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Partition function for a singular background

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Abstract

We present a method for evaluating the partition function in a varying external field. Specifically, we look at the case of a non-interacting, charged, massive scalar field at finite temperature with an associated chemical potential in the background of a delta-function potential. Whilst we present a general method, valid at all temperatures, we only give the result for the leading order term in the high temperature limit. Although the derivative expansion breaks down for inhomogeneous backgrounds we are able to obtain the high temperature expansion, as well as an analytic expression for the zero point energy, by way of a different approximation scheme, which we call the *local Born approximation* (LBA).

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In this Letter we discuss the evaluation of the partition function in the non-smooth background of a spherically symmetric shell, a particular motivation being some recent interest in singular potentials [1–3]. The delta-function profile is a useful approximation in modelling semi-transparent boundary conditions, which are naturally expected in many problems of physical interest. The Casimir energy has been evalu-

ated for a scalar field in the background of a spherical penetrable shell in [4], which used the Jost function technique along with contour integral methods, e.g., see [5] and the references therein.

However, here we shall investigate the partition function for a massive, charged scalar field at finite temperature with a non-zero chemical potential. We shall rely on the fact that the thermal partition function can be related (by partial wave analysis) to a radial momentum integral and angular momentum sum over the phase shifts. The phase shift method has a simple connection with the Jost function approach [5]. Numerous

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works have employed the partial waves technique to evaluate one loop and non-perturbative effects. Some of these are for example; the prefactor in bubble nucleation [6,7], quantum effects for solitons [8,9], the Casimir energy of a skyrmion [10] and instanton effects in QCD [11,12]. Indeed, the phase shift method appears to have been first used in the context of field theory by Schwinger [13].

Usually, the derivative expansion can be employed as an approximation to external fields that gradually vary, but for the case of potentials such as a delta-function this approximation clearly breaks down. However, recent work which deals with the heat kernel asymptotics of singular potentials [14,15] means that other approximation schemes can be devised. We shall explicitly show how by obtaining the high temperature limit using the *local Born approximation* (LBA).

In tandem we shall also apply the LBA to the calculation of the zero point energy, which gives surprisingly good agreement with exact results. The zero point energy must undergo regularisation; and of the many possible approaches, such as subtracting terms from the Born series [8], we tackle the problem by subtracting the relevant heat kernel coefficients, enabling an analytically continued expression for the zero point energy. As discussed in [9] the intrinsically local heat kernel coefficients can be related to the non-local Born series. Indeed a non-local generalisation of the heat kernel asymptotics exists in the guise of covariant perturbation theory, which has been applied to finite temperature field theory in [16].

As is well known, e.g., see [17], the factored one loop effective action for a charged scalar field is $W^\beta = W^\beta(\mu) + W^\beta(-\mu)$, where

$$W^\beta(\pm\mu) = \frac{1}{2} \log \det \ell^2 \left[-\square_E + m^2 - \mu^2 \pm 2i\mu \frac{\partial}{\partial t} \right], \quad (1)$$

and the parameter ℓ , with dimensions of length, keeps the argument of the determinant dimensionless. The connection between the Euclidean effective action and the canonical free energy is well known

$$F^\beta = \frac{1}{\beta} W^\beta \quad (2)$$

where we are ignoring any terms independent of the temperature, e.g., see [16]. We must deal with the

eigenvalues of the operator

$$\Delta_\pm \phi_\pm(x, \tau) = \lambda_{n,k} \phi_\pm(x, \tau), \quad (3)$$

where

$$\Delta_\pm = \left[-\square_{E\pm} + m^2 \right] \quad (4)$$

and the Euclidean d'Alembertian operator is

$$-\square_{E\pm} = -\left[(\partial_\tau \mp iA_0)^2 + \nabla^2 \right] \quad (5)$$

with $A_\mu = (A_0, \mathbf{0})$ and $A_0 = -i\mu$. It is related to the Lorentzian \square operator by the Wick rotation $-i\partial_t = \partial_\tau$. The vector A_μ is a fictitious Abelian gauge potential which represents the effect of an external charge density on the quantum system.

Consider the spatial Laplacian,

$$(-\nabla^2 + m^2 + V(x))\phi(x) = E^2\phi(x) \quad (6)$$

for a set of eigenvalues E^2 , where we shall assume a spatially dependent background coupling with spherical symmetry of the form

$$V(r) = \frac{\alpha}{R} \delta(r - R), \quad (7)$$

$\alpha > 0$, i.e., we are considering a massive, charged scalar field in the background of a repulsive spherical shell, at some radius R . We have chosen the inverse radius for our dimensionful parameter in the background delta function. Other choices can of course be made, see [4]. If we are interested in a massless field, $m = 0$, a slightly different approach must be applied, e.g., see [7].

After separating the eigenmodes into radial functions and spherical harmonics, the phase shift can be obtained from the solutions of the $(d+1)$ -dimensional radial wave equation

$$\left(-\partial_r^2 - \frac{d}{r} \partial_r + m^2 + \frac{\alpha}{R} \delta(r - R) + \frac{l(l+d-1)}{r^2} \right) \times u(r) = E^2 u(r) \quad (8)$$

with angular momentum l . The limit $\alpha \rightarrow \infty$ implies reflecting Dirichlet boundary conditions and the partial waves approach should reproduce the functional determinant for the Dirichlet ball which has been studied in detail in [5] (however, also see the comments in [4]). It is straightforward to show that the phase shift is (for $d = 2$)

$$\tan \delta_l(k) = \frac{\frac{\pi}{2} \alpha J_{l+1/2}^2(kR)}{\frac{\pi}{2} \alpha J_{l+1/2}(kR) N_{l+1/2}(kR) - 1}, \quad (9)$$

where the radial momentum is defined by

$$k = \sqrt{E^2 - m^2} \quad (10)$$

and $J_\nu(x)$, $N_\nu(x)$ are Bessel and Neumann functions, respectively. For such a case when the eigenvalues are not explicitly known it is possible to employ the phase shift method as follows.

From a knowledge of the phase shift it is straightforward to relate it to the heat kernel by

$$K(t) = \frac{2}{\pi} \int_0^\infty dk e^{-(k^2+m^2)t} kt \sum_l \chi_l \delta_l(k), \quad (11)$$

e.g., see [7,9]. We should mention that in this Letter we shall assume that there are no bound states, which is the case for background coupling with $\alpha > 0$ (e.g., see [6,9] for a discussion of the inclusion of any bound states). The degeneracy factor $\chi_l = (2l + 1)$ in three dimensions. There is also a free space contribution, which is encoded by the C_0 term in the heat kernel expansion. This term gives the usual constant background results, which have been well studied at finite temperature [17,18], so we shall not discuss it. The heat kernel can now be used to regularise the one loop effective action. Defining the generalised ζ -function [19] by

$$\zeta(s) = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} \text{tr} K(t) dt. \quad (12)$$

The analytic continuation of $\zeta(s)$ then gives the one loop effective action, which is related to the zeta-function by

$$W^\beta = W^\beta(\mu) + W^\beta(-\mu), \\ W^\beta(\pm\mu) = -\frac{1}{2}\zeta'_\pm(0) + \frac{1}{2}\zeta_\pm(0) \log \ell^2. \quad (13)$$

Because we are working on a static manifold, the field can be written in separable form as $\phi(\tau, x) = e^{-i\omega_n\tau} \phi(x)$, where $\omega_n = 2\pi n/\beta$ are the Matsubara frequencies with β the inverse temperature. Thus, the coincidence limit of the heat kernel takes the following form

$$K_\pm^\beta(t) = \sum_{n=-\infty}^\infty \frac{2}{\pi} \int_0^\infty dk e^{-(k^2+m^2)t} kt \\ \times \sum_l \chi_l \delta_l(k) e^{-(\omega_n \pm i\mu)^2 t}. \quad (14)$$

The thermal effective action for a charged scalar field is therefore

$$W^\beta(\pm\mu) = -\frac{1}{2} \int_0^\infty dt t^{s-1} \sum_{n=-\infty}^\infty \frac{2}{\pi} \int_0^\infty dk e^{-(k^2+m^2)t} kt \\ \times \sum_l \chi_l \delta_l(k) e^{-(\omega_n \pm i\mu)^2 t}. \quad (15)$$

The analytic continuation can be conveniently performed by using the Jacobi–Poisson resummation formula on the Matsubara modes, e.g., see [20]. After some formal manipulations we find the total thermal effective action to be

$$W^\beta = -\frac{\beta}{\pi} \int_0^\infty dk \sum_{l=0}^\infty (2l+1) \bar{\delta}_l(k) \\ - \frac{\beta}{\pi} \int_0^\infty \frac{k dk}{(k^2+m^2)^{1/2}} \\ \times \sum_{l=0}^\infty (2l+1) \frac{\delta_l(k)}{e^{\beta(E-\mu)} - 1} - (\mu \rightarrow -\mu) \\ = W^\infty + W^\beta(\mu) + W^\beta(-\mu). \quad (16)$$

In an abuse of our previous notation, see (13), the first term is the zero point energy ($\beta \rightarrow \infty$) which is ultraviolet divergent, hence $\bar{\delta}_l(k)$ (see below), while the other two terms contribute to the thermal part of the effective action, one for each charge $\pm\mu$. Similar expressions can be found in [6,7], however, here we have incorporated a chemical potential.

For numerical purposes, the analytic continuation of the zero point energy is best performed by subtracting terms from the heat kernel. As $t \rightarrow 0$, the heat kernel in $d + 1$ dimensions has the asymptotic expansion

$$K(t) \sim t^{-(d+1)/2} \sum_{n=0} C_n(r) t^n \quad (17)$$

where due to radial symmetry the heat kernel coefficients are only local functions of r . The leading terms, which cause the poles in the zeta-function, can be removed by replacing the sum over phase shifts in (11) by [7]

$$\sum_l \chi_l \bar{\delta}_l(k) = \sum_l \chi_l \delta_l(k) - \frac{\pi C_1(r)(k^2 + m^2)^{\frac{d-1}{2}}}{\Gamma(\frac{d+1}{2})} - \frac{\pi C_{3/2}(r)(k^2 + m^2)^{\frac{d-2}{2}}}{\Gamma(\frac{d}{2})} - \frac{\pi C_2(r)(k^2 + m^2)^{\frac{d-3}{2}}}{\Gamma(\frac{d-1}{2})} - \frac{\pi C_{5/2}(r)(k^2 + m^2)^{\frac{d-4}{2}}}{\Gamma(\frac{d-2}{2})}, \tag{18}$$

where for distributional sources the heat kernel coefficients only contribute to surface terms [14,15], see below. To obtain a finite regularised sum we only require up to C_2 for finite temperatures in three dimensions and zero temperature in four dimensions. However, in practice it is useful to include the $C_{5/2}$ term for better numerical convergence or to interpolate the large k behaviour. A useful check is that the leading asymptotic behaviour follows that of the $C_{5/2}$ term. Indeed, as we shall show, the dominant contribution to the LBA is given by the $C_{5/2}$ term.

The analytic continuation of the zero point energy can be found in [7,10], for example, and we obtain

$$W^\infty = -\frac{\beta}{\pi} \int_0^\infty dk \left(\sum_{l=0}^\infty (2l+1) \delta_l(k) - 2\sqrt{\pi} \sqrt{k^2 + m^2} C_1 - \pi C_{3/2} - \frac{\sqrt{\pi} C_2}{\sqrt{k^2 + m^2}} - \frac{\pi C_{5/2}}{k^2 + m^2} \right) + \frac{\pi \beta C_{5/2}}{2m} + \frac{\beta C_2}{\sqrt{4\pi}} \log m^2 \ell^2. \tag{19}$$

In Fig. 1 is a plot of the integrand (in brackets) in the above equation, given as blue solid lines for various values of the coupling α . The extra factor of two for the zero point energy (19) as compared to the expression given in [7] is due to the fact that we are considering a charged scalar field. Although in this Letter we do not give explicit results that depend on μ , apart from (16), the more general expression is required if one wishes to comment on things such as Bose–Einstein condensation, which we hope to report on in the near future.

For the spatial wave equation (6) with a potential of the form defined in (7) the heat kernel coefficients

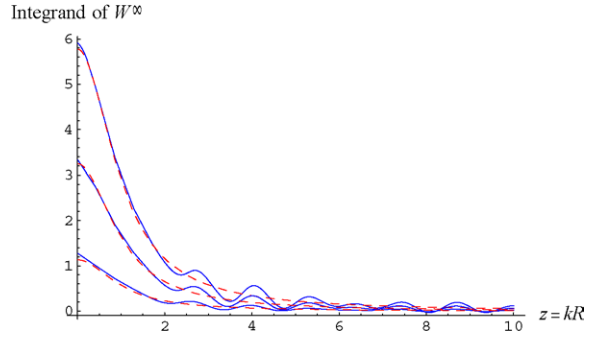


Fig. 1. A plot of the integrand in (19), solid lines (blue lines in the web version), and the contribution from the integrand in (23), dashed lines (red dashed lines in the web version), for values of increasing $\alpha = 1.5, 2.25, \text{ and } 2.75$, in units of $(mR)^{-1}$. For clarity the z axis has been shifted below the origin by a small amount.

are [14,15]:

$$C_1(r) = \frac{1}{(4\pi)^{(d+1)/2}} \int_\Sigma -\frac{\alpha}{R},$$

$$C_{3/2}(r) = \frac{1}{(4\pi)^{(d+1)/2}} \int_\Sigma \frac{\sqrt{\pi}}{4} \frac{\alpha^2}{R^2}, \tag{20}$$

$$C_2(r) = \frac{1}{(4\pi)^{(d+1)/2}} \int_\Sigma \left(-\frac{1}{6} \frac{\alpha^3}{R^3} + m^2 \frac{\alpha}{R} \right),$$

$$C_{5/2}(r) = \frac{1}{(4\pi)^{(d+1)/2}} \int_\Sigma \left(\frac{\sqrt{\pi}}{32} \frac{\alpha^4}{R^4} + \frac{\sqrt{\pi}}{4} m^2 \frac{\alpha^2}{R^2} \right), \tag{21}$$

where the volume of a spherical shell in $d + 1$ dimensions is given by

$$\int_\Sigma = \frac{2\pi^{(d+1)/2} R^d}{\Gamma(\frac{d+1}{2})} = 4\pi R^2|_{d=2}. \tag{22}$$

In fact, the leading order contribution comes from the $C_{5/2}$ term in (19), up to the renormalisation scale dependence, ℓ . As can be seen in Fig. 1, for example, the choice $\alpha = \frac{x}{mR}$ for various values of x gives surprisingly good agreement with the integrand of (19). That is, the zero point energy is dominated by the term

$$W^\infty \approx \frac{\beta}{\pi} \int_0^\infty dk \left(\frac{\pi C_{5/2}}{k^2 + m^2} \right) = \frac{\pi \beta C_{5/2}}{2m} \tag{23}$$

for which the integrand of the left-hand side (in brackets) we have plotted in Fig. 1 as dashed lines (red

dashed lines in the web version). Clearly, the accuracy of this approximation improves as the area of the integrand in (19) becomes larger and the oscillatory behaviour for the large k part has less effect. Including higher order corrections, such as the C_3 term, should improve the accuracy for smaller values of the area of the integrand in (19).

For large temperatures numerical evaluation of $W^\beta(\pm\mu)$ in (16) becomes difficult and it is useful to have analytic expressions valid in the high temperature limit, $\beta \rightarrow 0$. We can achieve this by using the LBA, as we have already done for the zero point energy. The high temperature expansion can be obtained in various ways, however, we shall simply adapt the method used in [18]. First, let us rewrite the thermal effective action explicitly in terms of k as

$$W^\beta(\pm\mu) = -\frac{\beta}{\pi} \int_0^\infty \frac{k dk}{(k^2 + m^2)^{1/2}} \times \sum_{l=0}^\infty (2l + 1) \frac{\delta_l(k)}{e^{\beta(k^2 + m^2)^{1/2}} e^{\pm\beta\mu} - 1}. \quad (24)$$

Our approach will be to substitute the sum over phase shifts [7]

$$\sum_l \chi_l \delta_l(k) \sim \sum_{n=1}^\infty \frac{\pi C_n (k^2 + m^2)^{\frac{d+1-2n}{2}}}{\Gamma(\frac{d+1-2n+2}{2})} \quad (25)$$

into our expression for W^β (24), i.e., $W^\beta(\pm r) = \sum_n W_n^\beta(\pm r)$

$$W_n^\beta(\pm r) = \frac{-\beta^{2n-d-1} C_n}{\Gamma(\frac{d+1-2n+2}{2})} \times \int_0^\infty x dx \frac{(x^2 + \bar{m}^2)^{\frac{d-2n}{2}}}{e^{(x^2 + \bar{m}^2)^{1/2}} e^{\pm r \bar{m}} - 1}, \quad (26)$$

where we have made the change of variables $x = \beta k$, $\bar{m} = \beta m$ and $r = \mu/m$.

In this Letter we shall only consider the leading order contribution to the high temperature expansion (for $d = 2$), which corresponds to $n = 1$, i.e.,

$$W_1^\beta(\pm r) = -\beta^{-1} \frac{C_1}{\Gamma(\frac{3}{2})} \times \int_0^\infty x dx \frac{1}{e^{(x^2 + \bar{m}^2)^{1/2}} e^{\pm r \bar{m}} - 1}. \quad (27)$$

The small \bar{m} expansion of the above integral is well known [18] and leads to the result

$$W_1^\beta(\pm r) = \frac{-2C_1}{\sqrt{\pi}\beta} g_2(\bar{m}, \pm r), \quad (28)$$

where the function $g_2(\bar{m}, r)$ is defined in Appendix A of [18]. Then, it is simple to show that

$$g_2(\bar{m}, r) + g_2(\bar{m}, -r) = \frac{\pi^2}{3} - 2\bar{m} + \bar{m}r \ln \left[\frac{(1+r)}{(1-r)} \right] + \frac{\bar{m}^2(1-r^2)}{2} + \mathcal{O}(\bar{m}^3) \quad (29)$$

and thus, the leading order contribution for small \bar{m} to the thermal part of the effective action is

$$W_1^\beta(\mu) + W_1^\beta(-\mu) = \left(\frac{-2C_1}{\sqrt{\pi}\beta} \right) \frac{\pi^2}{3} = \frac{1}{12\beta} \int_\Sigma \frac{\alpha}{R} = \frac{1}{12\beta} 4\pi\alpha R, \quad (30)$$

where the second equality is specific to a spherical shell. Thus, for the free space field theory, i.e., in a constant background, the leading order contribution to the free energy is $F_0^\beta \propto \beta^{-4}$, e.g., see [18], whereas the effect of a repulsive delta-function potential is to contribute to leading order $F_1^\beta \propto \beta^{-2}$.

The method we have discussed is sufficiently general such that we can choose any spherically symmetric background potential, smooth or inhomogeneous, the only requirement being a knowledge of the heat kernel coefficients. Of course if they are not known then the heat kernel coefficients can be derived by taking the local part of the Born approximation, which is an expansion in powers of small coupling of the phase shift. This is also true for the case when there is no analytic expression for the phase shift, where recourse can be made to the WKB method [6,12].

Furthermore, the finite temperature expression (24) is a general expression valid at any temperature, which requires numerics for the general case. However, it is instructive to have analytic expressions for a charged scalar field in the high temperature limit, for example, to consider Bose–Einstein condensation. In this Letter we showed how to obtain the leading order term. Indeed, next to leading order corrections will depend on the chemical potential, μ . The low temperature expansion can also be obtained in a similar way.

The *local Born approximation* (LBA) was also applied to give an approximate expression for the non-thermal part of the one loop effective action, i.e., the zero point energy. We employed zeta-function and heat kernel methods to subtract the divergences inherent in the zero point energy, this being one of the many commonly used subtraction procedures.

As well as for delta-function type potentials one could consider step function profiles, which are useful in modelling many physically interesting situations, such as instantons in bubble nucleation [7]. For such a case it would also be possible for the chemical potential, μ , to vary with the same radial profile as the mass, e.g., a step-function with profiles $\mu^2\theta(r - R)$ and $m^2\theta(r - R)$. However, this is a considerably more complicated set up, which we shall report on in forthcoming work, as well as other related issues.

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