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The Partition Function for Anharmonic Oscilator in the Strong-Coupling Regime

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Abstract

We consider a single anharmonic oscillator with frequency ω and coupling constant λ respectively, in the strong-coupling regime. We are assuming that the system is in thermal equilibrium with a reservoir at temperature β^{-1}. Using the strong-coupling perturbative expansion, we obtain the partition function for the oscillator in the regime $\lambda >> \omega$, up to the order $\frac{1}{\sqrt{\lambda}}$. To obtain this result, we follow two steps. First, we must give meaning to the first term of the strong-coupling perturbative expansion, i.e., the static ultra-local generating functional $Q_\beta(h)$. Second, we have to regularize and renormalize the kernel $K(\omega, \sigma, \tau - \tau')$ integrated over Euclidean time. In order to solve both problems, we make use of a combination of Klauder representation for the static ultra-local generating functional (Acta Phys. Austr. **41**, 237 (1975), Ann. Phys. **117**, 19 (1979)), and the generalized zeta-function method. The free energy and the mean energy, up to the order $\frac{1}{\sqrt{\lambda}}$, are also presented. We are showing that the thermodynamics quantities are nonanalytic in the coupling constant.

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1 Introduction

The strong-coupling regime in quantum field theory is one of the unsolved problems of theoretical physics of the last century. There are many situations where one has to account for non-perturbative coupling regions, and to discuss the physics of the strongly coupled systems. Let us quickly mention a few examples.

The standard case is QCD, where we believe there exists a deconfinement phase transition. It is expected that at sufficiently high temperatures, quarks and gluons become no longer bounded inside hadrons. There is also another phase transition which depends on the number of quark flavour: the chiral symmetry phase transition. The chiral symmetry is spontaneoulsly broken at zero temperature and it is restored at some finite temperature. Although QCD is asymptotically free in the ultraviolet limit, it has a coupling $g(\beta^{-1}) \approx 1$ near the phase transition, where β^{-1} is the temperature. Consequently a non-perturative approach must be used to deal with this situation. Lattice QCD is a means to study the phase transition from first principles.

In condensed matter physics we also have different situations in which the strong-coupling regime may occur. For example, in the theory of superconductors there is the strong-coupling regime in the electron-phonon interaction. In particular, the strong-coupling limit for the polaron problem has been investigated by many authors. A detailed exposition can be found in Ref. [1]. Also in models with a disordered ground state one can use the strong-coupling approach. A standard case is the $O(N)$ non-linear sigma model, describing lattice magnets, where there is a regime in which one can treat the coupling between different sites as a perturbation. Until now we pointed out that there are many situations in quantum field theory that cannot be described using the weak-coupling perturbation theory. Nevertheless, the use of the perturbative expansion outside the weak-coupling regime is also fundamental for our understanding of the whole perturbative renormalization program in quantum field theory.

Various types of harmonic oscillator have served for long as simple analogue systems for more general and complex situations in quantum field theory. Actually, the anharmonic oscillator, with a $\frac{\lambda}{4!}\,x^4(\tau)$ term is formally very similar to the field theory describing a scalar field with a quartic self-interaction. Therefore, in this paper we present a method for calculating the partition function and the Helmholtz free energy for a single oscillator with the anharmonic $\frac{\lambda}{4!}\,x^4(\tau)$ contribution in the strong-coupling regime up to the order $\frac{1}{\sqrt{\lambda}}$. In other words, our model belongs to the regime in which the coupling constant is much larger than the frequency, i.e., $\lambda >> \omega$. In fact, the oscillator with any anharmonic term of the kind $\frac{\lambda}{(2p)!}\,x^{2p}(\tau)$, $p > 3$ in the strong-coupling regime can be analysed by our method and also the generalization for N non-interacting anharmonic oscillators is straightforward. The anharmonic oscillator is described by the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2} m\,\omega^2\,x^2 + \frac{\lambda}{4!}\,x^4. \tag{1}$$

For simplicity we are assuming that our system is one-dimensional and is in thermal equilibrium with a reservoir at temperature β^{-1}. We are working in the imaginary time formalism and making use of the Kubo-Martin-Schwinger (KMS) condition [2] [3] [4].

To find the partition function and the Helmholtz free energy, our approach consists in the combination of two techniques used currently in the literature: the strong-coupling expansion [5] [6] [7] [8] [9] [10] and the zeta-function method [11] [12], which is a classical case of a general formalism concerning regularized products and determinants. For a review of the strong-coupling expansion in field theory, see for example Ref. [13] and also Ref. [14], and for a recent treatment of the strong-coupling expansion in quantum mechanics, see Ref. [15].

Let us briefly discuss the strong-coupling expansion in Euclidean field theory at zero temperature. The basic idea of the approach is the following: in a formal representation for the generating functional of complete Schwinger functions of the theory $Z(h)$, we treat the Gaussian part of the action as a perturbation with respect to the remaining terms of the functional integral, i.e., in the case for the $(\lambda\varphi^4)_d$ theory, the local self-interacting part, in the functional integral. In the literature this approach it has been called the strong-coupling expansion. A stimulating reading can be found in Ref. [16] and Ref. [17]. The main difference from the the standard perturbative expansion is that we have an expansion of the generating functional of complete Schwinger functions in inverse powers of the coupling constant. We are developing our perturbative expansion around the static ultra-local model $Q_0(h)$ [18] [19] [20] [21]. In the ultra-local approximation, different points of the Euclidean space are decoupled since the gradient terms are dropped. This representation of the Schwinger functional $Z(h)$ is defined by an unrenormalized perturbative series, which can be truncated in the order of the approximation. For example, if $Z(h) \equiv Q_0(h)$, we call it the ultra-local approximation or the zeroth-order approximation. It should be noted that although the static ultra-local functional $Q_0(h)$ is not a product of Gaussian integrals, it can be viewed formally as an infinite product of ordinary integrals, one for each point of the d-dimensional Euclidean space. The fundamental problem of the strong-coupling expansion is how to give meaning to the static ultra-local generating functional and to the unorthodox representation for the Schwinger functional. One attempt is to replace the Euclidean space by a hypercubic lattice. Actually, it may be quite subtle to disentangle lattice artifacts from continuous physics. A partial solution to this problem, was presented by Klauder and colaborators a long time ago [19] [22] [23]. They obtained a quite interesting representation for the ultra-local generating functional describing Euclidean free and also self-interacting scalar fields.

In this paper we show how it is possible to compute the partition function and the Helmholtz free energy of the anharmonic oscillator in the strong-coupling regime, up to the order $\frac{1}{\sqrt{\lambda}}$. Our results are showing that the thermodynamics quantities are nonanalytic in the coupling constant. This paper is organized as follows: In section II, the strong-coupling expansion for a single anharmonic oscillator is presented. In section III, we study the analytic structure of the static ultra-local generating-functional $Q_\beta(\sigma;h)$ in the complex plane of the coupling constant λ. In section IV we calculate the partition function and other thermodynamics quantities that are derived from it, as the Helmholtz free energy and the mean energy of the system. Finally, section V contains our conclusions. We assume that the physical quantities are dimensionless. Consequently, it is convenient to introduce an arbitrary parameter μ with mass dimension to define all dimensionless physical quantities. For simplicity, we assume that $\mu = 1$ since we are not interested in the scaling behavior of the model. As usual β^{-1} is the temperature of the thermal bath.

2 The partition function of a one-dimensional quantum mechanical system

Let us consider a one-dimensional quantum mechanical system. The partition function for the system assuming that it is in thermal equilibrium with a reservoir at temperature β^{-1} is given by

$$Z_\beta = \int_{x(0)=x(\tau)} [dx(\tau)]\;\exp\left[-\int_0^\beta d\tau\left(\frac{1}{2}m(\frac{dx}{d\tau})^2 + V(x(\tau))\right)\right], \tag{2}$$

where in the functional integral we require that $x(\tau)$ is periodic with period β, i.e., $x(\tau) = x(\tau+\beta)$. There are many different physical situations that can be analysed starting from the partition function. We would like to discuss the case of a single anharmonic oscillator, where the contribution of $V(x(\tau))$ is given by

$$V_1(x) = \frac{1}{2}\,\omega^2\,x^2 + \frac{\lambda}{4!}\,x^4. \tag{3}$$

For simplicity, we are choosing $m^2 = 1$. As we will see, it is not difficult to apply our method in non-polynomials theories. The second situation that can also be analysed is the non-polynomial model, i.e., the sinh-Gordon potential defined by the following expression

$$V_2(x) = \frac{\omega^4}{\lambda}\left[\cosh\left(\frac{\sqrt{\lambda}}{\omega}\,x(\tau)\right) - 1\right]. \tag{4}$$

In order to study the anharmonic oscillator, let us sketch the solution for the single harmonic oscillator. In the potential $V_1(x)$, choosing $\lambda = 0$ we obtain the harmonic oscillator, where the partition function can be found in texbooks and is given by

$$Z_\beta = \int_{x(0)=x(\tau)} [dx(\tau)]\ \exp\Bigg[-\int_0^\beta d\tau\,\left(\frac{1}{2}(\frac{dx}{d\tau})^2 + \frac{1}{2}\omega^2\,x^2(\tau)\right)\Bigg]. \tag{5}$$

To write the partition function in a more tractable way, let us perform an integration by parts, to obtain

$$Z_\beta = \int_{x(0)=x(\tau)} [dx(\tau)]\ \exp\Bigg[-\int_0^\beta d\tau\,\frac{1}{2}x(\tau)\left(-\frac{d^2}{d\tau^2} + \omega^2\right)x(\tau)\Bigg]. \tag{6}$$

It is a standard procedure to define the following kernel $K(\omega;\tau-\tau')$ by the equation

$$K(\omega;\tau-\tau') = \left(-\frac{d^2}{d\tau^2} + \omega^2\right)\delta(\tau-\tau'), \tag{7}$$

and substituting Eq.(7) in Eq.(6) the partition function Z_β becomes

$$Z_\beta = \int_{x(0)=x(\tau)} [dx(\tau)]\ \exp\Bigg[-\int_0^\beta d\tau\int_0^\beta d\tau'\,\frac{1}{2}x(\tau)K(\omega;\tau-\tau')x(\tau')\Bigg]. \tag{8}$$

As usual, we define the generating functional $Z_\beta(h)$ introducing an external source $h(\tau)$. At this point it is convenient to consider $h(\tau)$ to be complex. Consequently $h(\tau) = \mathrm{Re}(h) + i\,\mathrm{Im}(h)$. In the paper we are concerned with the case $\mathrm{Re}(h) = 0$. Therefore the generating functional $Z_\beta(h)$ is defined by

$$Z_\beta(h) = \int_{x(0)=x(\tau)} [dx(\tau)]\exp\Bigg[-\int_0^\beta d\tau\int_0^\beta d\tau'\frac{1}{2}x(\tau)K(\omega;\,\tau-\tau')x(\tau') + \int_0^\beta d\tau\,h(\tau)x(\tau)\Bigg]. \tag{9}$$

Note that we are using the same notation for functionals and functions, for example $Z_\beta(h)$ instead of the usual notation $Z_\beta[h]$. Since the integrations that appear in Eq.(9) are Gaussian it is straightforward to write

$$Z_\beta(h) = Z_\beta\,\exp\Bigg[-\int_0^\beta d\tau\int_0^\beta d\tau'\,\frac{1}{2}h(\tau)G(\omega;\,\tau-\tau')h(\tau')\Bigg], \tag{10}$$

where the partition function is defined by $Z_\beta = Z_\beta(h)|_{h=0}$, and the Green function $G(\omega;\,\tau-\tau')$ is the inverse kernel, defined by

$$\int_0^\beta d\tau'\,K(\omega,\tau-\tau')G(\omega,\tau'-\tau'') = \delta(\tau-\tau''). \tag{11}$$

Since we are assuming that $\tau\ \epsilon\ [0,\beta]$, the inverse kernel can be written as

$$G(\omega,\tau) = \frac{1}{2\omega}\Bigg[(1+n(\omega))\,e^{-\tau\omega} + n(\omega)\,e^{\omega\tau}\Bigg], \tag{12}$$

where $n(\omega) = \frac{1}{e^{\beta|\omega|}-1}$. At this point it is important to define the modified kernel $K(\omega,\sigma;\tau-\tau')$ by the equation

$$K(\omega,\sigma;\tau-\tau') = \left(-\frac{d^2}{d\tau^2} + (1-\sigma)\,\omega^2\right)\delta(\tau-\tau'), \tag{13}$$

where σ is a complex parameter defined in the region $0 \leq$ Re $(\sigma) < 1$. Note that in general, Re $(\sigma) \neq 1$, because Re $(\sigma) = 1$ introduce infrared divergences in the calculations. The zero frequency case ($\sigma = 1$) in the modified kernel can be assumed in some very special situations only, as for example to calculate the renormalized vacuum energy of a scalar field in the presence of boundaries, where Dirichlet boundary conditions are assumed. See for example Ref. [14]. To summarize, the choice of a suitable σ will simplify our calculations in some situations. This modification will be clarified in the next section.

Let us now suppose an anharmonic oscillator in the strong-coupling regime. We would like to stress that the semiclassical approximation (the WKB approximation) can also be used in the strong-coupling regime. The difficulty is to find the classical orbits which are stationary-phase points in the functional integral [24]. First, as we made in the non-interacting case, it is convenient to couple linearly the oscillator to a τ-dependent external source. Therefore the generating functional at finite temperature is given by

$$Z_\beta(h) = \int_{x(0)=x(\tau)} [dx(\tau)]$$
$$\exp\left[-\int_0^\beta d\tau \int_0^\beta d\tau'\,\frac{1}{2}x(\tau)\,K\,x(\tau') + \int_0^\beta d\tau\left(-\frac{1}{2}\sigma\omega^2 x^2(\tau) - \frac{\lambda}{4!}x^4(\tau) + h(\tau)x(\tau)\right)\right], \tag{14}$$

where we have also integrated over all periodic paths and $K \equiv K(\omega,\sigma;\tau-\tau')$. Functional differentiation gives the thermal average of a time-ordered of position operators i.e., the correlation functions for a stochastic process. For sake of completeness, we would like to present the simple result for the partition function of the anharmonic oscillator in the regime $\lambda << \omega$, in first order in λ. One finds [25]

$$Z_\beta = \left(2\sinh(\frac{\beta\omega}{2})\right)^{-1}\left(1 - \frac{3\lambda}{4!}\int_0^\beta d\tau \frac{1}{4}(\coth^2(\frac{\beta\omega}{2})) + O(\lambda^2)\right). \tag{15}$$

To find the partition function for the anharmonic oscillator in the strong-coupling regime it is natural to use an unorthodox perturbative theory, i.e., the strong-coupling perturbative expansion. The idea is to treat the Gaussian part of the action as a perturbation with respect to the non-Gaussian terms in the functional integral. We get the following formal representation for the generating functional at finite temperature $Z_\beta(h)$:

$$Z_\beta(h) = \exp\left(-\frac{1}{2}\int_0^\beta d\tau \int_0^\beta d\tau' \frac{\delta}{\delta h(\tau)}K(\omega,\sigma;\tau-\tau')\frac{\delta}{\delta h(\tau')}\right)\,Q_\beta(\sigma;\,h), \tag{16}$$

where $Q_\beta(\sigma;h)$, the new static ultra-local functional integral, is given by

$$Q_\beta(\sigma;h) = \mathcal{N}\int_{x(0)=x(\tau)} [dx(\tau)]\, \exp\left[\int_0^\beta d\tau\, \left(-\frac{1}{2}\sigma\,\omega^2\, x^2(\tau) - \frac{\lambda}{4!}x^4(\tau) + h(\tau)x(\tau)\right)\right], \quad (17)$$

and the modified kernel $K(\omega,\sigma;\tau-\tau')$ was defined by Eq.(13). The factor $\mathcal{N}$ is a normalization that can be found using that $Q_\beta(\sigma;h)|_{h=0} = 1$.

The main difference from the standard representation for the generating functional is that we have an expansion of the generating functional in inverse powers of the coupling constant. We are developing our perturbative expansion around the static ultra-local generating functional $Q_\beta(\sigma;h)$. We would like to stress that we are considering a modification of the strong-coupling expansion. We split the quadratic part in the functional integral, which is proportional to the frequency squared, into two parts; one contributes together with the derivative term in the action as the perturbation, and the other appears in the static ultra-local generating functional.

Since we are mainly interested in presenting the partition function, we can assume that the external source is constant. As we will see, this assumption will lead us to redefine Klauder's representation for the ultra-local generating functional. Assuming that the external source is constant, i.e. $h(\tau) = h$, one way to proceed is to neglect high-orders terms in the perturbative expansion. Therefore in the leading order, we have that $\ln Z_\beta(h)$ can be written as

$$\ln Z_\beta(h) = -\frac{1}{2Q_\beta(\sigma;h)}\frac{\partial^2 Q_\beta(\sigma;h)}{\partial h^2}\int_0^\beta d\tau \int_0^\beta d\tau'\, K(\omega,\sigma;\,\tau-\tau'). \quad (18)$$

Of course, the above assumption considerably simplifies our problem, but we still have some work to do. To evaluate $\ln Z_\beta(h)$, note that we have two steps to follow. The first one is to give meaning to the static ultra-local generating-functional, and the second one is to regularize and renormalize the kernel $K(\omega,\sigma;\,\tau-\tau')$ integrated over the volume $[0,\beta]$. Note that the parameter σ was introduced only to simplify our calculations in some situations. Therefore σ can be complex if we are able to work in all order of perturbation theory. The generating functional does not depends on the value for σ. Since we concentrate in the leading order, some care has to be taken to prevent a complex generating functional. A simple way to avoid the problem is assume that the parameter σ is real. Therefore we will impose that Im $(\sigma) = 0$. In this situation the static ultra-local functional $Q_\beta(\sigma;h)$ should be a normalized, positive definite functional. We will discuss this point latter.

Before using the Klauder's result and the generalized zeta-function method, we would like to discuss briefly one method to obtain some information about the static ultra-local generating functional (actually, the static ultra-local generating function) $Q_\beta(\sigma;h)$. In the next section we will study the analytic structure of the static ultra-local generating-functional $Q_\beta(\sigma;h)$ in the complex plane of the coupling constant λ.

3 The analytic structure of the ultra-local generating functional

In this section we would like to study the analytic structure of the static ultra-local generating-functional $Q_\beta(\sigma; h)$ in the complex plane of the coupling constant λ. Since we can interpret the static ultra-local model as an infinite product of ordinary integrals, let us discretize the space, i.e., introducing a lattice. In this way it is possible to analyse the generating function defined in each point of the lattice given by

$$z(\omega, \lambda; h) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, \exp\left(-\frac{1}{2}\omega^2 x^2 - \frac{\lambda}{4!} x^4 + h\, x\right), \tag{19}$$

where we are assuming, for the sake of convenience, that $\sigma = 1$. The zero-dimensional generating function in the absence of external source is defined as the zero-dimensional partition function, i.e., $z(\omega, \lambda;\, h)|_{h=0} \equiv z_0(\omega, \lambda)$. Our aim is first to analyse the zero-dimensional partition function $z_0(\omega, \lambda)$, given by

$$z_0(\omega, \lambda) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, \exp\left(-\frac{1}{2}\, \omega^2 x^2 - \frac{\lambda}{4!} x^4\right). \tag{20}$$

The integral given by Eq.(18) can be solved exactly for Re $\lambda \geq 0$ [26] [27], yielding

$$z_0(\omega, \lambda) = (\frac{3}{2\lambda})^{\frac{3}{4}} (\omega^2)\, \Psi\left(\frac{3}{4}, \frac{3}{2}; \frac{3\omega^4}{2\lambda}\right), \tag{21}$$

where $\Psi(a, c\,; z)$ is the confluent hypergeometric function of second kind [28], and we are using the principal branch of this function. The confluent hypergeometric function of second kind $\Psi(a, c\,; z)$ is a many valued analytic function of z, with a usual branch cut for $|\arg z| = \pi$, and a singularity at $z = 0$. Therefore $z_0(\omega, \lambda)$ can be defined as a multivalued analytic function on the complex plane λ, with a branch cut for $|\arg \lambda| = \pi$ and a singularity at $\lambda = 0$. So we have to consider its principal branch in the plane cut along the negative real axis. If someone is interested in define the zero-dimensional partition function $z_0(\omega, \lambda)$ in the whole complex plane of the coupling constant λ, it has to use only the principle of analytic continuation. The analytic continuation corresponds to the definition for $z_0(\omega, \lambda)$ in the whole coupling constant complex plane except for a branch cut for $|\arg z| = \pi$.

Now, we are able to introduce the sources to analyse the zero-dimensional generating function $z(\omega, \lambda;\, h)$. We have that the zero-dimensional generating function $z(\omega, \lambda;\, h)$ is given by

$$z(\omega, \lambda; h) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, \cosh(h\, x)\, \exp\left(-\frac{1}{2}\, \omega^2 x^2 - \frac{\lambda}{4!} x^4\right). \tag{22}$$

It is possible to find $z_0(\omega,\lambda)$ in a closed form. Nevertheless it is not possible to express $z(\omega,\lambda;h)$ in terms of known functions. If we try to expand $\exp(h\,x)$ in power series and, in order to solve the resulting integrals, we interchange the summation and the integration, we have problems because the power series is uniformly convergent only if $|h\,x|<1$. The result of this operation is $z^{(1)}(\omega,\lambda;h)$ which is the asymptotic expansion of $z(\omega,\lambda;h)$. We may write $z^{(1)}(\omega,\lambda;h)\sim z(\omega,\lambda;h)$. Thus we have

$$z^{(1)}(\omega,\lambda;h)=\sum_{k=0}^{\infty}h^{2k}f_k(\omega,\lambda) \tag{23}$$

where the coefficients f_k are given by

$$f_k(\omega,\lambda)=\frac{(-1)^k}{\sqrt{2\pi}}\frac{2^{k+1}}{2k!}\left(\frac{\partial}{\partial\omega^2}\right)^k z_0(\omega,\lambda). \tag{24}$$

Recall that $z_0(\omega,\lambda)$ is the generating function in the absence of sources. Using Eq.(21) we evaluate the partial derivatives of $z_0(\omega,\lambda)$ in the above formula. After some algebra, we have the asymptotic representation for $z(\omega,\lambda;h)$ in terms of derivatives of the confluent hypergeometric function of second kind,

$$z^{(1)}(\omega,\lambda;\,h)=(\frac{3}{2\lambda})^{\frac{3}{4}}\left(\sqrt{\frac{2}{\pi}}\,(\omega^2)\,\Psi\left(\frac{3}{4},\frac{3}{2};\frac{3\omega^4}{\lambda}\right)+\sum_{k=1}^{\infty}h^{2k}c_k\left(\frac{\partial}{\partial\omega^2}\right)^k\Psi\left(\frac{3}{4},\frac{3}{2};\frac{3\omega^4}{2\lambda}\right)\right) \tag{25}$$

where the coefficients c_k are given by $c_k=\frac{(-1)^k}{\sqrt{2\pi}}\frac{2^{k+1}}{2k!}$. Let us study the singularities of $z^{(1)}(\omega,\lambda;h)$ in the complex coupling constant for $0<|\lambda|<\infty$. The derivatives of the confluent hypergeometric functions of second kind are given by

$$\frac{d^n}{dz^n}\Psi(\alpha,\gamma;z)=(-1)^n(\alpha)_n\Psi(\alpha+n,\gamma+n;z), \tag{26}$$

where the coefficients $(\alpha)_k$ are defined by

$$(\alpha)_0=1,...\;(\alpha)_k=\frac{\Gamma(\alpha+k)}{\Gamma(\alpha)}=\alpha(\alpha+1)...(\alpha+k-1), \tag{27}$$

for $k=1,2,....$ Therefore, again we note that in the series representation for $z^{(1)}(\omega,\lambda;\,h)$ we find branch points at $\lambda=0$, $\lambda=\infty$ and a branch cut at $\arg(\lambda)=\pi$.

On closer inspection, great difficulties become apparent. If the $z^{(1)}(\omega,\lambda;\,h)>1$ in the limit $N\to\infty$, where N is the number of points of the lattice, the static ultra-local generating function becomes infinite and if $z^{(1)}(\omega,\lambda;\,h)<1$, in the same limit the ultra-local generating function becomes zero. In fact it is quite a subtle matter to give meaning to the static ultra-local generating functional once it is very dificult to disentangle the lattice from continuous physics. We can attempt a short cut, in the next section, we will use the Klauder representation for the static ultra-local generating functional, and also use the generalized zeta-function method to regularize and renormalize the kernel $K(\omega,\sigma;\tau-\tau')$ integrated over the Euclidean time.

4 The partition function for the anharmonic oscillator in the strong-coupling regime

In the present section we study the single anharmonic oscillator in the strong-coupling regime. Since all the thermodynamics quantiyies are derived from the Helmholtz free energy, let us proceed in deriving the free energy. The Helmholtz free energy can be obtained from $\ln Z_\beta(h)|_{h=0}$, i.e. $F_\beta = -\frac{1}{\beta}\ln Z_\beta(h)|_{h=0}$. To have a well defined meaning to the Helmholtz free energy that can be obtained from Eq.(18) we may proceed as follows. First, to give meaning to the static ultra-local generating functional $Q_\beta(\sigma;h)$, we may discretize the space, or else use to Klauder's result, as the formal definition of the ultra-local generating functional. Second, we have to regularize and renormalize the kernel $K(\omega,\sigma;\tau-\tau')$ integrated over the Euclidean time. As we will see, there is a practical advantage in going from the ultra-local defined in the lattice, to another representation derived by Klauder. The sucess of our method, depends critically on the possibility to handle the static ultra-local generating functional and the kernel integrated on the Euclidean time $[0,\beta]$.

Since we are concerned with the strong-coupling regime, to evaluate $\ln Z_\beta$ let us use the leading term. After some simple calculations we obtain

$$\ln Z_\beta(h) = \frac{1}{Q_\beta(\sigma;h)}\frac{\partial^2 Q_\beta(\sigma;h)}{\partial\, h^2}\left(-\frac{1}{2}+\frac{1}{2}\frac{d}{ds}\zeta(s)|_{s=0}\right), \tag{28}$$

where $\zeta(s)$ is the global generalized zeta-function associated with the operator $\left(-\frac{d^2}{d\tau^2}+(1-\sigma)\,\omega^2\right)$. There are some issues that we would like to discuss. Note also that, we assume thermal equilibrium and since we are working in the Euclidean formalism, the spectrum of the operator $D\equiv\left(-\frac{d^2}{d\tau^2}+(1-\sigma)\omega^2\right)$ has a denumerable contribution. Remind that σ is a complex parameter defined in the region $0\leq$ Re $(\sigma)<1$. At this point, let us impose that Im $(\sigma)=0$, since $Q_\beta(\sigma;h)$ should be a positive definite functional, i.e., a characterized functional of a generalized stochastic process.

The operator D is a positive definite eliptic operator, and has a complete set of orthonormal eigenfunctions $x_n(\tau)$ and associated eigenvalues a_n. We have

$$\left(-\frac{d^2}{d\tau^2}+(1-\sigma)\,\omega^2\right)x_n(\tau) = a_n\,x_n(\tau), \tag{29}$$

with the boundary conditions $x_n(0)=x_n(\beta)$. Note that we have $\int_0^\beta d\tau\, x_n(\tau)x_{n'}(\tau)=\delta_{nn'}$.

At this point, we would like to stress that a number of difficulties appear for complex σ. Since we are working in the leading order of the inverse power of the coupling constant, another problem related to the choice Im $(\sigma)\neq 0$, is related to the eigenvalue equation given by Eq.(29). For complex σ, the eigenvalue equation involve complex eigenvalues a_n and the eigenfunctions still form a complete, but not orthogonal set. See for example [29] [30]. Actually there is a program to study non-self adjoint operators and this is related to the Parisi-Wu stocastic quantization [31] with a complex Langevin equation [32] [33]. Actually complex Euclidean action also appears in different systems. For example the Euclidean action for a gauge theory with external static charge is complex. Effective actions with topological terms are complex in the Euclidean formalism. Such kind of problems also appear in lattice QCD, where the analysis of the phase diagram in the temperature-chemical potential plane has been investigated [33]. It is well known that in the SU(3) theory, the fermionic determinant is complex, giving to a complex Euclidean action. For the study of the Gross-Neveu model with a nonzero imaginary chemical potential, see Ref. [34]. Summarizing, complex Euclidean generating functional introduce new stimulated problems and deserves a carefull analysis of them.

Going back to the eigenvalue equation, the generalized zeta-function associated with the operator $\left(-\frac{d^2}{d\tau^2}+(1-\sigma)\omega^2\right)$, i.e., $\zeta_{-\frac{d^2}{d\tau^2}+(1-\sigma)\,\omega^2}(s)$ is defined by

$$\zeta_{-\frac{d^2}{d\tau^2}+(1-\sigma)\,\omega^2}(s)=\sum_{n=-\infty}^{\infty}a_n^{-s}, \tag{30}$$

where the spectrum is given by

$$a_n=\left[\left(\frac{2\pi n}{\beta}\right)^2+(1-\sigma)\,\omega^2\right],\quad n\,\varepsilon\,\mathrm{Z}. \tag{31}$$

Using the definition for the global generalized zeta-function and the spectrum of the operator given by Eq.(31) we have that the generalized zeta-function is given by

$$\zeta_{-\frac{d^2}{d\tau^2}+(1-\sigma)\,\omega^2}(s)=\sum_{n=-\infty}^{\infty}\left[\left(\frac{2\pi n}{\beta}\right)^2+(1-\sigma)\,\omega^2\right]^{-s}. \tag{32}$$

Here, it is useful to define the modified Epstein zeta-function in the complex plane s, i.e., the function $\zeta(s,\nu)$ by:

$$\zeta(s,\nu)=\sum_{n=-\infty}^{\infty}(n^2+\nu^2)^{-s},\qquad \nu^2\ >0. \tag{33}$$

The series defined by Eq.(33) converges absolutely and defines in the complex s plane an analytic function for Re(s) $>\frac{1}{2}$. It is possible to analytically extend the modified Epstein zeta-function where the integral representation is valid for $Re(s)<1$, [35] [36]:

$$\sum_{n=-\infty}^{\infty}(n^2+\nu^2)^{-s}=\nu^{1-2s}\left[\sqrt{\pi}\,\frac{\Gamma(s-\frac{1}{2})}{\Gamma(s)}+4\sin\pi s\int_1^{\infty}\frac{(t^2-1)^{-s}dt}{\mathrm{e}^{2\pi\nu t}-1}\right]. \tag{34}$$

For a different representation for the analytic extention of the modified Epstein zeta-function in terms of the modified Bessel function $K_\alpha(z)$ or the Macdonald's function, the reader can use for example Ref. [37].

It is not difficult to write the generalized zeta-function in terms of the modified Epstein zeta-function. We have

$$\zeta_{-\frac{d^2}{d\tau^2}+(1-\sigma)\,\omega^2}(s) = \left(\frac{\beta}{2\pi}\right)^{2s} \zeta\left(s, \sqrt{1-\sigma}(\frac{\omega\beta}{2\pi})\right), \tag{35}$$

where $\zeta(s,\nu)$, is the modified Epstein zeta-function. As we discussed, the series representation for $\zeta(s,\nu)$ converges for Re(z) $> \frac{1}{2}$ and its analytic continuation defines a meromorphic function of s which is analytic at $s=0$. The modified Epstein zeta-function has poles at $s=\frac{1}{2}, -\frac{1}{2}$, etc. Using Eq.(34) is not difficult to show that the values for the modified Epstein zeta-function $\zeta(s,\nu)$, at $s=0$ and $\frac{\partial}{\partial s}\zeta(s,\nu)|_{s=0}$ are given by

$$\zeta(s,\nu)|_{s=0} = 0, \tag{36}$$

and also

$$\frac{\partial}{\partial s}\zeta(s,\nu)|_{s=0} = -2\ln(2\,\sinh\pi\nu). \tag{37}$$

Since we are interested in calculating the derivative of the generalized zeta-function at the origin of the complex s plane, we have

$$\frac{1}{2}\frac{\partial}{\partial s}\zeta_{-\frac{d^2}{d\tau^2}+(1-\sigma)\,\omega^2}(s)|_{s=0} = \left(\frac{1}{2}\zeta(s,\nu)\frac{d}{ds}\left(\frac{\beta}{2\pi}\right)^{2s} + \frac{1}{2}\left(\frac{\beta}{2\pi}\right)^{2s}\frac{\partial}{\partial s}\zeta(s,\nu)\right)|_{s=0}. \tag{38}$$

Choosing $\sigma=0$, and using Eq.(36) and Eq.(37) in Eq.(38) we obtain the well known result in the literature. For the general case ($\sigma \neq 0$) we have

$$\frac{1}{2}\frac{\partial}{\partial s}\zeta_{-\frac{d^2}{d\tau^2}+(1-\sigma)\,\omega^2}(s)|_{s=0} = -\ln\left[(2\,\sinh\left((1-\sigma)\frac{\omega\beta}{2}\right)\right]. \tag{39}$$

Thus it is clear that the zeta function regularization can be used to control the divergences of the kernel $K(\omega,\sigma;\,\tau-\tau')$ integrated over the Euclidean time.

To give meaning to the static ultra-local generating functional $Q_\beta(\sigma;h)$, we may either discretize the space or use the Klauder's result, as the formal definition of the static ultra-local generating functional derived for scalar fields in a d-dimensional Euclidean space. This generating functional is a mean zero Gaussian functional integral and using the fact that the fields defined in each point of the Euclidean time are statistically independent we are able to write

$$Q_\beta(\sigma;h) = \exp\left(-\int d\tau\, L(\sigma;h(x))\right), \tag{40}$$

for some function $L(\sigma; h(x))$. The formula above is fundamental for our study. Let us see how it is possible to extract some information from it. Before studing the anharmonic oscillator, let us analyse a simple example, i.e., $\lambda = 0$. In this case we have

$$Z_\beta(h)|_{\lambda=0} = \exp\left(-\frac{1}{2}\int_0^\beta d\tau \int_0^\beta d\tau' \frac{\delta}{\delta h(\tau)} K(\omega,\sigma;\tau-\tau') \frac{\delta}{\delta h(\tau')}\right) Q_\beta(\sigma;\, h)|_{\lambda=0}, \tag{41}$$

where $Q_\beta(\sigma; h)$, the static ultra-local generating functional, is given by

$$Q_\beta(\sigma; h)|_{\lambda=0} = \mathcal{N}\int_{x(0)=x(\tau)} [dx(\tau)]\, \exp\left[\int_0^\beta d\tau\, \left(-\frac{1}{2}\sigma\,\omega^2\, x^2(\tau) + h(\tau)x(\tau)\right)\right], \tag{42}$$

where once more the modified kernel $K(\omega, \sigma; \tau - \tau')$ was defined by Eq.(13). The free ultra-local generating functional must satisfies $Q_\beta(\sigma; h)|_{h=\lambda=0} = 1$. Since we are assuming that $h = cte$, we have to normalize our expressions. Therefore we obtain

$$Q_\beta(\sigma; h)|_{\lambda=0} = \exp\left[-\frac{1}{2\beta\sigma\omega^2}\int_0^\beta d\tau\, h^2(\tau)\right]. \tag{43}$$

The generalization for the anharmonic oscillator in equilibrium with a termal bath can be done using the Klauder result. We would like to point out that in Klauder's derivation for the static ultra-local model a result was obtained which is well defined for all functions which are square integrable in R^n i.e., $h(x)\,\varepsilon\, L^2(R^n)$. This observation allow us to conclude that we need also to use a normalization. It is possible to show that the ultra-local generating functional can be written as

$$Q_\beta(\sigma; h) = \exp\left[-\frac{1}{2\beta}\int_0^\beta d\tau \int_{-\infty}^\infty \frac{du}{|u|}\,(1-\cos(hu))\exp\left(-\frac{1}{2}\,\sigma\,\omega^2\,u^2 - \frac{\lambda}{4!}\,u^4\right)\right]. \tag{44}$$

There is no need to go into details of this derivation. The reader can find it in Ref. [16] [19] [23]. It is important to stress that the static ultra-local generating functional defined by Eq.(44) do not reduce to the conventional free static ultra-local model given by Eq.(43), if we choose $\lambda = 0$. The non-gaussian contribution represents a discontinuous perturbation of the free theory, or using the Klauder's definition; a pseudo-free theory. Actually, this is the key point of the program developed by Klauder to investigate non-renormalizable models in field theory. For a interesting study of the pseudo-free harmonic oscillator see for example Ref. [38].

In order to study $Q_\beta(\sigma; h)$ let us define $E(\omega, \sigma, \lambda; h)$ given by

$$E(\omega,\sigma,\lambda; h) = \int_{-\infty}^\infty \frac{du}{|u|}\,(1-\cos(hu))\exp\left(-\frac{1}{2}\,\sigma\,\omega^2\,u^2 - \frac{\lambda}{4!}\,u^4\right). \tag{45}$$

Using a series representation for $\cos x$, the series obtained does not converge uniformly in the interval $[0, \infty)$, consequently the series can not be integrated term by term. In order to perform such operation we have to interpret the resuls as the asymptotic expansion for $E(\omega,\sigma,\lambda;h)$. It is not difficult to show that

$$E(\omega,\sigma,\lambda;h) = 2\sum_{k=1}^{\infty}\frac{(-1)^k}{(2k)!}h^{2k}\int_0^{\infty}du\,u^{2k-1}\exp\left(-\frac{1}{2}\,\sigma\,\omega^2\,u^2 - \frac{\lambda}{4!}\,u^4\right). \tag{46}$$

Now let use the fact that the σ parameter can be choosen in such a way that the calculations becomes tractable. Analysing only the static ultra-local generating functional it is not possible to write $Q_\beta(\sigma;h)$ in a closed form even in the case of constant external source. One way to obtain a closed expression is to choose $\sigma = 0$. Therefore we have

$$E(\omega,\sigma,\lambda;h)|_{\sigma=0} = 2\sum_{k=1}^{\infty}\frac{(-1)^k}{2k!}h^{2k}\int_0^{\infty}du\,u^{2k-1}\exp(-\frac{\lambda}{4!}\,u^4). \tag{47}$$

At this point let us use the following integral representation for the Gamma function [28]

$$\int_0^{\infty}dx\,x^{\nu-1}\exp(-\mu x^p) = \frac{1}{p}\mu^{-\frac{\nu}{p}}\,\Gamma\left(\frac{\nu}{p}\right), \quad \mathrm{Re}(\mu) > 0 \quad \mathrm{Re}(\nu) > 0 \;\; p > 0. \tag{48}$$

It is clear that the $(\lambda\,x^p)$ theory, for even $p > 4$, can also easily handle applying our method. Using the result given by Eq.(48) in Eq.(47) we have

$$E(\omega,\sigma,\lambda;h)|_{\sigma=0} = \sum_{k=1}^{\infty}g(k)\frac{h^{2k}}{\lambda^{\frac{k}{2}}}, \tag{49}$$

where the coefficients $g(k)$ are given by

$$g(k) = \frac{1}{2}\frac{(-1)^k}{(2k)!}(4!)^{\frac{k}{2}}\Gamma(\frac{k}{2}). \tag{50}$$

Substituting the Eq.(49) and Eq.(50) in Eq.(44) we obtain that the static static ultra-local generating functional $Q_\beta(\sigma;h)|_{\sigma=0}$ can be written as

$$Q_\beta(\sigma;h)|_{\sigma=0} = \exp\left[-\frac{1}{2\beta}\int_0^{\beta}d\tau\,\sum_{k=1}^{\infty}g(k)\frac{h^{2k}}{\lambda^{\frac{k}{2}}}\right]. \tag{51}$$

It is easy to calculate the second derivative for the ultra-local generating function with respect to h. Note that $Q_\beta(\sigma;h)|_{h=\sigma=0} = 1$. Thus we have

$$\frac{\partial^2 Q_\beta(\sigma;h)}{\partial\,h^2}|_{\sigma=0} = \left(-\frac{1}{2}\sum_{k=1}^{\infty}g(k)(2k)(2k-1)\frac{h^{2k-2}}{\lambda^{\frac{k}{2}}}\right)\exp\left(-\frac{1}{2}\sum_{k=1}^{\infty}g(k)\frac{h^{2k}}{\lambda^{\frac{k}{2}}}\right) + G(h), \tag{52}$$

where $G(h)$ is given by

$$G(h) = \left(\sum_{k,\,q=1}^{\infty}g(k,q)\frac{h^{2k+2q-2}}{\lambda^{\frac{k+q}{2}}}\right)\exp\left(-\frac{1}{2}\sum_{k=1}^{\infty}g(k)\frac{h^{2k}}{\lambda^{\frac{k}{2}}}\right), \tag{53}$$

and $g(k,q) = k\,q\,g(k)g(q)$. We are interested in the case $h=0$, therefore the double series does not contributes to the Eq.(52), since $lim_{h\rightarrow 0}G(h)=0$. Using the fact that we are interested in the case $h=0$, we have the simple result that in the Eq.(52) only the term $k=1$ contributes. We get

$$\frac{\partial^2 Q_\beta(\sigma;h)}{\partial\, h^2}|_{h=\sigma=0} = \sqrt{\frac{3\pi}{8\lambda}}. \tag{54}$$

Substituting the result obtained from the generalized zeta-function method given by Eq.(39) (choosing $\sigma=0$) and Eq.(54) in Eq.(28) we have that $\ln Z_\beta$ is given by

$$\ln Z_\beta = \sqrt{\frac{3\pi}{8\lambda}}\left[\frac{1}{2} - \ln\left(2\sinh(\frac{\omega\beta}{2})\right)\right]. \tag{55}$$

Therefore the partition function for the single oscillator is

$$Z_\beta = \frac{e^{\frac{1}{2}\sqrt{\frac{3\pi}{8\lambda}}}}{\left(2\sinh(\frac{\omega\beta}{2})\right)^{\sqrt{\frac{3\pi}{8\lambda}}}}. \tag{56}$$

It should be noted that for a system of N harmonic oscillators, the partition function is

$$Z_\beta = \frac{1}{\left(2\sinh(\frac{\omega\beta}{2})\right)^N}. \tag{57}$$

Therefore the identification $N=\sqrt{\frac{3\pi}{8\lambda}}$, the partition function for the strongly coupled single oscillator seem to be equivalent to the partition function of N harmonic oscillators, up to the order $\frac{1}{\sqrt{\lambda}}$.

Other thermodynamics quantities that we are able to find are the Helmholtz free energy and the mean energy. The Helmholtz free energy is given by $F_\beta = -\frac{1}{\beta}\ln Z_\beta(h)|_{h=0}$. Thus we have

$$F_\beta = \frac{1}{\beta}\sqrt{\frac{3\pi}{8\lambda}}\left[-\frac{1}{2} + \ln\left(2\sinh(\frac{\beta\omega}{2})\right)\right]. \tag{58}$$

It is possible to write this expression in the following way

$$F_\beta = \sqrt{\frac{3\pi}{8\lambda}}\left[-\frac{1}{2\beta} + \frac{\omega\beta}{2} + \frac{1}{\beta}\ln\left(1-e^{-\beta\omega}\right)\right]. \tag{59}$$

Finally the mean energy is defined by $E = -\frac{\partial}{\partial\beta}\ln\, Z_\beta$. Therefore we have

$$E = \sqrt{\frac{3\pi}{8\lambda}}\left[\frac{\omega}{2} + \frac{\omega}{e^{\omega\beta}-1}\right]. \tag{60}$$

We conclude with some observations. Usually, the free energy of a finite system is an analytic function of the parameters that define our physical system. Nevertheless, our results are showing that the thermodynamics quantities are nonanalytic in the coupling constant.

The picture emerging from the previous discussion is the following: in the strong-coupling perturbative expansion we may split the problem of defining the generating functional into two parts: how to define precisely the ultra-local generating functional and how to go beyond the static ultra-local approximation, taking into account the perturbation part. Our results show that the strong-coupling perturbative expansion, in combination with an analytic regularization procedure, is a useful method to compute global quantities, as the Helmholtz free energy, in the strong-coupling regime.

5 Conclusions

In this article we studied the strong-coupling regime in one-dimensional models, after analytic continuation to imaginary time. One-dimensional models is a very simple system for which we can apply our method in obtaining thermodynamics quantities in the leading order in the inverse of coupling constant. We calculate the partition function and the Helmholtz free energy for the anharmonic oscillator, using the strong-coupling perturbative expansion and the generalized zeta-function analytic regularization. It was possible to present expressions up to the order $\frac{1}{\sqrt{\lambda}}$ for the partition function and the other thermodynamic quantities derived from the the Helmholtz free energy.

The picture that emerges from our method is the following: in the strong-coupling perturbative expansion we may split the problem of defining the generating functional into two parts: the first is how to define precisely the static ultra-local generating functional; we may use of a lattice approximation to give a mathematical meaning to the non-Gaussian functional (actually, it is not easy to recover the continuum limit) or use the Klauder's representation for the ultra-local generating functional. The second part is to go beyond the ultra-local approximation and take into account the perturbation part. This problem can be controled using an analytic regularization. Besides these technical problems, we still have the problem of obtaining the Green's functions from this approach. The strong-coupling perturbative expansion is not fit to obtain local quantities, as the Green's functions of the model. On the other hand, our results show that the strong-coupling perturbative expansion, in combination with an analytic regularization procedure, is a useful method to compute global quantities, as the Helmholtz free energy, in the strong-coupling regime.

There are several directions for investigations, using the Klauder's result and an analytic regularization procedure. It should be possible for applying the method to more realistic theories. To mention a few: since scalar fields play a fundamental role in the standard model, the study of the strongly coupled $(\lambda\varphi^4)_d$ theory at finite temperature and also the renormalized vacuum energy of scalar quantum fields in the presence of macroscopic structures deserves future investigations.

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