta] = S[q_0] + \frac{1}{2} \int_0^{\Theta} d\theta \left\{ \eta(\theta) \left[ -\frac{d^2}{d\theta^2} + \overline{\Sigma}^2 \right] \eta(\theta) + 2\alpha \sqrt{g} \eta(\theta) \right\} , \]  
(46)

and

\[ S_I[q_0, \eta] = \int_0^{\Theta} d\theta \left[ \sqrt{\Theta} q_0 \eta^3(\theta) + \frac{g}{4} \eta^4(\theta) \right] , \]  
(47)

where \( \overline{\Sigma}^2 = 3 \eta_0^2 + 1 \) and \( \alpha = \eta_0^2 + q_0 \). One obtains a quadratic approximation for the partition function by considering

\[ Z_2 = \int dq_0 \int_{\eta(0) = \eta(\Theta) = 0} [D\eta] e^{-S_2[q_0, \eta]} . \]  
(48)

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

\[ \zeta(\theta) = \eta(\theta) + \frac{\alpha}{\sqrt{g}} \int_0^{\Theta} d\theta' G_\eta(\theta, \theta') \]  
(49)

where the Green function \( G_\eta \), defined by

\[ \left[ -\frac{d^2}{d\theta^2} + \overline{\Sigma}^2 \right] G_\eta(\theta, \theta') = \delta(\theta - \theta') , \]  
(50a)

\[ G_\eta(0, \theta') = G_\eta(\Theta, \theta') = 0 , \]  
(50b)

is given by

\[ G_\eta(\theta, \theta') = \frac{\sinh[\overline{\Sigma}(\theta - \Theta)] \sinh[\overline{\Sigma}(\Theta - \theta')]}{\overline{\Sigma} \sinh(\overline{\Sigma} \Theta)} . \]  
(51)

The result for \( Z_2 \) is then

\[ Z_2 = \int dq_0 (\det G_\eta)^{1/2} \exp\{-S[q_0] + \Sigma_\eta\} , \]  
(52)

where

\[ \det G_\eta = \frac{\overline{\Sigma}}{2 \pi \sinh(\overline{\Sigma} \Theta)} \]  
(53)

and

\[ \Sigma_\eta = \frac{\alpha}{2g} \int_0^{\Theta} d\theta d\theta' G_\eta(\theta, \theta') . \]  
(54)

To go beyond the quadratic order in \( \eta \), we use the following approximation:

\[ e^{-S_2[q_0, \eta]} \approx 1 - \int_0^{\Theta} d\theta \left[ \sqrt{\Theta} q_0 \eta^3(\theta) + \frac{g}{4} \eta^4(\theta) \right] . \]  
(55)

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

\[ \delta^{(1)} Z = - \int dq_0 \int_0^{\Theta} d\theta \left[ \sqrt{\Theta} q_0 \eta^3(\theta) + \frac{g}{4} \eta^4(\theta) \right] , \]  
(56)

with

\[ \langle \eta(\theta_1) \ldots \eta(\theta_k) \rangle = \int [D\eta] e^{-S_2[q_0, \eta]} \eta(\theta_1) \ldots \eta(\theta_k) . \]  
(57)

As usual, we can introduce a linear coupling of \( \eta \) with an external current \( j \):

\[ Z_2[j] = \int dq_0 \int_{\eta(0) = \eta(\Theta) = 0} [D\eta] \exp\left\{ -S_2[q_0, \eta] + \int d\theta j(\theta) \eta(\theta) \right\} , \]  
(58)

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

\[ Z_2[j] = \int dq_0 (\det G_\eta)^{1/2} \exp\{-S[q_0] + \Sigma_\eta[j]\} , \]  
(59)

where

\[ \Sigma_\eta[j] = \frac{1}{2} \int_0^{\Theta} d\theta d\theta' \sigma(\theta) G_\eta(\theta, \theta') \sigma(\theta') , \]  
(60)

and \( \sigma(\theta) = \alpha/\sqrt{g} - j(\theta) \). Finally, we use

\[ e^{-\Sigma_\eta} \left[ \frac{\delta^3}{\delta j^3(\theta)} \right]_{j=0} e^{\Sigma_\eta[j]} = I_0^3(\theta) + 3 I_0(\theta) G_\eta(\theta, \theta) \]  
(61)

and

\[ e^{-\Sigma_\eta} \left[ \frac{\delta^4}{\delta j^4(\theta)} \right]_{j=0} e^{\Sigma_\eta[j]} = I_0^4(\theta) + 6 I_0^2(\theta) G_\eta(\theta, \theta) \]  

+ 3 G_\eta^2(\theta, \theta) , \]  
(62)
where \( I_0(\theta) \) plays the role of an expectation value of \( \eta(\theta) \):

\[
I_0(\theta) = -\frac{\alpha}{\sqrt{g}} \int_0^\Theta d\theta' G_{\eta}(\theta, \theta') = \frac{\alpha}{\sqrt{g}} \cosh \Theta - \sinh \Theta \tanh \Theta/2 - 1. \tag{63}
\]

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

Notice that the integrand of (52) is dominated by the quadratic approximation near \( T_\text{min} \), for the region where \( q_0 = 0 \), where the quadratic action reaches its minimum value. For small temperatures, that integrand becomes sharply peaked at zero, while for large \( T \) a broad range of \( q_0 \) substantially contributes. Therefore, one can estimate the importance of the correction term (56) using the following quantity:

\[
\langle S_I(0, \eta) \rangle = \frac{3q}{4} \int_0^\Theta d\theta \tilde{G}_\eta^2(\theta, \theta) \approx \frac{3g\Theta}{16}. \tag{64}
\]

The temperature \( T_\text{min} \) where \( \langle S_I(0, \eta) \rangle \) goes to 1 is displayed in Fig. 2 as a function of the coupling constant \( \lambda \). \( T_\text{min} \) provides a rough estimate for the validity of the quadratic approximation. From Fig. 2, we see that \( T_\text{min} \) is of order 1 for \( \lambda \) as large as 50.

The results for the free energy and for the specific heat are displayed in Fig. 3 and Fig. 4, respectively. In the figures, classical corresponds to calculation using Eq. (33), quadratic uses Eq. (52), improved includes the correction corresponding to Eq. (56), semiclassical refers to the semiclassical result obtained in Ref. [4], 1-loop stands for the usual 1-loop perturbative result, and exact corresponds to results from Refs. [12, 13] combined with WKB estimates.

The first remarkable thing in the plots is the failure of the perturbative result in the high-temperature region \( (T \gg m) \). As seen in Ref. [4], that region is well described by the semiclassical curve, and asymptotically, by the classical one. This is evident from both plots. It is interesting that, for \( g = 0.4 \), the agreement extends to temperatures down to \( T \approx m/2 \), a region where the character of the system is far from classical. However, it is surprising that our simple calculation using (52) 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 (31) for the quartic potential. In practice, one has to deal with rather involved Jacobi elliptic functions [4, 14]. In contrast, using the expansion (34) 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. 3) reveals a non-monotonic behavior for low temperatures: the free energy passes by a maximum and decreases towards the free value 0.5. This is a general feature regardless of the value of \( m \) and \( \lambda \), and it is a clear signal of the breakdown of the approximation below \( T_\text{min} \) (see Fig. 2). The improved free energy diverges at \( T_\text{min} \), 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 \( T = 0 \). 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.

Fig. 4 compares different predictions for the specific heat for \( \lambda = 0.4, m = 1 \) and \( \omega = 1 \). Notice that all curves, except for the perturbative one, have the correct high-temperature limit. The anomalous behavior of the quadratic approximation near \( T_\text{min} \) is even more evident in this plot. The improvement obtained in the
FIG. 4: Specific heat of the anharmonic oscillator as a function of the temperature for $\lambda = 0.4$, $m = 1$ and $\omega = 1$ (see text for details).

Finally, Fig. 5 displays the quadratic result for the specific heat when $\lambda = 0.4$ and $m = 1$ in the limit of zero $\omega$. For large temperatures, the curve converges to the classical value 0.75. As discussed in Section II, with the separation of the zero mode, the finiteness of the theory for the $\eta$ variable is not affected in the infrared limit, and we see in this specific case that the interaction makes the effective zero-mode theory well defined.

V. CONCLUSIONS AND OUTLOOK

The theoretical description of the thermodynamics of a given interacting many-body system kept in thermal equilibrium by the contact with a heat bath is an issue of capital importance in most realms of physics, from cosmology to condensed matter settings. 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. Nevertheless, whenever collective (massless) bosonic modes are relevant, as is the case in practically any plasma, infrared divergences are unavoidable in a plain perturbative treatment, forcing a reorganization of the series that grants special attention to the zeroth Matsubara mode. As discussed in this paper, we also need a separate treatment of the static mode already in the context of quantum statistical mechanics in order to improve the convergence of the perturbative expansion in the high-temperature limit.

The choice of the traditional Matsubara mode expansion, combined with the trace requirement that the paths (configurations) coincide at the two boundaries of the compact euclidean time, implies a restriction to periodic paths in the process of functional integration to compute the partition function. However, 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. We have shown that, in order to allow for non-periodicity, one has to define a modified expansion into Matsubara modes.

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 non-periodic trajectories, for which the usual Matsubara expansion leads to an incorrect result for the action of the trajectory. As was shown above, one can properly incorporate the contribution of non-periodic paths by using a modified Matsubara series expansion in which the zero mode is identified with the boundary value of the path. The latter turns out to be the stochastic variable that

| $\lambda$ | $E_0$ (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      |

TABLE I: Ground state energy of the quartic oscillator for different values of the coupling $\lambda$ ($m = \omega = 1$). Exact data were extracted from Ref. [13], whereas $E_0$ (quadratic) was obtained using Eq. (52).
survives in the final effective theory.

The approach proposed in this paper has, thus, the advantage of providing a natural separation of the physics of the zero mode. In fact, we built a very simple effective theory for the zero mode in the nontrivial problem of the anharmonic oscillator, obtaining very precise results for practically the whole range of temperatures, and in a framework that is free of spurious divergences. In particular, we were able to describe the semiclassical (high-temperature) limit of the anharmonic oscillator without any information about the classical solutions. We expect that other potentials can profit from the simplicity of the present method in quantum mechanical systems.

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 onto the problem of infrared divergences. Results in this direction will be presented elsewhere [15]

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[1] M. Le Bellac, Thermal Field Theory (Cambridge University Press, 2000). J. I. Kapusta and C. Gale, Finite-Temperature Field Theory: Principles and Applications (Cambridge University Press, 2006). A. Das, Finite Temperature Field Theory (World Scientific, 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, JHEP 0708, 007 (2007).
[4] C. A. A. de Carvalho, R. M. Cavalcanti, E. S. Fraga and S. E. Jorás, Annals Phys. 273, 146 (1999).
[5] C. A. A. de Carvalho, R. M. Cavalcanti, E. S. Fraga and S. E. Jorás, Phys. Rev. E 61, 6392 (2000).
[6] C. A. A. de Carvalho, R. M. Cavalcanti, E. S. Fraga and S. E. Jorás, Phys. Rev. E 65, 056112 (2002).
[7] U. Kraemmer and A. Rebhan, Rept. Prog. Phys. 67, 351 (2004).
[8] J. O. Andersen and M. Strickland, Annals Phys. 317, 281 (2005).
[9] E. Braaten, Nucl. Phys. A 702, 13 (2002).
[10] V. N. Popov, Functional Integrals and Collective Excitations (Cambridge University Press, 1991).
[11] H. Kleinert, Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets (World Scientific, Singapore, 2004).
[12] S. N. Biswas, K. Datta, R. P. Saxena, P. K. Srivastava, and V. S. Varma, J. Math. Phys. 14, 1190 (1973).
[13] F. T. Hioe and E. W. Montroll, J. Math. Phys. 16, 1945 (1975).
[14] M. Abramowitz and I. A. Stegun (eds.), Handbook of Mathematical Functions (Dover, New York, 1965).
[15] A. Bessa, C. A. A. de Carvalho and E. S. Fraga, work in progress.