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AN IMPROVED GAUSSIAN APPROXIMATION FOR QUANTUM FIELD THEORY

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Abstract. *We present a new approximation technique for quantum field theory. The standard one-loop result is used as a seed for a recursive formula that gives a sequence of improved Gaussian approximations for the generating functional. In a different setting, the basic idea of this recursive scheme is used in the second part of the paper to substantially speed up the standard Monte Carlo algorithm.*

1. INTRODUCTION

Quantum field theory is compactly written in terms of path integrals. Path integrals have been specially useful in dealing with symmetries, quantizing gauge theories, etc. At some point, however, we need to calculate the path integrals. The problem is that the only path integrals that we know how to solve correspond to free theories (Gaussian integrals). We would be in a very sorry state if we didn't have a generic approximation scheme at our disposal. Semi-classical or loop expansion is just such an approximation scheme. In fact, much of what we know about quantum field theory comes from one-loop results. The one-loop result is obtained by Taylor expanding the action around classical fields and disregarding cubic and higher terms. In this way the path integral is approximated by a Gaussian.

In this paper we will consider another Gaussian approximation to the path integral. Unlike the one-loop result, here we will Taylor expand about the average field $\phi \equiv \langle \phi \rangle$. We shall show that this leads to an improved approximation given in terms of a recursive relation.

2. THE GAUSSIAN APPROXIMATION

The central object in quantum field theory is the generating functional $Z[J]$. Functional derivatives of $Z[J]$ with respect to the external fields $J(x)$ give the Green's functions of the theory. The generating functional is determined from the (Euclidian) action $S[\phi]$ through the path integral

$$Z[J] = \int [d\phi] e^{-\frac{1}{\hbar}(S[\phi] - \int dx J(x)\phi(x))}. \quad (1)$$

The integration measure is, formally, simply

$$[d\phi] = \prod_{x \in \mathbf{R}^d} d\phi(x) \quad (2)$$

where d is the dimension of space-time. We are interested in looking at a set of approximations to the above path integral. The approximations are valid in all d . In this letter, however, we are going to look at the simpler case of $d = 0$ theories, where it is easy to compare our results with exact numerical calculations. In $d = 0$ functionals become functions, and the path integral reverts to a single definite integral over the whole real line.

$$Z[J] = \int d\phi e^{-\frac{1}{\hbar}(S(\phi) - J\phi)}. \quad (3)$$

An even more useful object is $W(J)$ – the generator of connected diagrams, defined by

$$Z(J) = Z(0) e^{-\frac{1}{\hbar}W(J)}. \quad (4)$$

In statistical mechanics parlance this is the free energy. The quantum average of the field ϕ is

$$\phi \equiv \langle \phi \rangle = -\frac{\partial}{\partial J} W(J). \quad (5)$$

In the Gaussian approximation, we Taylor expand the action in the path integral around some reference point ϕ_{ref} , and keep terms that are at most quadratic in $\phi - \phi_{ref}$. Thus, we use

$$S(\phi) \approx S(\phi_{ref}) + S'(\phi_{ref})(\phi - \phi_{ref}) + \frac{1}{2} S''(\phi_{ref})(\phi - \phi_{ref})^2. \quad (6)$$

The integral in (3) is now a Gaussian and we find, up to an unimportant constant, that

$$W_{Gauss}(J, \phi_{ref}) \approx S(\phi_{ref}) - J\phi_{ref} + \frac{\hbar}{2} \ln S''(\phi_{ref}) - \frac{1}{2} \frac{(S'(\phi_{ref}) - J)^2}{S''(\phi_{ref})}. \quad (7)$$

For this approximation to make sense, the integral must get its dominant contribution from the vicinity of the reference point ϕ_{ref} . The standard Gaussian approximation corresponds to the choice $\phi_{ref} = \phi_{class}(J)$, where ϕ_{class} is the solution of the classical equation of motion $S' = J$. The classical solution is the maximum of the integrand in (3). This specific choice of ϕ_{ref} gives us the standard one-loop result

$$W(J) \approx W_1(J) \equiv S(\phi_{class}) - J\phi_{class} + \frac{\hbar}{2} \ln S''(\phi_{class}). \quad (8)$$

As is well known, loop expansion is just an expansion in powers of \hbar . The one-loop result gives us the first quantum correction to classical physics. From now on we set $\hbar = 1$.

3. IMPROVING THE GAUSSIAN APPROXIMATION

In this section we will choose a *different* expansion point ϕ_{ref} for our general Gaussian formula (7). The idea is to expand around the average field ϕ . Although the classical solution gives the maximum of the integrand, expansion around ϕ gives a better approximation for the area under the curve. This is in particular true for large values of J . We will work with ϕ^4 theory in $d = 0$, whose action is given by

$$S(\phi) = \frac{1}{2} \phi^2 + \frac{1}{4!} g \phi^4. \quad (9)$$

The classical equation of motion is now a cubic algebraic equation. We easily find the unique real solution. In this way we get a closed form expression for the one-loop approximation $W_1(J)$. The Gaussian approximation around the average field ϕ is simply

$$S(\phi) - J\phi + \frac{1}{2} \ln S''(\phi) - \frac{1}{2} \frac{(S'(\phi) - J)^2}{S''(\phi)}. \quad (10)$$

To be able to calculate this *in closed form* we need to know $\phi(J)$, which is tantamount to knowing how to do the theory exactly, since ϕ and its derivatives give all the connected Green's functions. The use of equation (10) comes about when one solves it iteratively. We use equations (5) and (7) as the basis for the following iterative process.

$$\phi_{n+1}(J) = -\frac{d}{dJ} W_{Gauss}(J, \phi_n(J)). \quad (11)$$

Differentiating (7) we find

$$\phi_{n+1} = \phi_n - \frac{S'(\phi_n) - J}{S''(\phi_n)} - \frac{S'''(\phi_n)}{2} \left(\frac{S'(\phi_n) - J}{S''(\phi_n)} \right)^2 + \frac{1}{S''(\phi_n)} \frac{d\phi_n}{dJ}. \quad (12)$$

For the seed of this iteration we choose the classical field, i.e. $\phi_0 = \phi_{class}$. In this way we obtain a sequence of points $\phi_0, \phi_1, \phi_2, \dots$ or equivalently of approximations to the connected generating functional W_1, W_2, W_3, \dots given by $W_{n+1}(J) = W_{Gauss}(J, \phi_n(J))$. The idea behind this is obvious – we want to obtain a sequence of $W_n(J)$'s that give better and better approximations to $W(J)$. The following two figures show that this really works.

From Figure 1 we see that the sequence of ϕ_n 's converges to ϕ_∞ . In iterating (12) we necessarily discretize the J 's. The coarseness of this discretization effects the speed of convergence of the ϕ_n 's. The standard way out of this problem is to introduce a small mixing parameter ϵ . Instead of the recursive relation $\phi_{n+1} = f(\phi_n)$ one then considers

$\varphi_{n+1} = (1 - \varepsilon)\varphi_n + \varepsilon f(\varphi_n)$. Note that $\varphi_\infty \neq \varphi$. The reason for this is obvious: We used the Gaussian approximation W_{Gauss} in defining our recursive relation, and there is no reason to expect that this converges to the exact result. It does, however, converge and φ_∞ represents an excellent approximation to φ . To see this, in Figure 2 we have plotted the ratio $\left| \frac{\varphi - \varphi_0}{\varphi - \varphi_\infty} \right|$. This ratio represents a direct measure of the improvement of approximations in going from the one-loop result $W_1(J) = W_{Gauss}(J, \varphi_0(J))$ to our improved Gaussian result $W_\infty(J) = W_{Gauss}(J, \varphi_\infty(J))$.

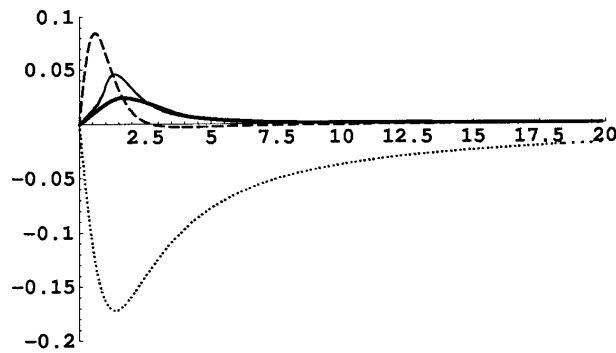


Fig. 1. Plots of $\varphi - \varphi_0$ (dotted line), $\varphi - \varphi_1$ (dashed line), $\varphi - \varphi_2$ (thin line) and $\varphi - \varphi_\infty$ (thick line) as functions of J . Here we had $g = 1$.

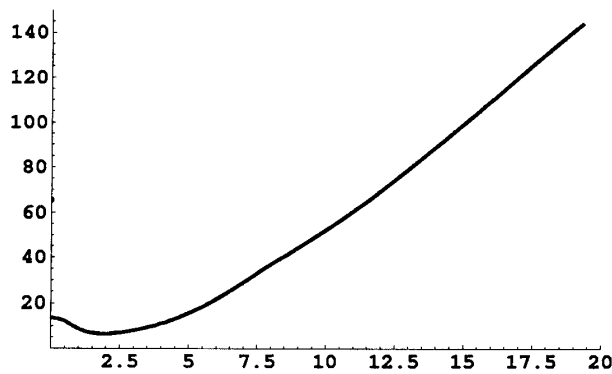


Fig. 2. Plot of the ratio $|\varphi - \varphi_0|/|\varphi - \varphi_\infty|$ as a function of J . This is a direct measure of how the new approximation outperforms the standard one-loop result. Here we had $g = 1$.

As we have already mentioned, our new approximation was tailored to work well for large J . This can be read off directly from Figure 2. For example, for $J = 15$ the improved Gaussian is about one hundred times better than the one-loop result. The new

approximation is poorest for $J \approx 2$, but even there it beats the old approximation by a factor of seven. Most of the time we are interested in working with small or zero external fields. In the vicinity of $J = 0$ the new approximation is fourteen times better than the old one.

4. MONTE CARLO

The aim of our investigations so far has been to develop better analytic approximation schemes that can be applied to general quantum field theories. We worked in $d = 0$ in order to be able to make a simple comparison with exact (numerical) results. In this section we will look at the numerical techniques themselves. We used the Monte Carlo algorithm [1] for calculating path integrals. In $d = 0$ Monte Carlo is not the most efficient way to do things – its advantages become apparent as we look at larger and larger numbers of integrations. We use Monte Carlo in order to investigate the algorithm itself in light of what we have learned in the previous two sections.

We start with a brief introduction of the method. In order to calculate the definite integral $\int f(\phi) d\phi$ we choose a non-negative function $p(\phi)$ normalized so that $\int p(\phi) d\phi = 1$. Therefore, $p(\phi)$ is a probability distribution. The integral is now

$$\int f(\phi) d\phi = \int \frac{f(\phi)}{p(\phi)} p(\phi) d\phi \equiv \left\langle \frac{f}{p} \right\rangle_p, \quad (13)$$

where $\langle F \rangle_p$ represents the mean value of F with respect to the probability distribution p . Therefore, the integral of f is given as the mean value of f/p on a sample of random numbers whose probability distribution is given by p . In practice, this mean value is estimated using a finite number N_{mc} of Monte Carlo samples, and the error of such an estimate is itself estimated to be $\sigma_{f/p} = \sqrt{\sigma_{f/p}^2}$, where the variance equals

$$\sigma_{f/p}^2 = \frac{\left\langle \left(\frac{f}{p} \right)^2 \right\rangle - \left\langle \frac{f}{p} \right\rangle_p^2}{N_{mc} - 1}. \quad (14)$$

The central limit theorem guarantees that the Monte Carlo algorithm converges to $\int f d\phi$ for an arbitrary choice of distribution p . The only condition that must be met is $\sigma_{f/p}^2 < \infty$.

This freedom in the choice of p is used to speed-up the convergence of the algorithm. The speed of convergence is measured by the efficiency ϵ , given by

$$\epsilon = \frac{1}{T \sigma_{f/p}^2}, \quad (15)$$

where T represents the total computation time. Note that a hundred fold increase of efficiency corresponds to one extra significant figure in the final result.

In our calculation we chose $p(\phi)$ to be the Gaussian normal distribution

$$p(\phi) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(\phi-a)^2}{2\sigma^2}\right), \quad (16)$$

where a and σ completely determine the distribution. There are two reasons for using this distribution. First of all, the function we are integrating can be approximated by a Gaussian over a wide range of parameters J and g . A good choice of a and σ makes f/p almost constant over the range of integration, thus making the variance small. Second, there exists a specific algorithm for generating random numbers conforming to a Gaussian distribution. The Box-Muller algorithm [3] is much more efficient than the standard Metropolis algorithm [2] since it doesn't give rise to autocorrelations of generated numbers. In the Metropolis algorithm autocorrelations can be pronounced, and their removal substantially slows down the simulation.

The choice of probability distribution has a great effect on the efficiency. For example, the efficiency corresponding to the uniform distribution on the interval $\phi \in [-100, 100]$ is $3.5 \cdot 10^{10}$ times smaller than the efficiency achieved by the Gaussian distribution centered at $a = \phi_{class}$ with optimal choice of width σ . Having chosen p to be a Gaussian, the computation time T depends only on the number of Monte Carlo samples N_{mc} . Therefore, in our case, maximalization of efficiency is equivalent to a minimalization of the variance $\sigma_{f/p}^2$.

In the previous sections we saw that it is even better to expand around ϕ . In the Monte Carlo setting this should translate into a further increase in efficiency. This is *precisely* what we see. By varying the center of the Gaussian a (always using optimal width for that given a), we find maximum efficiency precisely at $a = \phi$ as we can see in Figure 3.

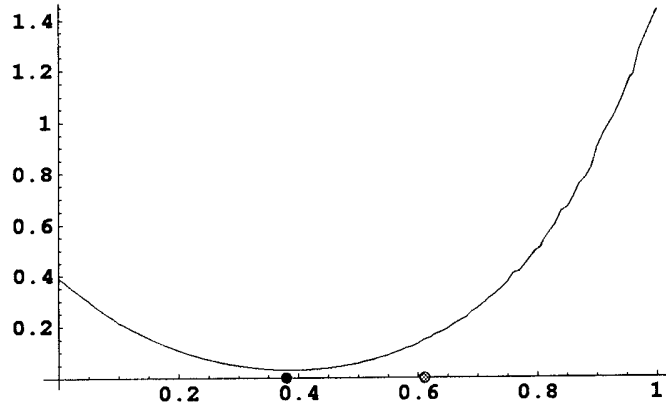


Fig. 3. The variance as a function of a . The plot is for $g = 10, J = 1$. The variance is minimized for $\phi(1) = 0.376799$ (black dot). The classical field is $\phi_{class}(1) = 0.614072$ (grey dot).

Figure 4 compares the efficiencies ϵ_C of simulations about ϕ_{class} and ϵ_Q for simulations

about φ for various values of J . It is seen that we get a two fold improvement in efficiency. This may not seem spectacular, and in $d = 0$ it really is not. However, once we consider theories in $d > 0$ we are dealing with true path integrals. If we approximate the path integral with N integrals then the expansion around φ gives a jump in efficiency of 2^N . Even for a modest simulation with $N = 20$ this corresponds to an increase of six orders of magnitude.

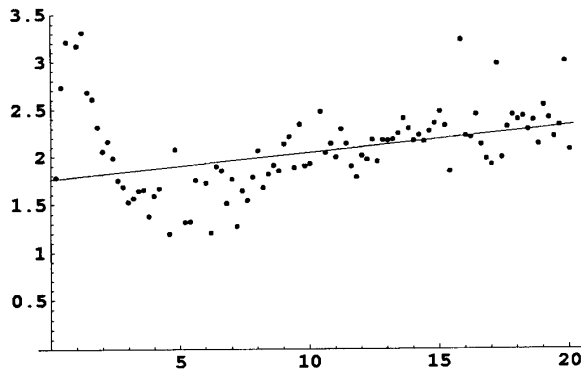


Fig. 4. The ratio $\varepsilon_Q/\varepsilon_C$ as a function of J for $g = 1$.

The problem with this calculation is that we already need to have the exact result for φ in order to get the stated increase in speed. The way out is obvious and is reminiscent of the step we made in the previous section in going from (10) to (11). Therefore, we need to start Monte Carlo with a Gaussian distribution centered about φ_{class} . After a while this gives us an approximation to φ say φ_1^{mc} . Using this as the center of a new probability distribution we obtain φ_2^{mc} , etc. Unlike the series $\varphi_0, \varphi_1, \varphi_2, \dots$ of the previous section, this one necessarily converges to the exact result – even ordinary Monte Carlo does that. The improved Monte Carlo scheme, however, can be tailored to yield an efficiency very near to the ideal value ε_Q [4].

5. CONCLUSION

We have looked at two different ways how one can take advantage of the (rather intuitive) fact that in quantum field theory Gaussians are best centered about the average field $\varphi \equiv \langle \phi \rangle$. We cast the Gaussian approximation about φ as a recursive relation. Working of ϕ^4 theory in $d = 0$ we have shown that the iterates of this equation present better and better approximations to $W(J)$. This sequence of approximations ends with $W_\infty(J)$, i.e. the best Gaussian approximation. The first iterate in this sequence is the standard one-loop result. The second (W_2) is not much more complicated, and is already much better than the one-loop approximation. In looking at theories in $d > 0$ it may be possible to use W_2 to get a better analytic approximation to (say) the effective potential.

The second use for the newly centered Gaussians is in Monte Carlo calculations. The Monte Carlo algorithm is most efficient when one generates random numbers through Gaussian probability distributions centered about φ . We have shown that this can substantially speed up the algorithm. For an N -fold integral the speed up is roughly 2^N . We are currently working on applying the improved Monte Carlo algorithm to models in $d \geq 1$.

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POBOLJŠANA GAUSOVSKA APROKSIMACIJA U KVANTNOJ TEORIJI POLJA

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Dat je prikaz nove aproksimativne tehnike u kvantnoj teoriji polja. Standardni rezultat do na jednu petlju je iskorišćen kao početna tačka rekurzivne formule koja daje niz poboljšanih gausovskih aproksimacija generišućeg funkcionala. Sa druge strane, u drugom delu članka, osnovna ideja ove rekurzivne sheme je iskorišćena za suštinsko ubrzanje standardnog Monte Carlo algoritma.