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Semiclassical thermodynamics of scalar fields

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Abstract: We present a systematic semiclassical procedure to compute the partition function for scalar field theories at finite temperature. The central objects in our scheme are the solutions of the classical equations of motion in imaginary time, with spatially independent boundary conditions. Field fluctuations — both field deviations around these classical solutions, and fluctuations of the boundary value of the fields — are resummed in a Gaussian approximation. In our final expression for the partition function, this resummation is reduced to solving certain ordinary differential equations. Moreover, we show that it is renormalizable with the usual 1-loop counterterms.

Keywords: Thermal Field Theory, Phenomenological Models.

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1. Introduction

Finite-temperature field theory [1] is the natural framework for the study of phase transitions, and of the thermodynamic properties of equilibrium states. Applications range from the investigation of the phase structure of the strong and electroweak interactions, and the related applications to the early universe, to the low-energy effective field theories in particle physics and condensed matter systems.

However, finite-temperature field theories often face a major difficulty: the plain perturbation expansion [5 – 8] is ill-defined due to the presence of infrared divergences in the bosonic sector, and often gives meaningless results. In the case of hot QCD, for instance, one can say that the domain of validity of the naive weak-coupling expansion is the empty set [2]. This challenge stimulated the development of resummation techniques that reorganize the perturbative series, and resum certain classes of diagrams, thereby improving the perturbative expansion (see [3, 4] for recent reviews). Some of these techniques amount

to using an effective theory in order to separate the scales T, gT, and g^2T [9 – 14]. Others use modified quasi-particles as the starting point of the perturbative expansion [15], leading to a significant improvement of the convergence of the expansion when the mass of these quasi-particles is properly chosen (one can also mention refs. [27, 28], where a simple phenomenological model of massive quasi-particles was successfully used in order to reproduce the pressure of the quark-gluon plasma obtained in lattice simulations). In other approaches that aim at maintaining thermodynamical consistency, one reorganizes the perturbative expansion of the thermodynamical potential around two-particle irreducible skeleton diagrams [16 – 21]. Finally, some of these techniques are based on a systematic use of the Hard Thermal Loop effective action [22 – 26], i.e., on the assumption that the HTLs provide a good description of the quasi-particles in the plasma, and of their interactions.

A somewhat different approach, which can also be interpreted as a resummation of an infinite set of perturbative diagrams, is provided by the semiclassical approximation [29, 30]. Since the partition function of a given system can be cast in the form of a path integral whose weight is the exponential of minus the Euclidean action, an expansion around *Euclidean* classical solutions is quite natural. This program has been carried out in the case of one-dimensional quantum statistical mechanics for particles in a single-well potential in [31], and also for double wells [32]. From the mere knowledge of the classical Euclidean solutions of the equation of motion, the full semiclassical series for the partition function was constructed.[1] Later, these results were generalized to the case of a particle in a central potential in an arbitrary number of dimensions [35]. In both cases, excellent results were obtained, for instance, for the ground state energy and the specific heat, in the case of the quartic potential.

In this paper we develop a similar semiclassical procedure to compute the partition function for thermal scalar field theories with a single-well potential. We expand around Euclidean classical fields, whose value on the boundaries of the time interval are taken to be independent of space. These solutions are assumed to be known to all orders in the interaction potential (either analytically or numerically). Then, we incorporate fluctuations around these classical trajectories, as well as space-dependent fluctuations of the boundary value of the classical fields. All these fluctuations are kept only in a Gaussian approximation, although it is in principle possible to go systematically beyond this approximation. We also provide a diagrammatic interpretation of our results, connecting our formalism to the ordinary perturbative expansion, and identifying the classes of diagrams that are resummed in our approach. The implementation of the renormalization procedure in this semiclassical treatment is discussed in detail at the end.

Since the procedure we propose is infrared finite, we believe it represents an interesting alternative to other rearrangements of perturbation theory at finite temperature. In this paper, we present the general semiclassical framework for an arbitrary potential. We leave the application to the case of a scalar theory with quartic self-interactions, and comparisons

[1] The equivalent problem in quantum mechanics at zero temperature was previously studied by DeWitt-Morette [33] for arbitrary potentials, and by Mizrahi [34] for the single-well quartic anharmonic oscillator, using similar techniques. For a more complete list of references on the semiclassical series in quantum mechanics, see [31]

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with other methods to a following publication [38].

The paper is organized as follows:

In section 2, we discuss the computation of the partition function, starting from its expression in terms of a functional integral, within the semiclassical approximation. Although the main result is, of course, well known, we focus our discussion on the role played by the boundary conditions in Euclidean time at finite temperature. We also recall the diagrammatic interpretation of the integration over quadratic fluctuations around the classical field.

In section 3, we present a systematic procedure to incorporate effects from fluctuations of the boundary value of the field in the computation of the partition function. We explain how one can perform an expansion in those fluctuations in a consistent way, provided that one knows the classical solutions for the problem with constant boundary conditions. We derive formulas that incorporate the effects of these fluctuations up to quadratic order. These formulas depend only on the classical field itself, and on a basis of solutions for the equation of motion for small fluctuations around the classical field.

In section 4, we expand the classical action to second order in the boundary fluctuations, and discuss diagrammatically the meaning of this expansion in terms of the boundary value of the field. This leads to our final expression for the partition function in terms of quantities that can be straightforwardly obtained in explicit form for a given potential once one knows the classical solution mentioned previously (at least numerically). This expression, however, still needs to be renormalized.

The renormalization procedure, which resembles the usual perturbative procedure, is discussed in section 5. There, we show how to obtain a finite expression for the partition function through the introduction of only two counterterms in the action, plus the subtraction of the zero point energy.

We present our conclusions and outlook in section 6. Finally, in appendix A, we illustrate the procedure in the case of the free theory and in appendix B we demonstrate a useful relation. As mentioned above, the non-trivial example of the quartic potential will be addressed in detail in another publication.

2. Small fluctuations around a classical solution

We want to calculate the partition function $Z \equiv \mathrm{Tr} e^{-\beta H}$ for a system of interacting scalar fields, making use of a semiclassical approximation. Our starting point is the expression of Z in terms of path integrals:

$$Z = \int [D\varphi(\boldsymbol{x})] \int\limits_{\phi(-\beta/2,\boldsymbol{x})=\phi(\beta/2,\boldsymbol{x})=\varphi(\boldsymbol{x})} [D\phi(\tau,\boldsymbol{x})] \quad e^{-S_{_E}[\phi]} \,, \tag{2.1}$$

where $S_{_E}[\phi]$ is the Euclidean action of the field:

$$S_{_E}[\phi] = \int\limits_{-\beta/2}^{+\beta/2} d\tau d^3\boldsymbol{x} \left[\frac{1}{2}\partial_\mu\phi\partial^\mu\phi + \frac{1}{2}m^2\phi^2 + U(\phi)\right] \,. \tag{2.2}$$

Assume, for the time being, that we know the solution $\phi_c(\tau, \boldsymbol{x})$ of the classical equation of motion, that takes the value $\varphi(\boldsymbol{x})$ on the boundaries of the time interval:

$$\begin{aligned}(\Box_{_E} + m^2)\phi_c(\tau, \boldsymbol{x}) + U'\left(\phi_c(\tau, \boldsymbol{x})\right) &= 0 \ , \\ \phi_c(-\beta/2, \boldsymbol{x}) = \phi_c(\beta/2, \boldsymbol{x}) &= \varphi(\boldsymbol{x}) \ ,\end{aligned} \tag{2.3}$$

where we denote by $\Box_{_E} \equiv -(\partial_\tau^2 + \boldsymbol{\nabla}^2)$ the Euclidean D'Alembertian operator.

A classical solution is a (local) minimum of S_E. Next, in the functional integration over $\phi(\tau, \boldsymbol{x})$ in eq. (2.1), one assumes that the integral is dominated by field configurations in the vicinity of that classical solution, i.e., by small fluctuations around this classical solution. In order to evaluate the integral in this approximation, one writes:

$$\phi(\tau, \boldsymbol{x}) \equiv \phi_c(\tau, \boldsymbol{x}) + \eta(\tau, \boldsymbol{x}) \ , \tag{2.4}$$

and expands the Euclidean action to second order in the fluctuation $\eta(\tau, \boldsymbol{x})$:

$$S_{_E}[\phi] = S_{_E}[\phi_c] + \frac{1}{2}\int (d^4x_1)_{_E}(d^4x_2)_{_E} \ \left.\frac{\delta^2 S_{_E}[\phi]}{\delta\phi(x_1)\delta\phi(x_2)}\right|_{\phi=\phi_c} \eta(x_1)\eta(x_2) + \mathcal{O}(\eta^4) \ . \tag{2.5}$$

In this equation, we have used the shorthands $x \equiv (\tau, \boldsymbol{x})$ and $\int (d^4x)_{_E} \equiv \int_{-\beta/2}^{\beta/2} d\tau \int d^3\boldsymbol{x}$. For the sake of brevity, let us also introduce the following notation:

$$\eta^T A[\phi_c]\eta \equiv \int (d^4x_1)_{_E}(d^4x_2)_{_E} \ \left.\frac{\delta^2 S_{_E}[\phi]}{\delta\phi(x_1)\delta\phi(x_2)}\right|_{\phi=\phi_c} \eta(x_1)\eta(x_2) \ , \tag{2.6}$$

where $A[\phi_c]$ is a symmetric "matrix" that depends on the classical solution ϕ_c (with continuous indices spanning $[-\beta/2, \beta/2] \times \mathbb{R}^3$).

The Gaussian functional integration over the fluctuation η must be performed with the constraint that the fluctuation $\eta(\tau, \boldsymbol{x})$ vanishes at the time boundaries,

$$\forall \boldsymbol{x} \ , \quad \eta(-\beta/2, \boldsymbol{x}) = \eta(\beta/2, \boldsymbol{x}) = 0 \ , \tag{2.7}$$

because the classical background field already saturates the boundary conditions. Let us therefore call $A^*[\phi_c]$ the restriction of the operator $A[\phi_c]$ to the subspace of fluctuations η that obey these boundary conditions. We can write:

$$Z \approx \int [D\varphi(\boldsymbol{x})] \ e^{-S_{_E}[\phi_c]} \ \left[\det \ (A^*[\phi_c])\right]^{-1/2} \ . \tag{2.8}$$

In order to compute the semiclassical calculation of Z, one must now integrate over the boundary value of the field, $\varphi(x)$. However, before we pursue this calculation, it is useful to recall the nature of the diagrams that are contained in the square root of the functional determinant. It is well known that the Gaussian integration over fluctuations above a given background field amounts to calculating the one-loop correction to the effective action. However, for this correspondence to be valid, one must integrate over *all the periodic fields* $\eta(x)$. In our case, the Gaussian integration involves only fields η that vanish on the time boundaries (see eq. (2.7)), i.e., only a subset of all the periodic fields. Therefore,

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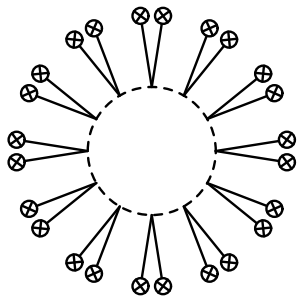

Figure 1: Typical 1-loop diagram included in the integration over fluctuations around the classical solution in the Gaussian approximation. The lines terminated by a cross denote the classical solution with a fixed boundary condition $\varphi(\boldsymbol{x})$. The dashed line can be seen as the propagator around the classical field, for a fluctuation that vanishes at the time boundaries.

the quantity $\left[\det\left(A^*[\phi_c]\right)\right]^{-1/2}$ is a part of the one-loop effective action, but does not contain all the terms that would normally enter in the effective action at this order.[2] With this caveat in mind, a typical diagram included in this quantity is displayed in figure 1, in the case of a field theory with a quartic coupling. It is important to remember that the propagator represented by the dashed line differs from the complete time ordered propagator, because it corresponds to a subset of all the periodic modes.

Both the classical action and the determinant in eq. (2.8) depend on the field $\varphi(\boldsymbol{x})$ on the boundary, through the dependence of the classical solution ϕ_c on the boundary conditions in eq. (2.3). In fact, the classical solution ϕ_c can be represented diagrammatically as the sum of all the tree diagrams terminated by the boundary field $\varphi(\boldsymbol{x})$. The easiest way to see this is to write Green's formula for the solution of eq. (2.3). Let us first introduce a Green's function of the operator $\Box_E + m^2$:

$$\left[\partial_{\tau'}^2 + \boldsymbol{\nabla}_{\boldsymbol{x}'}^2 - m^2\right] G^0(\tau, \boldsymbol{x}; \tau', \boldsymbol{x}') = \delta(\tau - \tau')\delta(\boldsymbol{x} - \boldsymbol{x}') \; . \tag{2.9}$$

This Green's function is not unique, but we can postpone its choice for later. Let us multiply this equation by the classical field $\phi_c(\tau', \boldsymbol{x}')$, and integrate over τ' and $\boldsymbol{x}'$. This gives:

$$\phi_c(\tau, \boldsymbol{x}) = \int_{-\beta/2}^{\beta/2} d\tau' \int d^3\boldsymbol{x}' \; \phi_c(\tau', \boldsymbol{x}') \left[\partial_{\tau'}^2 + \boldsymbol{\nabla}_{\boldsymbol{x}'}^2 - m^2\right] G^0(\tau, \boldsymbol{x}; \tau', \boldsymbol{x}') \; . \tag{2.10}$$

Now, multiply the equation of motion for $\phi_c(\tau', \boldsymbol{x}')$ by the Green's function $G^0(\tau, \boldsymbol{x}; \tau', \boldsymbol{x}')$, integrate over τ', and subtract the resulting equation from the previous one. This leads to:

$$\begin{aligned} \phi_c(\tau, \boldsymbol{x}) = & \int_{-\beta/2}^{\beta/2} d\tau' \int d^3\boldsymbol{x}' \; G^0(\tau, \boldsymbol{x}; \tau', \boldsymbol{x}') \; U'(\phi_c(\tau', \boldsymbol{x}')) \\ & + \int_{-\beta/2}^{\beta/2} d\tau' \int d^3\boldsymbol{x}' \; G^0(\tau, \boldsymbol{x}; \tau', \boldsymbol{x}') \Big[\; \overrightarrow{\partial_{\tau'}^2} + \overrightarrow{\boldsymbol{\nabla}_{\boldsymbol{x}'}^2} - \overleftarrow{\partial_{\tau'}^2} - \overleftarrow{\boldsymbol{\nabla}_{\boldsymbol{x}'}^2} \; \Big] \phi_c(\tau', \boldsymbol{x}') \; , \end{aligned} \tag{2.11}$$

[2] This distinction can also be seen by studying the eigenfunctions of the operator $A[\phi_c]$, on the space of periodic functions and on the space of functions that vanish at $\tau = \pm\beta/2$ respectively.

where the arrows on the differential operators on the second line indicate on which side they act. The second line can be rewritten as a boundary term, by noting that:

$$A\Big[\overrightarrow{\partial_\mu^2} - \overleftarrow{\partial_\mu^2}\Big]B = \partial^\mu \left\{ A\Big[\overrightarrow{\partial_\mu} - \overleftarrow{\partial_\mu}\Big]B \right\} . \tag{2.12}$$

In eq. (2.11), the boundary in the spatial directions does not contribute to the classical field at the point $\boldsymbol{x}$ because the free propagator decreases fast enough when the spatial separation increases. Thus, we are left with only a contribution from the boundaries in time. At this point, since the boundary conditions for ϕ_c consist in specifying the value of the field at $\tau' = \pm\beta/2$, while its first time derivative is not constrained, it is very natural to choose a Green's function G^0 that obeys the following conditions:[3]

$$G^0(\tau, \boldsymbol{x}; -\beta/2, \boldsymbol{x}') = G^0(\tau, \boldsymbol{x}; +\beta/2, \boldsymbol{x}') = 0 . \tag{2.13}$$

With this choice of the propagator, we obtain the following formula for $\phi_c(\tau, \boldsymbol{x})$:

$$\begin{aligned} \phi_c(\tau, \boldsymbol{x}) = &\int_{-\beta/2}^{\beta/2} d\tau' \int d^3\boldsymbol{x}'\; G^0(\tau, \boldsymbol{x}; \tau', \boldsymbol{x}')\; U'(\phi_c(\tau', \boldsymbol{x}')) \\ &- \int d^3\boldsymbol{x}'\; \varphi(\boldsymbol{x}')\; \Big[\partial_{\tau'} G^0(\tau, \boldsymbol{x}; \tau', \boldsymbol{x}')\Big]_{\tau'=-\beta/2}^{\tau'=+\beta/2} , \end{aligned} \tag{2.14}$$

This formula tells us how the classical solution ϕ_c depends on the boundary value $\varphi(\boldsymbol{x})$. If the first term in the right hand side — involving the derivative U' of the potential — were not there, then the relationship between ϕ_c and the boundary value φ would be linear. This only happens in a free theory. When there are interactions, one can solve eq. (2.14) iteratively in powers of U'. This expansion can be represented diagrammatically by the sum of the tree diagrams whose "leaves" are made of the boundary field $\varphi(\boldsymbol{x})$. An example of such a diagram is illustrated in figure 2, in the case of a ϕ^4 interaction of the fields. Notice that, when the boundary field is small,[4] this sum of trees can be approximated by the zeroth order in the expansion in powers of U', which is independent of the interactions. On the other hand, for large values of φ, it is important to keep the full sum of tree diagrams that are summed in ϕ_c, because all the terms in the expansion can be equally important. Therefore, we already see an important feature of our approximation scheme: although the quantum fluctuations are only included at the 1-loop level, it treats the boundary field to all orders, allowing a correct treatment even for non-perturbatively large values of $\varphi(\boldsymbol{x})$.

[3] It is in general always possible to impose two conditions on a Green's function of $\Box_E + m^2$, because the zero modes of this operator form a linear space of dimension 2. The conditions of eq. (2.13) are explicitly realized by:

$$\begin{aligned} G^0(\tau, \boldsymbol{x}; \tau', \boldsymbol{x}') = \int \frac{d^3\boldsymbol{k}}{(2\pi)^2}\, e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')} \Bigg\{ &\theta(\tau-\tau') \frac{\sinh(\omega_{\boldsymbol{k}}(\tau - \frac{\beta}{2}))\sinh(\omega_k(\tau' + \frac{\beta}{2}))}{\omega_{\boldsymbol{k}}\, \sinh(\omega_{\boldsymbol{k}}\beta)} \\ &+ \theta(\tau'-\tau) \frac{\sinh(\omega_{\boldsymbol{k}}(\tau' - \frac{\beta}{2}))\sinh(\omega_k(\tau + \frac{\beta}{2}))}{\omega_{\boldsymbol{k}}\, \sinh(\omega_{\boldsymbol{k}}\beta)} \Bigg\} , \end{aligned}$$

where we denote $\omega_{\boldsymbol{k}} \equiv \sqrt{\boldsymbol{k}^2 + m^2}$.

[4] By this, we mean that the interaction term is smaller than the kinetic term in the action. This condition depends on the particular momentum modes one is interested in.

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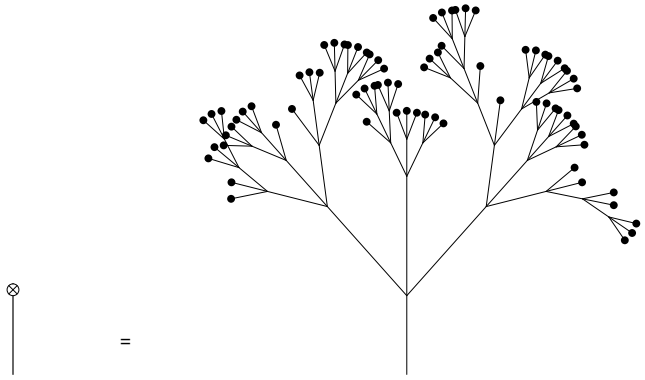

Figure 2: Diagrammatic expansion of the classical field in terms of the boundary value of the field (black dots).

3. Expansion in fluctuations of the boundary

3.1 Preliminary discussion

The integration over boundary configurations that remains to be performed in eq. (2.8) makes the semiclassical approximation for Z rather involved; first, we must solve the partial differential equation (2.3) for an arbitrary $\varphi(\boldsymbol{x})$, and this will not be feasible analytically in general. Even numerically, this is a very complicated task. Besides that, the only functional integral over φ that one is able to perform analytically is a Gaussian integral. In order to circumvent these problems, we are forced to perform some further approximations.

One can see readily in eqs. (2.3) that the classical equation of motion reduces to an ordinary differential equation in the case where the field $\varphi(\boldsymbol{x})$ on the boundary is a constant φ_0. In this case, the classical solution $\phi_c(\tau, \boldsymbol{x})$ becomes a function $\phi_0(\tau)$ of the time only:

$$\begin{aligned} (-\partial_\tau^2 + m^2)\phi_0(\tau) + U'\left(\phi_0(\tau)\right) &= 0 \,, \\ \phi_0(-\beta/2) &= \phi_0(\beta/2) = \varphi_0 \,. \end{aligned} \tag{3.1}$$

Such a simplification of the classical equation of motion would make the problem much more tractable by analytical or numerical methods. This remark suggests that we decompose the boundary field $\varphi(\boldsymbol{x})$ into a constant part φ_0, and a fluctuation $\xi(\boldsymbol{x})$:

$$\varphi(\boldsymbol{x}) = \varphi_0 + \xi(\boldsymbol{x}) \,. \tag{3.2}$$

The solution of the classical equation of motion can therefore be expanded in a similar manner:

$$\phi_c(\tau, \boldsymbol{x}) = \phi_0(\tau) + \phi_1(\tau, \boldsymbol{x}) + \phi_2(\tau, \boldsymbol{x}) + \cdots \,, \tag{3.3}$$

where ϕ_n is of order n in ξ (there are terms of arbitrarily high order in ξ if the equation of motion is non linear). Having done this, we can rewrite the path integral over $\varphi(\boldsymbol{x})$ in

eq. (2.8) as follows:

$$Z \approx \int_{-\infty}^{+\infty} d\varphi_0 \int_{\langle \xi(\boldsymbol{x}) \rangle = 0} [D\xi(\boldsymbol{x})]\, e^{-S_E[\phi_c]}\, [\det\, (A^*[\phi_c])]^{-1/2}\ . \tag{3.4}$$

Notice that the integration over $\xi(\boldsymbol{x})$ must be performed with the constraint that

$$\langle \xi(\boldsymbol{x}) \rangle \equiv \int d^3\boldsymbol{x}\, \xi(\boldsymbol{x}) = 0\ , \tag{3.5}$$

since the "uniform component" (i.e., the zero mode) of the boundary condition is already included in φ_0. An unrestricted integration of $\xi(\boldsymbol{x})$ would therefore overcount the contribution of this zero mode.

In the following, we are going to assume that the first term $\phi_0(\tau)$ can be determined with an arbitrary accuracy — it can be determined analytically in certain cases, while in general it is obtained by solving numerically an ordinary differential equation. Moreover, the dependence on ϕ_0 will always be treated exactly. Only the terms that are of higher order in the fluctuation ξ of the boundary field will be treated in some approximate way. Doing this allows us to preserve the benefits of treating correctly the interaction term when the boundary field is large, since only the fluctuations of the boundary field are assumed to be perturbative.

A natural approximation to obtain the dependence on ξ is to do a Gaussian approximation around $\xi = 0$. As we shall see shortly, in order to find the classical action $S_E[\phi_c]$ at order two in the fluctuation $\xi(\boldsymbol{x})$ of the boundary, it is enough to obtain the classical solution ϕ_c at order one in $\xi(\boldsymbol{x})$.

Moreover, to be consistent with the Gaussian approximation for $S_E[\phi_c]$, we only need to evaluate the determinant at lowest order in $\xi(\boldsymbol{x})$, i.e., at order zero. Indeed, the Gaussian integration over the fluctuations ξ corresponds to a one-loop correction in the background ϕ_0. However, as we have seen in the previous section, the functional determinant in eq. (3.4) is already a one-loop correction. Therefore, keeping the ξ dependence in this determinant would give higher loop corrections when we integrate over ξ, but only a certain subset of all the 2-loop corrections would be included. Doing so is not forbidden by any fundamental principle, but it would arguably make the calculation more complicated; and moreover this would alter the renormalization of the final result. Indeed, as we shall see later, by expanding in ξ the functional determinant in eq. (3.4), we will eventually obtain an expression whose ultraviolet divergences are precisely those of the one-loop effective action. For these reasons, we are going to evaluate

$$Z \approx \int_{-\infty}^{+\infty} d\varphi_0\ [\det\, (A^*[\phi_0])]^{-1/2} \int_{\langle \xi(\boldsymbol{x}) \rangle = 0} [D\xi(\boldsymbol{x})]\, e^{-S_E[\phi_c]}\ . \tag{3.6}$$

3.2 Correction to ϕ_c due to boundary fluctuations

The next step is to find the correction $\phi_1(\tau, \boldsymbol{x})$ to the classical solution ϕ_c. In order to find the equation obeyed by ϕ_1, simply replace ϕ_c by $\phi_0 + \phi_1$ in eq. (2.3). By dropping all the

terms that are of order higher than unity in ϕ_1 (since they are at least of order two in ξ), and using the equation obeyed by ϕ_0, we obtain the following (linearized) equation for ϕ_1:

$$\Big[(\Box_{_E} + m^2) + U''\left(\phi_0(\tau)\right)\Big]\phi_1 = 0\ , \tag{3.7}$$

with the boundary condition:

$$\phi_1(-\beta/2, \boldsymbol{x}) = \phi_1(\beta/2, \boldsymbol{x}) = \xi(\boldsymbol{x})\ . \tag{3.8}$$

In the following, we also need the Green's formula for the variation ϕ_1 of the classical field. The derivation is very similar to the derivation of eq. (2.14), and we shall not reproduce it here. The main difference compared to eq. (2.14) is that we need a Green's function for the operator $\left(\Box_{_E} + m^2 + U''\left(\phi_0(\tau)\right)\right)$,

$$\left[\partial^2_{\tau'} + \boldsymbol{\nabla}^2_{\boldsymbol{x}'} - m^2 - U''\left(\phi_0(\tau')\right)\right] G(\tau, \boldsymbol{x}; \tau', \boldsymbol{x}') = \delta(\tau - \tau')\delta(\boldsymbol{x} - \boldsymbol{x}')\ , \tag{3.9}$$

instead of the free propagator G^0 that we have introduced earlier. Again, this propagator must obey the boundary condition

$$G(\tau, \boldsymbol{x}; -\beta/2, \boldsymbol{x}') = G(\tau, \boldsymbol{x}; \beta/2, \boldsymbol{x}') = 0\ . \tag{3.10}$$

In terms of the fluctuation ξ and of the propagator, the first order correction to the classical solution reads:

$$\phi_1(\tau, \boldsymbol{x}) = \int d^3\boldsymbol{x}'\ \xi(\boldsymbol{x}')\left[\partial_{\tau'} G(\tau, \boldsymbol{x}; \tau', \boldsymbol{x}')\right]^{\tau'=+\beta/2}_{\tau'=-\beta/2}\ . \tag{3.11}$$

Notice that, since the background field ϕ_0 does not depend on space, the propagator G depends only on the difference $\boldsymbol{x} - \boldsymbol{x}'$. Thus, we can get rid of the spatial convolution by going to Fourier space:

$$\phi_1(\tau, \boldsymbol{k}^2) = \xi(\boldsymbol{k})\left[\partial_{\tau'} G(\tau, \tau', \boldsymbol{k}^2)\right]^{\tau'=+\beta/2}_{\tau'=-\beta/2}\ , \tag{3.12}$$

where the propagator in Fourier space is defined by

$$\left[\partial^2_{\tau'} - (\boldsymbol{k}^2 + m^2) - U''\left(\phi_0(\tau')\right)\right] G(\tau, \tau', \boldsymbol{k}^2) = \delta(\tau - \tau')\ , \tag{3.13}$$

and

$$G(\tau, -\beta/2, \boldsymbol{k}^2) = G(\tau, \beta/2, \boldsymbol{k}^2) = 0\ . \tag{3.14}$$

3.3 Propagator in the background ϕ_0

It is fairly easy to determine the propagator G that obeys eqs. (3.13) and (3.14) in terms of two linearly independent solutions of the homogeneous linear differential equation:

$$\left[\partial^2_{\tau} - (m^2 + \boldsymbol{k}^2) - U''\left(\phi_0(\tau)\right)\right] \eta(\tau, \boldsymbol{k}^2) = 0\ . \tag{3.15}$$

Let $\eta_a(\tau, \boldsymbol{k}^2)$ and $\eta_b(\tau, \boldsymbol{k}^2)$ be two such independent solutions[5] of (3.15). In order to construct from $\eta_{a,b}$ a solution of eqs. (3.13) and (3.14), let us first introduce the following object:

$$\Omega(\tau, \tau', \boldsymbol{k}^2) \equiv \eta_a(\tau, \boldsymbol{k}^2)\eta_b(\tau', \boldsymbol{k}^2) - \eta_b(\tau, \boldsymbol{k}^2)\eta_a(\tau', \boldsymbol{k}^2) \; . \tag{3.17}$$

It is trivial to check that $\Omega(\tau, \tau', \boldsymbol{k}^2)$ satisfies eq. (3.15), both with respect to the variable τ and to the variable τ'. Let us then consider the following quantity:

$$\begin{aligned} H(\tau, \tau', \boldsymbol{k}^2) &\equiv \frac{\Omega(\beta/2, \tau, \boldsymbol{k}^2)\Omega(\tau', -\beta/2, \boldsymbol{k}^2)}{\Omega(\beta/2, -\beta/2, \boldsymbol{k}^2)} \qquad \text{if } \tau > \tau' \; , \\ H(\tau, \tau', \boldsymbol{k}^2) &\equiv \frac{\Omega(\beta/2, \tau', \boldsymbol{k}^2)\Omega(\tau, -\beta/2, \boldsymbol{k}^2)}{\Omega(\beta/2, -\beta/2, \boldsymbol{k}^2)} \qquad \text{if } \tau < \tau' \; . \end{aligned} \tag{3.18}$$

This quantity obeys eq. (3.13) if $\tau \neq \tau'$. Moreover, although $H(\tau, \tau', \boldsymbol{k}^2)$ is continuous at $\tau = \tau'$, its first time derivative is not, and one has:

$$\begin{aligned} &\lim_{\epsilon \to 0^+} \left(\partial_{\tau'} H(\tau, \tau', \boldsymbol{k}^2)\big|_{\tau'=\tau+\epsilon} - \partial_{\tau'} H(\tau, \tau', \boldsymbol{k}^2)\big|_{\tau'=\tau-\epsilon} \right) \\ &\qquad = \eta_a(\tau, \boldsymbol{k}^2)\dot{\eta}_b(\tau, \boldsymbol{k}^2) - \dot{\eta}_a(\tau, \boldsymbol{k}^2)\eta_b(\tau, \boldsymbol{k}^2) \equiv -W \; . \end{aligned} \tag{3.19}$$

as can be checked by an explicit calculation. The right hand side of the previous equation is nothing but the Wronskian W of the pair of solutions $\eta_{a,b}$ and is independent of τ in the case of eq. (3.15). Let us denote by W the value of the Wronskian for the pair of solutions $\eta_{a,b}$. The discontinuity of $\partial_{\tau'} H(\tau, \tau', \boldsymbol{k}^2)$ across $\tau' = \tau$ is therefore equal to W, which means that the second time derivative indeed contains a term $W\,\delta(\tau - \tau')$. Finally, from the obvious property

$$\Omega(\tau, \tau, \boldsymbol{k}^2) = 0 \; , \tag{3.20}$$

one easily sees that $H(\tau, \tau', \boldsymbol{k}^2)$ satisfies the boundary condition of eq. (3.14). Therefore, $W^{-1}\, H(\tau, \tau', \boldsymbol{k}^2)$ is the propagator we are looking for:

$$G(\tau, \tau', \boldsymbol{k}) = -\frac{\Omega(\beta/2, \max(\tau, \tau'), \boldsymbol{k}^2)\Omega(\min(\tau, \tau'), -\beta/2, \boldsymbol{k}^2)}{W\; \Omega(\beta/2, -\beta/2, \boldsymbol{k}^2)} \; . \tag{3.21}$$

In general, the solutions $\eta_{a,b}$ will not be found analytically for a non-zero $\boldsymbol{k}$, and will have to be found numerically.

3.4 Calculation of the functional determinant

As we have already explained, we need to calculate the determinant that appears in eq. (3.4), $\det\left(\mathrm{A}^*[\phi_{\mathrm{c}}]\right)$, to order zero in the fluctuation $\xi(\boldsymbol{x})$ of the boundary, i.e.,

[5] When $\boldsymbol{k} = 0$, it is straightforward to verify that:

$$\begin{aligned} \eta_a(\tau; \boldsymbol{0}) &= \dot{\phi}_0(\tau) \; , \\ \eta_b(\tau; \boldsymbol{0}) &= \dot{\phi}_0(\tau) \int_0^\tau \frac{d\tau'}{\dot{\phi}_0^2(\tau')} \; . \end{aligned} \tag{3.16}$$

obey (3.15). However, this construction fails when $\boldsymbol{k} \neq 0$.

$\det\left(\mathrm{A}^*[\phi_0]\right)$. Integrating by parts the kinetic term, the Euclidean action can be rewritten as:

$$S_{_E}[\phi_0+\eta] \approx S_{_E}[\phi_0] + \int (d^4x)_{_E} \left[\frac{1}{2}\eta\Box_{_E}\eta + \frac{1}{2}m^2\eta^2 + U''(\phi_0)\eta^2\right] . \tag{3.22}$$

Notice that the integration by parts does not introduce any boundary term here, thanks to the boundary condition obeyed by η (see eq. (2.7)). Therefore, we have for the operator A^* the following expression:

$$\begin{aligned} A^*[\phi_0]_{\tau,\boldsymbol{x};\tau',\boldsymbol{y}} &\equiv \left.\frac{\delta^2 S_{_E}}{\delta\phi(\tau,\boldsymbol{x})\delta\phi(\tau',\boldsymbol{y})}\right|_{\phi=\phi_0} \\ &= \delta(\tau-\tau')\delta(\boldsymbol{x}-\boldsymbol{y})\left[\Box_{_E} + m^2 + U''\left(\phi_0(\tau)\right)\right] . \end{aligned} \tag{3.23}$$

Notice that here we have already written ϕ_0 explicitly as a field that depends only on time (because we are calculating the determinant only at order zero in the fluctuations of the boundary). Thus, we can perform a Fourier transform with respect to space, and use $\boldsymbol{k}$ instead of $\boldsymbol{x}$. The eigenvalues g_i and eigenfunctions η_i of the operator $A^*[\phi_0]$ are functions $\eta(\tau,\boldsymbol{x})$ that obey the following system of equations:[6]

$$\begin{aligned} \left[\partial_\tau^2 - (m^2+\boldsymbol{k}^2) - U''\left(\phi_0(\tau)\right)\right]\eta_i(\tau,\boldsymbol{k}^2) &= g_i\eta_i(\tau,\boldsymbol{k}^2) , \\ \forall\boldsymbol{x} \ , \quad \eta_i(-\beta/2,\boldsymbol{k}^2) = \eta_i(\beta/2,\boldsymbol{k}^2) &= 0 . \end{aligned} \tag{3.24}$$

This equation is of the same type as eq. (3.15), the only difference being that $\boldsymbol{k}^2$ is now replaced by $\boldsymbol{k}^2+g_i$. Therefore, it has two independent solutions that are given by $\eta_a(\tau,\boldsymbol{k}^2+g_i)$ and $\eta_b(\tau,\boldsymbol{k}^2+g_i)$, and its general solution can be written as:

$$\eta_i(\tau,\boldsymbol{k}^2) = C_a\eta_a(\tau,\boldsymbol{k}^2+g_i) + C_b\eta_b(\tau,\boldsymbol{k}^2+g_i) , \tag{3.25}$$

where $C_{a,b}$ are two integration constants. In order to have a non-zero η_i that obeys the required boundary conditions, we need to have the following property:

$$\eta_a(-\beta/2,\boldsymbol{k}^2+g_i)\eta_b(\beta/2,\boldsymbol{k}^2+g_i) = \eta_a(\beta/2,\boldsymbol{k}^2+g_i)\eta_b(-\beta/2,\boldsymbol{k}^2+g_i) . \tag{3.26}$$

This equation determines the allowed eigenvalues g_i. This equation can also be written as:

$$\Omega(\beta/2,-\beta/2,\boldsymbol{k}^2+g_i) = 0 , \tag{3.27}$$

where Ω has been introduced in eq. (3.17). The determinant of the operator A^* is of course obtained as the product of its eigenvalues:

$$\det A^*[\phi_0,\boldsymbol{k}^2] = \prod_{g|\Omega(\beta/2,-\beta/2,\boldsymbol{k}^2+g)=0} g . \tag{3.28}$$

(We denote by $A^*[\phi_0,\boldsymbol{k}^2]$ the restriction of the operator $A^*[\phi_0]$ to field fluctuations of Fourier mode $\boldsymbol{k}$.) If we denote by z_n the (possibly complex) zeros of the function

[6] For many more informations about properties of Hill's equations and their solutions, the reader may consult [36].

$\Omega(\beta/2, -\beta/2; z)$, then the solutions of $\Omega(\beta/2, -\beta/2, \boldsymbol{k}^2+g) = 0$ are the numbers $g = z_n - \boldsymbol{k}^2$. Therefore, we can write

$$\det A^*[\phi_0, \boldsymbol{k}^2] = \prod_n (z_n - \boldsymbol{k}^2) \,, \tag{3.29}$$

where multiple zeros are repeated as many times as needed in the product. The right hand side of this equation is an entire function of $\boldsymbol{k}^2$, that obviously vanishes at all the z_n's. Since $\Omega(\beta/2, -\beta/2, \boldsymbol{k}^2)$ shares the same property, there exists an entire function $p(\boldsymbol{k}^2)$ such that [37]:

$$\det A^*[\phi_0, \boldsymbol{k}^2] = \Omega(\beta/2, -\beta/2, \boldsymbol{k}^2)\, e^{p(\boldsymbol{k}^2)} \,. \tag{3.30}$$

From eq. (3.17) we see that, if we chose the functions η_a and η_b in such a way that their value at $\tau = -\beta/2$ is independent of $\boldsymbol{k}^2$, then the limit

$$\lim_{\boldsymbol{k}^2 \to \infty} |\Omega(\beta/2, -\beta/2, \boldsymbol{k}^2)|\, e^{-M\sqrt{\boldsymbol{k}^2}} \tag{3.31}$$

is bounded for any $M > \beta$. By Hadamard's theorem [37], we conclude that the function $p(\boldsymbol{k}^2)$ is a constant.[7] The constant factor e^p must in fact be proportional to the inverse of the Wronskian of the pair of solutions η_a and η_b that we are using, $e^p = \text{const}/\beta W$, because the determinant must be independent of this choice (the factor β in the denominator has been included by hand in order to have a dimensionless determinant). The normalization constant can be absorbed as an overall multiplicative constant in Z.

Finally, the determinant of $A^*[\phi_0]$ is obtained by multiplying the previous result for all $\boldsymbol{k}$'s, which gives:

$$\det A^*[\phi_0] = \exp V \int \frac{d^3\boldsymbol{k}}{(2\pi)^3} \ln\left(\frac{\Omega(\beta/2, -\beta/2, \boldsymbol{k}^2)}{\beta W}\right) \,. \tag{3.32}$$

In order to see how the volume V appears in this formula, it is useful to consider first that the system is in a finite box, and to rewrite the sum over the corresponding discrete Fourier modes as an integral.

4. Integration over the boundary fluctuations

4.1 Expansion of the classical action

The final step in the analytic part of this calculation is to calculate the functional integral over the fluctuation $\xi(\boldsymbol{x})$ of the boundary in eq. (3.4). Before doing this integration, we must expand the classical action $S_{_E}[\phi_c]$ to quadratic order in ξ, using the expansion of eq. (3.3) for ϕ_c. We have:

$$S_{_E}[\phi_c] = S_{_E}[\phi_0] + \delta^{(1)} S_{_E} + \delta^{(2)} S_{_E} + \mathcal{O}(\xi^3) \,. \tag{4.1}$$

[7] Strictly speaking, this result only proves the independence of the function p with respect to $\boldsymbol{k}^2$, but it does not exclude a dependence on the other parameters of the problem: the mass m and the coupling constants contained in the potential $U(\phi)$. However, as is clear from the operator whose determinant we are calculating, this dependence only arises from the combination $(m^2 + U''(\phi_0(\tau)))$ which means that it can enter in the final result only via the solutions η_a and η_b, i.e., via the function Ω. Thus, the prefactor $\exp(p(\boldsymbol{k}^2))$ cannot contain any implicit dependence on these parameters.

Notice that we could be in trouble because a priori we must keep ϕ_2 — the term of order ξ^2 in the classical solution ϕ_c — in the second term of the right hand side, which would be much more difficult to obtain. We will not need this term however, because ϕ_0 is an exact solution of the classical equations of motion. Indeed, one can write

$$\delta^{(1)}S_{_E} = \int (d^4x)_{_E}\, \frac{1}{2}\left[-\ddot{\phi}_0(\tau) + m^2\phi_0(\tau) + U'(\phi_0(\tau))\right](\phi_1(x)+\phi_2(x)) + \int d^3\boldsymbol{x}\left[\dot{\phi}_0(\tau)(\phi_1(x)+\phi_2(x))\right]_{\tau=-\beta/2}^{\tau=+\beta/2} . \tag{4.2}$$

The integrand in the first term of the right hand side vanishes identically because $\phi_0(\tau)$ obeys the classical equation of motion associated to the action $S_{_E}$. The second term — a boundary term — can be rewritten as follows:

$$\int d^3\boldsymbol{x}\left[\dot{\phi}_0(\tau)(\phi_1(x)+\phi_2(x))\right]_{\tau=-\beta/2}^{\tau=+\beta/2} = \left[\dot{\phi}_0(+\beta/2) - \dot{\phi}_0(-\beta/2)\right]\int d^3\boldsymbol{x}\xi(\boldsymbol{x}) , \tag{4.3}$$

and it vanishes because the fluctuation $\xi(\boldsymbol{x})$ of the field at the boundary has a vanishing average. The second order variation of the action — the third term in the right hand side of eq. (4.1) — can be written as

$$\begin{aligned}\delta^{(2)}S_{_E} &= \frac{1}{2}\int (d^4x)_{_E}\left[\Big(\partial_\mu\phi_1(x)\Big)\Big(\partial^\mu\phi_1(x)\Big) + m^2\phi_1^2(x) + U''(\phi_0(\tau))\phi_1^2(x)\right] \\ &= \frac{1}{2}\int (d^4x)_{_E}\,\partial_\mu\Big[\phi_1(x)\partial^\mu\phi_1(x)\Big] \\ &\qquad + \frac{1}{2}\int (d^4x)_{_E}\,\phi_1(x)\Big[\Box_{_E} + m^2 + U''(\phi_0(\tau))\Big]\phi_1(x) .\end{aligned} \tag{4.4}$$

The integrand of the second term vanishes because of the equation of motion obeyed by the field $\phi_1(x)$. Therefore, the second order variation of the classical action comes entirely from the boundary term

$$\delta^{(2)}S_{_E} = \frac{1}{2}\int d^3\boldsymbol{x}\,[\phi_1(\tau,\boldsymbol{x})\partial_\tau\phi_1(\tau,\boldsymbol{x})]_{\tau=-\beta/2}^{\tau=+\beta/2} . \tag{4.5}$$

By rewriting this integral in momentum space, and by making use of the boundary condition obeyed by $\phi_1(\tau,\boldsymbol{x})$ and of eq. (3.12), we can rewrite this as follows:[8]

$$\delta^{(2)}S_{_E} = \frac{1}{2}\int \frac{d^3\boldsymbol{k}}{(2\pi)^3}\, C(\boldsymbol{k})\;\xi(\boldsymbol{k})\xi(-\boldsymbol{k}) , \tag{4.6}$$

where we denote

$$C(\boldsymbol{k}) \equiv \Big[\Big[\partial_\tau\partial_{\tau'}G(\tau,\tau',\boldsymbol{k}^2)\Big]_{\tau'=-\beta/2}^{\tau'=+\beta/2}\Big]_{\tau=-\beta/2}^{\tau=+\beta/2} . \tag{4.7}$$

[8] In order to obtain this formula, we use the relation

$$\big[\partial_{\tau'}G(\tau,\tau',\boldsymbol{k}^2)\big]_{\tau'=-\beta/2}^{\tau'=+\beta/2} = \frac{\Omega(\tau,-\frac{\beta}{2},\boldsymbol{k}^2)+\Omega(\frac{\beta}{2},\tau,\boldsymbol{k}^2)}{\Omega(\frac{\beta}{2},-\frac{\beta}{2},\boldsymbol{k}^2)} .$$

Therefore, this quantity is equal to 1 at $\tau = \pm\beta/2$.

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Therefore, the Gaussian functional integral over ξ leads to the following result:

$$\frac{e^{-S_E[\phi_0]}}{\sqrt{\prod_{\boldsymbol{k}\neq 0} \beta C(\boldsymbol{k})}} = e^{-S_E[\phi_0]} \, \exp\left[-\frac{V}{2}\int \frac{d^3\boldsymbol{k}}{(2\pi)^3} \ln\left(\beta C(\boldsymbol{k})\right)\right] \, . \tag{4.8}$$

The constraint $k \neq 0$ serves to remove the contribution of the zero-modes, i.e., the functions $\xi(\boldsymbol{x})$ that are constant, since these are taken into account in the quantity φ_0. Factors of β have been introduced in order to make the arguments of the log and of the square root dimensionless.

4.2 Calculation of $C(k)$

The quantity $C(\boldsymbol{k})$ defined in eq. (4.7) involves the calculation of two derivatives of the Green's function evaluated at the boundaries. This may pose a problem because the derivative of G is not continuous at coincident points. It is crucial to note that eq. (4.7) imposes a very definite order when taking the limits $\tau, \tau' \to \pm\beta/2$. This leads to an unambiguous expression for $C(\boldsymbol{k})$:

$$\begin{aligned} C(\boldsymbol{k}) = & \lim_{\substack{\tau,\tau'\to+\beta/2 \\ \tau<\tau'}} \partial_\tau\partial_{\tau'} G(\tau,\tau',\boldsymbol{k}^2) + \lim_{\substack{\tau,\tau'\to-\beta/2 \\ \tau>\tau'}} \partial_\tau\partial_{\tau'} G(\tau,\tau',\boldsymbol{k}^2) \\ & - \lim_{\substack{\tau'\to+\beta/2 \\ \tau\to-\beta/2}} \partial_\tau\partial_{\tau'} G(\tau,\tau',\boldsymbol{k}^2) - \lim_{\substack{\tau'\to-\beta/2 \\ \tau\to+\beta/2}} \partial_\tau\partial_{\tau'} G(\tau,\tau',\boldsymbol{k}^2) \, . \end{aligned} \tag{4.9}$$

From eq. (3.21), we see that, depending on the order of τ and τ', the double derivative of the propagator reads:

$$\begin{aligned} \partial_\tau\partial_{\tau'} G(\tau,\tau',\boldsymbol{k}) &= -\frac{\partial_\tau\Omega(\beta/2,\tau,\boldsymbol{k}^2)\partial_{\tau'}\Omega(\tau',-\beta/2,\boldsymbol{k}^2)}{W\ \Omega(\beta/2,-\beta/2,\boldsymbol{k}^2)} \qquad \text{if } \tau' < \tau \, , \\ \partial_\tau\partial_{\tau'} G(\tau,\tau',\boldsymbol{k}) &= -\frac{\partial_{\tau'}\Omega(\beta/2,\tau',\boldsymbol{k}^2)\partial_\tau\Omega(\tau,-\beta/2,\boldsymbol{k}^2)}{W\ \Omega(\beta/2,-\beta/2,\boldsymbol{k}^2)} \qquad \text{if } \tau' > \tau \, . \end{aligned} \tag{4.10}$$

Using the explicit form of $\Omega(\tau,\tau',\boldsymbol{k}^2)$ given in eq. (3.17), a straightforward calculation gives:

$$C(\boldsymbol{k}) = \frac{\det\begin{pmatrix} \Delta\eta_a(\boldsymbol{k}^2) & \Delta\dot\eta_a(\boldsymbol{k}^2) \\ \Delta\eta_b(\boldsymbol{k}^2) & \Delta\dot\eta_b(\boldsymbol{k}^2) \end{pmatrix}}{\det\begin{pmatrix} \eta_a(\frac{\beta}{2},\boldsymbol{k}^2) & \eta_a(-\frac{\beta}{2},\boldsymbol{k}^2) \\ \eta_b(\frac{\beta}{2},\boldsymbol{k}^2) & \eta_b(-\frac{\beta}{2},\boldsymbol{k}^2) \end{pmatrix}} \, , \tag{4.11}$$

where we denote

$$\Delta\eta_{a,b}(\boldsymbol{k}^2) \equiv \Big[\eta_{a,b}(\tau,\boldsymbol{k}^2)\Big]_{\tau=-\beta/2}^{\tau=+\beta/2} \quad , \quad \Delta\dot\eta_{a,b}(\boldsymbol{k}^2) \equiv \Big[\dot\eta_{a,b}(\tau,\boldsymbol{k}^2)\Big]_{\tau=-\beta/2}^{\tau=+\beta/2} \, . \tag{4.12}$$

Notice that the form of $C(\boldsymbol{k})$ given in eq. (4.11) makes obvious the fact that $C(\boldsymbol{k})$ does not depend upon the choice of the two solutions η_a and η_b that one takes, as long as they are linearly independent. Indeed, the coefficients $C(\boldsymbol{k})$ are a property of the classical

action itself, and should be independent on the basis chosen for the fluctuations around the classical field.

If we take two solutions $\overline{\eta}_a$ and $\overline{\eta}_b$ such that

$$\begin{aligned} &\overline{\eta}_a(-\beta/2, \boldsymbol{k}^2) = 1 \ , \quad \dot{\overline{\eta}}_a(-\beta/2, \boldsymbol{k}^2) = 0 \ , \\ &\overline{\eta}_b(-\beta/2, \boldsymbol{k}^2) = 0 \ , \quad \dot{\overline{\eta}}_b(-\beta/2, \boldsymbol{k}^2) = 1/\beta \ , \end{aligned} \tag{4.13}$$

then

$$C(\boldsymbol{k}) = \frac{2\left(\overline{\eta}_a(\beta/2, \boldsymbol{k}^2) - 1\right)}{\beta \overline{\eta}_b(\beta/2, \boldsymbol{k}^2)} \, , \tag{4.14}$$

where we use the relation

$$\beta \dot{\overline{\eta}}_b(\beta/2, \boldsymbol{k}^2) = \overline{\eta}_a(\beta/2, \boldsymbol{k}^2) \tag{4.15}$$

which is demonstrated in appendix B. We will suppose that $(m^2 + U'')$ is positive.[9] In this case, one can easily show from (3.15) that $\overline{\eta}_a$ is monotonically increasing in $[-\beta/2, \beta/2]$. This implies that $C(\boldsymbol{k}) > 0$ and $\delta^{(2)} S_{_E} > 0$, which means that the fluctuations of the boundary field always increase the value of the action compared to the configuration with a uniform boundary condition. This can be seen as an a posteriori justification for the choice of expanding around configurations with a uniform boundary condition; indeed, such configurations have a smaller action than those with fluctuations of the boundary condition, and thus are the leading contribution to the partition function.

4.3 Diagrammatic interpretation

The Gaussian integration of $\exp(-S_{_E}[\phi_c])$ over the fluctuations of the field on the time boundary also corresponds to some one loop corrections. To begin with, let us recall the obvious fact that the classical action $S_{_E}[\phi_c]$ only contains terms that are quadratic or quartic in the classical field ϕ_c. Moreover, we have already seen at the end of section 2 that the classical field ϕ_c is the sum of all the tree diagrams with one external leg, terminated on the other side by the boundary field φ (see figure 2). Thus, $S_{_E}[\phi_c]$ is a sum of tree diagrams that have no external legs, with the boundary field φ at the endpoints of the tree. A typical diagram of that sort has been represented in figure 3.

At this point, these diagrams represent the classical action for an arbitrary field φ as the boundary condition. Writing $\varphi(\boldsymbol{x}) = \varphi_0 + \xi(\boldsymbol{x})$ and doing a Gaussian approximation means that, for each diagram like the one displayed in figure 3, all the black dots except two of them are replaced by a uniform boundary field φ_0 and the remaining two are replaced by the fluctuation $\xi(\boldsymbol{x})$ of the boundary. Then, integrating out the field ξ means that the endpoints where the ξ's are attached are linked together, thereby forming a loop. To this loop can be attached an arbitrary number of tree diagrams terminated by φ_0: each of these trees is a contribution to $\phi_0(\tau)$, the classical solution with boundary value φ_0.

Thus, we conclude that the terms resulting from the Gaussian average over the fluctuations of the boundary field are also 1-loop contributions in a background made of the field $\phi_0(\tau)$. These terms are therefore on the same footing as the terms included via the

[9] In other terms, the spectrum of the semiclassical propagator has no bound states [36].

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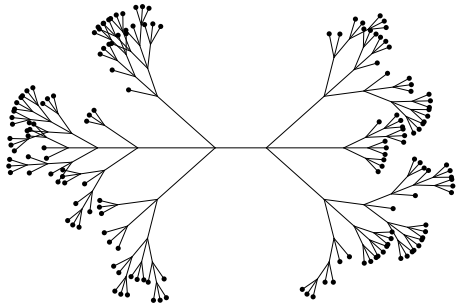

Figure 3: Diagrammatic expansion of the classical action $S_{_E}[\phi_c]$ in terms of the boundary value of the field (black dots).

determinant $\det\left(A^*[\phi_0]\right)$. Moreover, this analysis of the diagrammatic content of our approximate expressions confirms the self-consistency of these approximations: it would have been inconsistent to keep Gaussian fluctuations of the boundary in $\det\left(A^*[\phi_c]\right)$, because by doing this we would include two-loop terms in the background field ϕ_0.

As we shall see in section 5, another consistency check of our final formula can be made based on the structure of its ultraviolet divergences: it contains exactly the divergences one expects of the 1-loop effective action in the background field $\phi_0(\tau)$, and is thus straightforward to renormalize. It is important to realize that we need both the 1-loop corrections coming from $\det\left(A^*[\phi_c]\right)$, and those coming from the Gaussian integration over the fluctuations of the boundary field in order to reproduce the usual pattern of 1-loop ultraviolet divergences. Failing to include one of the types of terms, one would have spurious divergences that could not be removed by the usual renormalization procedure.

4.4 Final formula for the partition function

Collecting everything together, we can write the following formula for the (non-renormalized) partition function:

$$Z \approx \int_{-\infty}^{+\infty} d\varphi_0 \; e^{-S_{_E}[\phi_0]} \; \exp -\frac{V}{2} \int \frac{d^3\boldsymbol{k}}{(2\pi)^3} \ln \left[\frac{1}{W} \begin{vmatrix} \Delta\eta_a(\boldsymbol{k}^2) & \Delta\dot{\eta}_a(\boldsymbol{k}^2) \\ \Delta\eta_b(\boldsymbol{k}^2) & \Delta\dot{\eta}_b(\boldsymbol{k}^2) \end{vmatrix} \right] \;, \tag{4.16}$$

which is valid for arbitrary choices of $\boldsymbol{k}^2$-independent initial conditions. Indeed, the ratio of the determinant and the Wronskian inside the logarithm does not depend on any particular choice for the two solutions η_a and η_b. In practice, one can take advantage of this freedom in order to simplify the numerical calculations. In particular, for the initial conditions defined in (4.13) we have

$$\frac{1}{W} \begin{vmatrix} \Delta\eta_a(\boldsymbol{k}^2) & \Delta\dot{\eta}_a(\boldsymbol{k}^2) \\ \Delta\eta_b(\boldsymbol{k}^2) & \Delta\dot{\eta}_b(\boldsymbol{k}^2) \end{vmatrix} \;=\; 2\left(\overline{\eta}_a(\beta/2, \boldsymbol{k}^2) - 1\right) \;. \tag{4.17}$$

Thus, we have obtained a fairly compact formula that resums (in the Gaussian approximation) the fluctuations around the classical solution and the fluctuations of the boundary

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condition. At this stage, the calculation only involves solutions of some ordinary differential equations, which is in principle straightforward to obtain numerically. For each φ_0, one must determine the following quantities:

1. the classical solution $\phi_0(\tau)$,
2. the classical action $S_{_E}[\phi_0]$,
3. for each $\boldsymbol{k}^2$, two independent solutions $\eta_a(\tau, \boldsymbol{k}^2)$ and $\eta_b(\tau; \boldsymbol{k}^2)$ of the equation of fluctuations around the classical solution $\phi_0(\tau)$.

Notice that all the quantities that depend on $\boldsymbol{k}$ in fact only depend on $|\boldsymbol{k}|$. This means that the integration over $\boldsymbol{k}$ is in fact a one dimensional integral.

5. Renormalization

Our final expression, eq. (4.16), is plagued by ultraviolet divergences if taken at face value. These divergences arise from the integration over the momentum $\boldsymbol{k}$ in the second line. It is in fact easy to convince oneself that these divergences can be dealt with by the usual 1-loop renormalization procedure. In order to see this, one must write the solutions η_a and η_b as series in the interaction term $U''(\phi_0)$ with the background field. Indeed, if we denote by $\eta_{a,b}^{(n)}$ the term in $\eta_{a,b}$ that has n powers of $U''(\phi_0)$, we have the following relations:

$$\begin{aligned}(\partial_\tau^2 - \omega_{\boldsymbol{k}}^2)\eta_{a,b}^{(0)} &= 0\,,\\ (\partial_\tau^2 - \omega_{\boldsymbol{k}}^2)\eta_{a,b}^{(n+1)} &= U''(\phi_0)\eta_{a,b}^{(n)}\,.\end{aligned} \tag{5.1}$$

From these equations, one can see that $\eta_{a,b}^{(n+1)}$ has an extra power of $1/\boldsymbol{k}^2$ at large $\boldsymbol{k}$ compared to $\eta_{a,b}^{(n)}$. Thus, we expect that only a finite number of terms in this expansion will actually contain ultraviolet divergences. To check this, let us calculate explicitly the first three terms in the expansion of the right hand side of eq. (4.17). The solutions $\overline{\eta}_{a,b}^{(0)}$ that obey the boundary conditions of eq. (4.13) are given by:

$$\begin{aligned}\overline{\eta}_a^{(0)}(\tau, \boldsymbol{k}^2) &= \cosh\left(\omega_{\boldsymbol{k}}\left(\tau + \frac{\beta}{2}\right)\right)\,,\\ \overline{\eta}_b^{(0)}(\tau, \boldsymbol{k}^2) &= \frac{\sinh\left(\omega_{\boldsymbol{k}}\left(\tau + \frac{\beta}{2}\right)\right)}{\beta\omega_{\boldsymbol{k}}}\,.\end{aligned} \tag{5.2}$$

Notice that these 0th-order solutions already saturate the boundary conditions at $\tau = -\beta/2$ in eq. (4.13). Thus, the higher order terms in $\overline{\eta}_{a,b}$ should vanish and have a vanishing first time derivative at $\tau = -\beta/2$. In order to find these terms, it is useful to first construct a Green's function $\overline{G^0}(\tau, \tau', \boldsymbol{k}^2)$ of the operator $\partial_\tau^2 - \omega_{\boldsymbol{k}}^2$ that obeys the following conditions:

$$\begin{aligned}(\partial_\tau^2 - \omega_{\boldsymbol{k}}^2)\overline{G^0}(\tau, \tau', \boldsymbol{k}^2) &= \delta(\tau - \tau')\,,\\ \overline{G^0}\left(\tau = -\frac{\beta}{2}, \tau', \boldsymbol{k}^2\right) &= 0\,,\\ \partial_\tau\overline{G^0}\left(\tau = -\frac{\beta}{2}, \tau', \boldsymbol{k}^2\right) &= 0\,.\end{aligned} \tag{5.3}$$

It is straightforward to check that the propagator obeying these conditions is given by

$$\overline{G^0}(\tau,\tau',\boldsymbol{k}^2) = \theta(\tau-\tau')\frac{\sinh(\omega_{\boldsymbol{k}}(\tau-\tau'))}{\omega_{\boldsymbol{k}}}\,, \tag{5.4}$$

which is nothing but the retarded Green's function of $\partial_\tau^2 - \omega_{\boldsymbol{k}}^2$. With this Green's function, one can write

$$\overline{\eta}_{a,b}^{(n+1)}(\tau,\boldsymbol{k}^2) = \int_{-\beta/2}^{+\beta/2} d\tau'\; \overline{G^0}(\tau,\tau',\boldsymbol{k}^2)\; U''(\phi_0(\tau'))\; \overline{\eta}_{a,b}^{(n)}(\tau',\boldsymbol{k}^2)\,. \tag{5.5}$$

Notice that, since the classical solution $\phi_0(\tau)$ does not depend on space, the relationship between $\overline{\eta}_{a,b}^{(n+1)}$ and $\overline{\eta}_{a,b}^{(n)}$ is local in $\boldsymbol{k}$.

At this point, it is a straightforward matter of algebra to obtain $\overline{\eta}_{a,b}$ up to second order in U''. We obtain

$$\begin{aligned} 2\left(\overline{\eta}_a(\beta/2,\boldsymbol{k}^2)-1\right) = e^{\beta\omega_{\boldsymbol{k}}}\Bigg\{ & 1 + \int_{-\beta/2}^{+\beta/2} d\tau'\; \frac{U''(\phi_0(\tau'))}{2\omega_{\boldsymbol{k}}} + \frac{1}{2}\left[\int_{-\beta/2}^{+\beta/2} d\tau'\; \frac{U''(\phi_0(\tau'))}{2\omega_{\boldsymbol{k}}}\right]^2 \\ & -\frac{1}{2}\int_{-\beta/2}^{+\beta/2} d\tau' d\tau''\; \frac{e^{-2\omega_{\boldsymbol{k}}|\tau'-\tau''|}}{(2\omega_{\boldsymbol{k}})^2}\; U''(\phi_0(\tau'))\; U''(\phi_0(\tau'')) \\ & +\mathcal{O}(e^{-\beta\omega_{\boldsymbol{k}}}) + \mathcal{O}((U'')^3)\Bigg\}\,. \end{aligned} \tag{5.6}$$

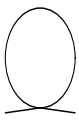
Inside the curly brackets, we have dropped all the terms that would go to zero exponentially when $|\boldsymbol{k}| \to +\infty$. Indeed, these terms do not contribute to the ultraviolet divergences we are studying in this section. In this expression, we recognize the time-ordered propagator, which reads

$$\overline{G_{_F}^0}(\tau,\tau',\boldsymbol{k}^2) = \frac{e^{-\omega_{\boldsymbol{k}}|\tau-\tau'|}}{2\omega_{\boldsymbol{k}}}\,. \tag{5.7}$$

It is a remarkable feature of eq. (4.17) that, while having a fairly natural expression in terms of a retarded propagator, it can be rearranged as an expression involving the time-ordered propagator (at least for the terms that will contribute to the ultraviolet divergences).

The terms that appear in the curly bracket in eq. (5.6) have a fairly simple interpretation in terms of Feynman diagrams. For a scalar theory with a ϕ^4 coupling, the first non-trivial term can be represented as

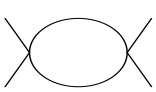
$$\int_{-\beta/2}^{+\beta/2} d\tau'\; \frac{U''(\phi_0(\tau'))}{2\omega_{\boldsymbol{k}}} \quad = \quad$$



. (5.8)

Notice that, in this expression, $1/2\omega_{\boldsymbol{k}}$ is the equal-time value of the time-ordered propagator. Similarly, the term on the third line can be represented as

$$-\frac{1}{2}\int_{-\beta/2}^{+\beta/2} d\tau' d\tau''\; \frac{e^{-2\omega_{\boldsymbol{k}}|\tau'-\tau''|}}{(2\omega_{\boldsymbol{k}})^2}\; U''(\phi_0(\tau'))\; U''(\phi_0(\tau'')) \;=\;$$



. (5.9)

The second term on the second line of eq. (5.6) would be represented by a graph made of two disconnected components, each of which is given in eq. (5.8) (the factor 1/2 is the symmetry

factor that results from the possibility of exchanging the two connected components). In fact, when we take the logarithm (as required by eq. 4.16), these disconnected contributions simply drop out:

$$\frac{1}{2}\ln\left[2\left(\overline{\eta}_a(\beta/2,\boldsymbol{k}^2)-1\right)\right] = \frac{\beta\omega_{\boldsymbol{k}}}{2} + \frac{1}{2}\int_{-\beta/2}^{+\beta/2} d\tau' \, \frac{U''(\phi_0(\tau'))}{2\omega_{\boldsymbol{k}}} \\ -\frac{1}{4}\int_{-\beta/2}^{+\beta/2} d\tau' d\tau'' \, \frac{e^{-2\omega_{\boldsymbol{k}}|\tau'-\tau''|}}{(2\omega_{\boldsymbol{k}})^2} \, U''(\phi_0(\tau'))U''(\phi_0(\tau'')) + \cdots \tag{5.10}$$

One can check that the cancellation of the disconnected terms when one takes the logarithm is in fact quite general, and works to all orders. Finally, when we integrate over $\boldsymbol{k}$, the first term gives the usual zero-point energy, and the next two terms are the first two non-trivial terms of the zero temperature[10] 1-loop effective action (for this, it was important to be able to rewrite the expression in terms of time-ordered propagators). All these terms are ultraviolet divergent. If calculated with a momentum cutoff Λ, they behave respectively as Λ^4, Λ^2, and $\ln(\Lambda)$, if there are 3 spatial dimensions. All the higher order terms in the expansion in powers of U'' are ultraviolet finite, because they have at least one extra power of $1/\boldsymbol{k}^2$ when $|\boldsymbol{k}| \to +\infty$.

This identification tells us that, in order to renormalize our final expression, we must follow the following procedure:

1. subtract the "zero point energy" in $\ln(Z)$, i.e., subtract $\beta\omega_{\boldsymbol{k}}/2$ from the integrand in the integration over $\boldsymbol{k}$,

2. add the one-loop counterterms to the classical action $S_{_E}[\phi_0]$, and simultaneously regularize the integration over $\boldsymbol{k}$.

Notice that the regularization scheme employed for calculating the counterterms must be identical to that used when computing the integral over $\boldsymbol{k}$. Thus, a regularization by an ultraviolet cutoff seems the most convenient method here. Once the above two steps have been carried out, one will have a Λ dependent expression that tends to a finite result when $\Lambda \to +\infty$.

This expression of Z is free of any ultraviolet divergence. But, naturally, it is now expressed in terms of couplings and masses that are scheme dependent (because one must chose a particular renormalization scheme[11] in order to define uniquely the counterterms that are added to the classical action). The standard procedure at this point is to express other physical quantities in terms of the same scheme-dependent parameters, and to eliminate them in order to have relationships that involve only physical quantities.

6. Conclusions

We have derived a semiclassical approximation for the partition function of a system of scalar fields in the presence of an arbitrary single-well interaction potential. In the path-

[10] We recover the well known fact that, if a theory is renormalizable at $T = 0$, it is also renormalizable at finite T, with the counterterms evaluated at $T = 0$.

[11] The renormalization scheme should not be confused with the regularization scheme.

integral formalism, the partition function is an integral over periodic configurations in imaginary time, and is dominated by classical trajectories. The non-perturbative information contained in the classical solutions serves as the starting point for this semiclassical approximation.

Euclidean classical solutions are usually not known for arbitrary (periodic) boundary conditions. However, by first considering classical solutions that correspond to a spatially independent boundary condition (finding these special solutions amounts to solving an ordinary differential equation), one can construct approximate classical solutions obeying arbitrary boundary conditions in a systematic fashion. We have calculated the contribution of quantum fluctuations around those classical solutions in a self-consistent scheme. Our final formula for Z admits a simple expression in terms of two independent solutions of the equation of small fluctuations around the classical solutions, and is thus easily amenable to a numerical evaluation. Despite its simplicity, our expression treats exactly the mean value of the field on the boundary, no matter how large. Moreover, we have shown that this expression is renormalizable by the subtraction of the standard one-loop counterterms, and by the subtraction of the free-field energy.

The formula we have obtained for the partition function is non-perturbative in the sense that it resums the interactions to all orders for the configurations where the mean value of the field on the boundary is large. This can be seen by investigating which classes of diagrams of the usual perturbation theory are taken into account in our approach. We expect that thermodynamical properties derived from this semiclassical expression for Z will be valid in a wider domain in the parameter space $(T, \{\lambda\})$ (where $\{\lambda\}$ represents the coupling constants) as compared to results obtained from the plain perturbative expansion. We are currently investigating in detail the case of a theory with a $\lambda\phi^4$ coupling. Results, including a detailed comparison with those obtained by other resummation schemes, will be presented in a future publication.

Natural candidates for a direct application of the result derived in this paper are condensed matter systems containing scalar order parameters, such as density or magnetization. Extensions to potentials with more that one minimum, and other field theories can also be pursued.

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A. The free case

The action in the free theory is given by

$$S[\phi] = \int_{-\beta/2}^{\beta/2} d^3x d\tau \left[\frac{1}{2} \partial_\mu \phi \partial^\mu \phi + \frac{1}{2} m^2 \phi^2 \right], \tag{A.1}$$

leading to the equation of motion:

$$\left[\partial_\tau^2 - m^2\right]\phi_0 = 0\,. \tag{A.2}$$

The classical solution satisfying $\phi_0(-\beta/2) = \phi_0(\beta/2) = \varphi_0$ is

$$\phi_0 = \varphi_0\left[\cosh(m(\tau+\beta/2)) + \frac{(1-\cosh(\beta m))}{\sinh(\beta m)}\sinh(m(\tau+\beta/2))\right]. \tag{A.3}$$

It is easy to show that $S_E[\phi_0] = \alpha\varphi_0^2$, with $\alpha = mV(\cosh(\beta m)-1)/\sinh(\beta m)$, where V is the volume. Following our main result, we need two solutions of

$$\left[\partial_\tau^2 - (m^2+k^2)\right]\eta = 0\,, \tag{A.4}$$

obeying eq. (4.13). We have already seen these solutions in eq. (5.2). We obtain

$$\begin{aligned} 2\left(\overline{\eta}_a(\beta/2,\boldsymbol{k}^2)-1\right) &= 2(\cosh(\beta\omega_{\boldsymbol{k}})-1) \\ &= (1-\exp(-\beta\omega_{\boldsymbol{k}}))^2\exp(\beta\omega_{\boldsymbol{k}})\,. \end{aligned} \tag{A.5}$$

Finally, we have

$$Z \approx \int_{-\infty}^{+\infty} d\varphi_0\; e^{-\alpha\varphi_0^2}\,\exp\left[-V\int\frac{d^3\boldsymbol{k}}{(2\pi)^3}\left(\ln(1-e^{-\beta\omega_{\boldsymbol{k}}})+\frac{\beta\omega_{\boldsymbol{k}}}{2}\right)\right] \tag{A.6}$$

$$= \sqrt{\frac{\pi}{\alpha}}\exp\left[-V\int\frac{d^3\boldsymbol{k}}{(2\pi)^3}\left(\ln(1-e^{-\beta\omega_{\boldsymbol{k}}})+\frac{\beta\omega_{\boldsymbol{k}}}{2}\right)\right] \tag{A.7}$$

that is (up to an overall factor, irrelevant after taking the thermodynamic limit) the known result for the harmonic oscillator (not yet renormalized). We see that our approximation scheme leads to the exact result in the case of the free theory. Naturally, this is due to the fact that, in the absence of any interactions, the Gaussian approximation represents exactly the fluctuations in the system.

B. Proof of relation (4.15)

From eq. (3.1), it follows that $\phi_0(-\tau) = \phi_0(\tau)$. As a consequence, the equation for the fluctuations is invariant under parity. That invariance implies that the following solution (ignoring the trivial dependency on $\boldsymbol{k}^2$):

$$\eta_e(\tau) = \overline{\eta}_a(\tau) + \frac{1-\overline{\eta}_a(\beta/2)}{\overline{\eta}_b(\beta/2)}\overline{\eta}_b(\tau)\,,$$

which obeys $\eta_e(-\beta/2) = \eta_e(\beta/2) = 1$, is even. Therefore, $\dot{\eta}_e$ is odd. In particular, $\dot{\eta}_e(\beta/2) = -\dot{\eta}_e(-\beta/2)$, and we obtain

$$\begin{aligned} \dot{\overline{\eta}}_a(\beta/2) + \frac{1-\overline{\eta}_a(\beta/2)}{\overline{\eta}_b(\beta/2)}\dot{\overline{\eta}}_b(\beta/2) &= -\dot{\overline{\eta}}_a(-\beta/2) - \frac{1-\overline{\eta}_a(\beta/2)}{\overline{\eta}_b(\beta/2)}\dot{\overline{\eta}}_b(-\beta/2) \\ &= \frac{\overline{\eta}_a(\beta/2)-1}{\beta\,\overline{\eta}_b(\beta/2)}\,. \end{aligned}$$

Multiplying by $\beta\,\overline{\eta}_b(\beta/2)$, we have

$$\beta\,\overline{\eta}_b(\beta/2)\dot{\overline{\eta}}_a(\beta/2) - \beta\,\overline{\eta}_a(\beta/2)\dot{\overline{\eta}}_b(\beta/2) + \beta\,\dot{\overline{\eta}}_b(\beta/2) = \overline{\eta}_a(\beta/2) - 1\,.$$

Using that the wronskian is equal to $1/\beta$, the identity follows.

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