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PAPER: Quantum statistical physics, condensed matter, integrable systems

Monte Carlo evaluation of the continuum limit of $(\phi^{12})_3$

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Abstract. We study canonical and affine versions of non-renormalizable Euclidean classical scalar field-theory with twelfth-order power-law interactions on three dimensional lattices through the Monte Carlo method. We show that while the canonical version of the model turns out to approach a ‘free-theory’ in the continuum limit, the affine version is perfectly well defined as an interaction model.

Keywords: integrable quantum field theory

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1. Introduction

Classical versions of all covariant scalar field-theory models with positive interactions admit acceptable solutions, but some models will lead to divergences when trying to solve them when using canonical quantum versions [1].

Although classical covariant models, such as $(\phi^{12})_3$, lead to acceptable solutions, canonical quantization leads only to free solutions, as if the interaction term was not present. There are simple classical models, e.g. a half-harmonic oscillator that is limited to $0 < q < \infty$, which also fails using canonical quantization. A newer procedure, called affine quantization [2–5], differs from canonical quantization only because it promotes different canonical variables to quantum operators. It has been shown that affine quantization can successfully quantize the oscillator example, and the purpose of this paper is to demonstrate that affine quantization, in effect, just adds one additional term, which is proportional to \hbar^2 , to the Hamiltonian. Which extra term to add is guided by affine quantization, and the result leads to a valid quantization of $(\phi^{12})_3$ ¹.

The problem treated in this work deals with covariant scalar fields with power-law interactions. For the $(\phi^r)_d$ theory, the Euclidean time version of the action functional is then given by,

$$S[\phi] = \int \left\{ \frac{1}{2} \left[\sum_{\mu=0}^s \left(\frac{\partial \phi(x)}{\partial x_\mu} \right)^2 + m^2 \phi^2(x) \right] + g \phi^r(x) \right\} d^d x, \tag{1.1}$$

with $x = (x_0, x_1, \dots, x_s)$ for s spatial dimensions, x_0 being time, and $d = s + 1$ for the number of space-time dimensions, m is the bare mass, $g > 0$ is the interaction term coupling constant and $r = 4, 6, 8, 10 \dots$ is the power of the interaction term.

Monte Carlo (MC) [6–8] studies in 1982 [9] showed that these models were correct for $r = 4$ and $d = 3$ but when $r = 4$ and $d = 4$ they led only to free models, with a vanishing renormalized coupling constant in the continuum limit, and this was later confirmed by analytic studies and that even became simply free models when $r = 4$ and $d > 4$, which includes non-renormalizable models as well.

All of the above stories used canonical procedures, which then failed when $r \geq 2d/(d - 2)$ [2–4]. It is believed that affine quantization procedures will solve those problems.

In this work, we chose the $(\phi^{12})_3$ theory. Classically, this is a straightforward problem that in the $g \rightarrow 0$ limit reduces to a free-theory. But in its canonical version it is non-renormalizable, which means that the domain of the free model, $\mathcal{D}_{g=0}$, is larger than

¹The example $(\phi^{12})_3$ has been deliberately chosen to be highly nonrenormalizable, while requiring the least amount of computer time.

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that of the interacting model $\mathcal{D}_{g>0}$ (integrating ϕ^{12} will be finite for less ϕ than in the free model). In the continuum limit, the domains disagree and by continuity the new domain for the ‘free’ version (we can call it a ‘pseudofree’ situation) is the domain $\mathcal{D}_{g>0}$, not $\mathcal{D}_{g=0}$. That is the source of having free models using canonical quantization, such as $(\phi^r)_d$ with $r > 2d/(d - 2)^2$. On the other hand, affine quantization will lead to a non-free model to begin with and so it is appropriate when $g \rightarrow 0$. In parallel to the covariant theory, one can also define an ultralocal theory that is obtained by neglecting the kinetic part of the action (the term $\sum_{\mu=1}^s (\partial\phi(x)/\partial x_\mu)^2$) [3]. It turns out that such a theory will have a divergent perturbation series already for $r > 2$ for any $d \geq 2$. In these cases, the field theory will lead to a free-theory, non-renormalizable. So, with $r = 12$ there should be an even greater difference between the canonical and affine versions.

Various efforts have been tried in literature [10] to get a good result for the $(\phi^4)_4$ models, only to find that every effort came to the same conclusion that the result was a ‘free-theory’. Hence, the affine approach is the first to find an acceptable result [11].

2. Affine version of the field-theory

Our model has a standard classical Hamiltonian given by,

$$H[\pi, \phi] = \int \left\{ \frac{1}{2} \left[\pi^2(x) + \sum_{\mu=1}^s \left(\frac{\partial\phi(x)}{\partial x_\mu} \right)^2 + m^2\phi^2(x) \right] + g\phi^r(x) \right\} d^s x, \quad (2.1)$$

where s denotes the number of spatial coordinates and x_0 is the time. The momentum field $\pi(x) = \partial\phi(x)/\partial x_0$ and the canonical action $S = \int H dx_0$ is the one of equation (1.1).

Next, we introduce the affine field $\kappa(x) \equiv \pi(x)\phi(x)$, with $\phi(x) \neq 0$ and modify the classical Hamiltonian to become [2–4],

$$H'[\kappa, \phi] = \int \left\{ \frac{1}{2} \left[\kappa(x)\phi^{-2}(x)\kappa(x) + \sum_{\mu=1}^s \left(\frac{\partial\phi(x)}{\partial x_\mu} \right)^2 + m^2\phi^2(x) \right] + g\phi^r(x) \right\} d^s x. \quad (2.2)$$

In an affine quantization, the operator term $\widehat{\kappa}(x)\phi^{-2}(x)\widehat{\kappa}(x) = \widehat{\pi}^2(x) + \hbar^2(3/4)\delta^{2s}(0)\phi^{-2}(x)$, which leads to an extra ‘3/4’ potential [12] term (see appendix A), so that the new affine action will formally read,

$$S'[\phi] = \int \left\{ \frac{1}{2} \left[\sum_{\mu=0}^s \left(\frac{\partial\phi(x)}{\partial x_\mu} \right)^2 + m^2\phi^2(x) \right] + g\phi^r(x) + \frac{3}{8}\hbar^2 \frac{\delta^{2s}(0)}{\phi^2(x) + \epsilon} \right\} d^d x, \quad (2.3)$$

where $\epsilon > 0$ is a parameter used to regularize the ‘3/4’ extra term. In the $g \rightarrow 0$ limit, this model remains different from a free-theory, exactly due to the new $(3/8)\hbar^2\delta^{2s}(0)/[\phi^2(x) + \epsilon]$ interaction term.

²One requires that $\int d^d x [\nabla\phi(x)]^2 < [\int d^d x \phi^r(x)]^{2/r}$.

3. The lattice formulation of the field-theory model

We used a lattice formulation of the field theory. The theory considers a real scalar field ϕ taking the value $\phi(x)$ on each site of a periodic, hypercubic, d -dimensional lattice of lattice spacing a and periodicity na . The canonical action for the field, equation (1.1), is then approximated by

$$S[\phi] \approx \left\{ \frac{1}{2} \left[\sum_{x,\mu} a^{-2} (\phi(x) - \phi(x + e_\mu))^2 + m^2 \sum_x \phi^2(x) \right] + g \sum_x \phi^r(x) \right\} a^d, \quad (3.1)$$

where e_μ is a vector of length a in the $+\mu$ direction. The vacuum expectation of a functional observable $F[\phi]$ is

$$\langle F \rangle \approx \frac{\int F[\phi] \exp(-S[\phi]) \prod_x d\phi(x)}{\int \exp(-S[\phi]) \prod_x d\phi(x)}. \quad (3.2)$$

We will approach the continuum limit by choosing $na = 1$ fixed and increasing the number of discretizations n of each component of the space-time, so that the lattice spacing $a = 1/n \rightarrow 0^3$.

4. Simulation details and relevant observables

From each real field $\phi(x)$, we extract the Fourier transform

$$\tilde{\phi}(p) = \int d^d x e^{ip \cdot x} \phi(x), \quad (4.1)$$

with $\tilde{\phi}^*(p) = \tilde{\phi}(-p)$, so that the action of equation (1.1) becomes

$$S[\tilde{\phi}] = \int \frac{1}{2} [p^2 + m^2] |\tilde{\phi}(p)|^2 \frac{d^d p}{(2\pi)^d} + g I_r[\tilde{\phi}], \quad (4.2)$$

where we denote with I_r the power-law interaction functional.

We then find the ensemble averages $\langle \tilde{\phi}^2(0) \rangle$ and $\langle \tilde{\phi}^4(0) \rangle$ and construct the following observable (a renormalized unitless coupling constant at zero momentum),

$$g_R = \frac{3 \langle \tilde{\phi}^2(0) \rangle^2 - \langle \tilde{\phi}^4(0) \rangle}{\langle \tilde{\phi}^2(0) \rangle^2}, \quad (4.3)$$

so that clearly, using path integrals in the Fourier transform of the field, we immediately find for the canonical version of the theory,

$$g_R \xrightarrow{g \rightarrow 0} 0. \quad (4.4)$$

³Note that one could change the field $\phi \rightarrow \phi' a^{1-d/2}$ so that for example the kinetic term of the action goes to simply $\sum_{x,\mu} [\phi'(x) - \phi'(x + e_\mu)]^2 / 2$.

This remains true even for the calculation on a discrete lattice.

We then choose the momentum p with one component equal to $2\pi/na$ and all other components zero and calculate the ensemble average $\langle |\tilde{\phi}(p)|^2 \rangle$. We then construct the renormalized mass

$$m_R^2 = \frac{p^2 \langle |\tilde{\phi}(p)|^2 \rangle}{\langle \tilde{\phi}^2(0) \rangle - \langle |\tilde{\phi}(p)|^2 \rangle}. \tag{4.5}$$

When $g = 0$ the canonical version of the theory can be solved, exactly yielding

$$m_R \xrightarrow{g \rightarrow 0} [\pi/n \sin(\pi/n)]m. \tag{4.6}$$

Following Freedman *et al* [9], we will call g_R a dimensionless renormalized coupling constant and we will use it to test the ‘freedomness’ of our field theories in the continuum limit. Note that the sum-rules of equations (4.4) and (4.6) do not hold for the affine version (2.3) of the field theory due to the additional $(3/8)\hbar^2\delta^{2s}(0)/[\phi^2(x) + \epsilon]$ interaction term.

Our MC simulations use the Metropolis algorithm [6, 8] to calculate the discretized version of equation (3.2), which is a n^d multidimensional integral. The simulation is started from the initial condition $\phi = 0$. One MC step consisted in a random displacement of each one of the n^d components of ϕ as follows

$$\phi \rightarrow \phi + (\eta - 1/2)\delta, \tag{4.7}$$

where η is a uniform pseudo random number in $[0, 1]$ and δ is the amplitude of the displacement. Each one of these n^d moves is accepted if $\exp(-\Delta S) > \eta$, where ΔS is the change in the action due to the move (it can be efficiently calculated considering how the kinetic part and the potential part change by the displacement of a single component of ϕ) and rejected otherwise. The amplitude δ is chosen in such a way to have acceptance ratios as close as possible to $1/2$ and is kept constant during the evolution of the simulation. One simulation consisted of $N = 10^6$ steps. The statistical error on the average $\langle F \rangle$ will then depend on the correlation time necessary to decorrelate the property F , τ_F , and will be determined as $\sqrt{\tau_F \sigma_F^2 / (N n^d)}$, where σ_F^2 is the intrinsic variance for F , as shown in appendix B.

5. Simulation results

We first chose the Euclidean covariant scalar interaction model with $d = 3$ and $r = 12$. In its canonical version (see the action of equation (1.1)), this is a non-renormalizable model and, following a perturbation expansion of g , there is an infinite number of different, divergent terms; or, if treated as a whole, such a model collapses to a ‘free-theory’ with a vanishing interaction term [13, 14]. This is even more true for the ultralocal version of the theory.

Following Freedman *et al* [9], in our MC simulation, for each n and g , we adjusted the bare mass m in such a way to maintain the renormalized mass approximately constant $m_R \approx 3$ (for large g it was necessary to take a complex bare mass so that m^2

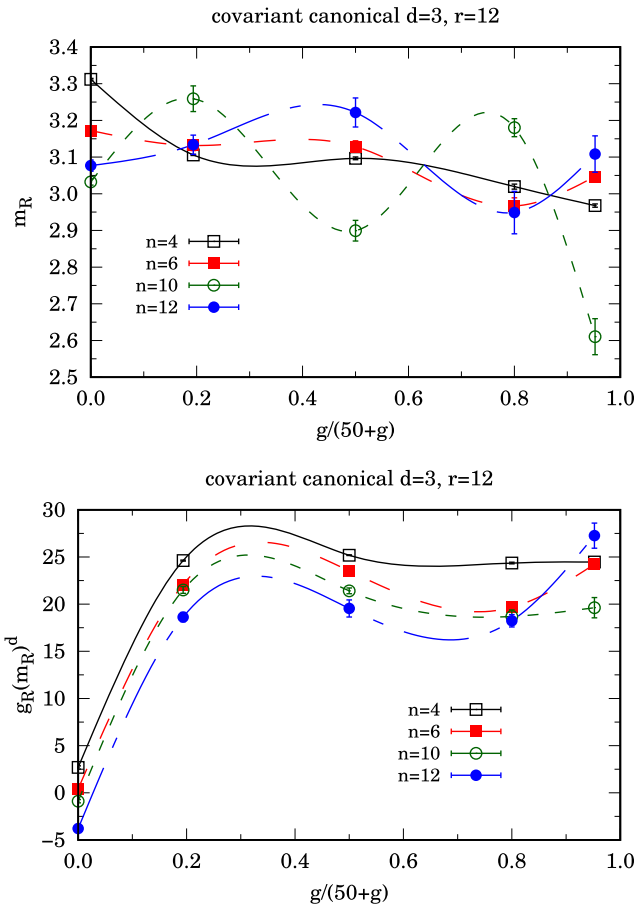


Figure 1. We show the renormalized mass m_R of equation (4.5) (top) and the renormalized coupling constant $g_R m_R^d$ of equation (4.3) (bottom) as calculated from equation (3.2) for $m_R \approx 3$ and various values of the bare coupling constant g at decreasing values of the lattice spacing $a = 1/n$ ($n \rightarrow \infty$ continuum limit) for the canonical $(\phi^{12})_3$ Euclidean scalar field theory described by the action in equation (1.1). The lines connecting the simulation points are just a guide for the eye.

was negative), to within a few percent (in all cases less than 15%), and we measured the renormalized coupling constant g_R of equation (4.3) for various values of the bare coupling constant g at a given small value of the lattice spacing $a = 1/n$. Thus, with na and m_R fixed, as a was made smaller, whatever change we found in $g_R m_R^d$ as a function of g could only be due to the change in a . We generally found that a depression in m_R produced an elevation in the corresponding value of g_R and vice-versa. The results are shown in figure 1 for the covariant version, where, following Freedman *et al* [9], we decided to compress the range of g for display by choosing the horizontal axis to be $g/(50 + g)$. As we can see from the figure the renormalized mass was made to stay around a value of 3, even if this constraint was not easy to implement, since for each n and g we had to run the simulation several (5–10) times with different values of the bare mass m .

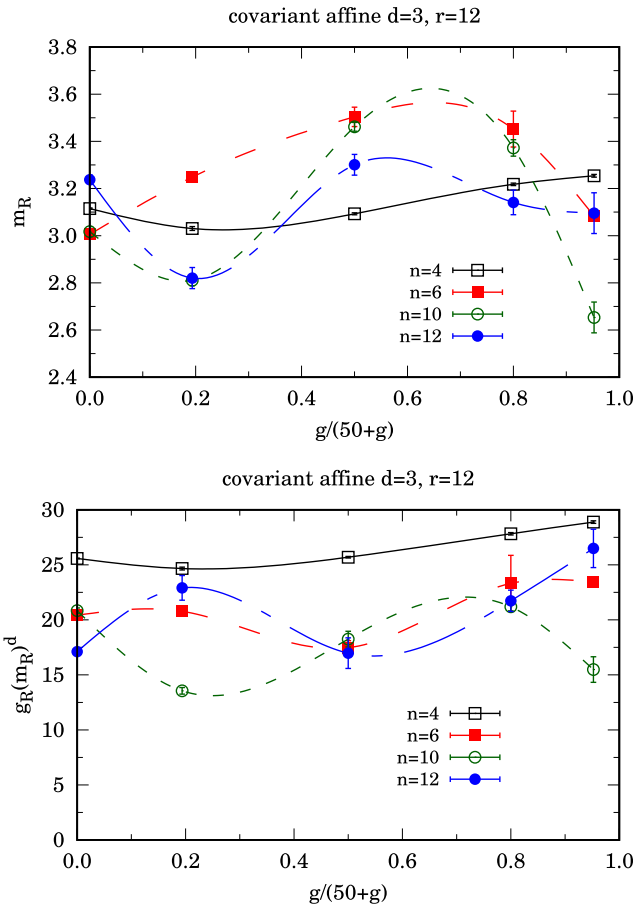


Figure 2. We show the renormalized mass m_R of equation (4.5) (top) and the renormalized coupling constant $g_R m_R^d$ of equation (4.3) (bottom) as calculated from equation (3.2) for $m_R \approx 3$ and various values of the bare coupling constant g at decreasing values of the lattice spacing $a = 1/n$ ($n \rightarrow \infty$ continuum limit) for the affine $(\phi^{12})_3$ Euclidean scalar field theory described by the action in equation (1.1). The lines connecting the simulation points are just a guide for the eye.

In figure 2, we show the same calculation but for the regularized affine field-theory (see the action of equation (2.3)), where we take $\hbar = 1$ and $\epsilon = 10^{-10}$.

From figure 1, we can see how at all finite values for the bare coupling constants g the renormalized coupling at zero momentum $g_R m_R^d$ appears to move to zero uniformly as the lattice spacing gets small, for $n \rightarrow \infty$. This numerically suggests that the canonical theory becomes asymptotically a free-theory in the continuum limit of large n , which is in agreement with the well known theoretical results [2–4]. This does not happen for the affine theory as shown in figure 2, where the renormalized coupling of the theory stays far from zero in the continuum limit for all values of the bare coupling constant.

6. Conclusions

Using MC simulations, we determined the dimensionless renormalized coupling constant of a Euclidean classical scalar field-theory with twelfth-order power-law interactions on a three-dimensional lattice. Our results for the canonical version of the theory are consistent with a noninteracting continuum limit. The renormalized coupling constant tends to zero at each finite value of the bare coupling constant as the lattice spacing gets small.

We then formulated an affine version of the same field-theory with the ‘3/4’ interaction term and observed that the MC results for the renormalized coupling constant stays far from zero for all values of the bare coupling constant as the lattice spacing diminishes. This means that the affine model remains a well-defined interacting model in the continuum limit.

A classical model, such as $(\phi^{12})_3$ with a positive coupling constant, has a natural behavior, while it becomes a free-theory with a positive coupling constant using canonical quantization. Canonical quantization also fails for a half-harmonic oscillator, e.g. $0 < q < \infty$ as well. Affine quantization solves both of these problems. There is a genuinely new procedure that permits various problem models to achieve a proper quantization. Affine quantization just selects different classical variables to promote to operators, and then it proceeds just like canonical quantization thereafter.

The present paper shows that the model $(\phi^{12})_3$ also generates a nontrivial behavior with an affine quantization. It is designed to feature a region where canonical quantization fails and there is a new procedure that can help. The classical limit of this quantized model leads back to a classical model with a positive coupling constant. That does not happen for canonical quantization. This implies that while canonical quantization is good for some models, affine quantization is needed for other models.

There are many other models that canonical quantization cannot solve, or struggle to quantize, that may be possible to quantize using affine quantization. Some of those models may be useful to specific problems in present-day high energy physics.

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Appendix A. The origin of the ‘3/4’ extra term

The operator corresponding to the affine field κ will be the dilation operator $\hat{\kappa} = (\hat{\pi}\hat{\phi} + \hat{\phi}\hat{\pi})/2$, where the regularized basic quantum Schrödinger operators are given by $\hat{\phi}(x) = \phi(x)$ and $\hat{\pi}(x) = -i\hbar\delta_{\phi(x)} = -i\hbar\delta/\delta\phi(x)$ so that the commutator $[\hat{\phi}(x), \hat{\pi}(y)] = i\hbar\delta^s(x-y)$, where $\delta^s(x)$ is a s -dimensional Dirac delta function since $\delta_{\phi(x)}\phi(y) = \delta^s(x-y)$. Multiplying this by $\hat{\phi}$, we find $[\hat{\phi}, \hat{\phi}\hat{\pi}] = [\hat{\phi}, \hat{\pi}\hat{\phi}] = [\hat{\phi}, \hat{\kappa}] = i\hbar\delta^s\hat{\phi}$,

which is only valid for $\phi \neq 0$. Then $\widehat{\kappa} = -i\hbar\{\delta_{\phi(x)}[\phi(x)] + \phi(x)\delta_{\phi(x)}\}/2 = -i\hbar\{\delta^s(0)/2 + \phi(x)\delta_{\phi(x)}\}$. Now, for $\phi(x) \neq 0$, we will have that affine quantization sends $\widehat{\pi}^2(x)$ to

$$\begin{aligned} \widehat{\kappa}(x)\phi^{-2}(x)\widehat{\kappa}(x) &= -\hbar^2\{\delta^s(0)/2 + \phi(x)\delta_{\phi(x)}\}\phi^{-2}(x)\{\delta^s(0)/2 + \phi(x)\delta_{\phi(x)}\} \\ &= -\hbar^2\{\delta^{2s}(0)\phi^{-2}(x)/4 + \delta^s(0)\phi(x)\delta_{\phi(x)}[\phi^{-2}(x)]/2 \\ &\quad + \delta^s(0)\phi^{-1}(x)\delta_{\phi(x)}/2 \\ &\quad + \delta^s(0)\phi^{-1}(x)\delta_{\phi(x)}/2 - \delta^s(0)\phi^{-1}(x)\delta_{\phi(x)} + \delta_{\phi(x)}^2\} \\ &= -\hbar^2\{\delta^{2s}(0)\phi^{-2}(x)/4 - 2\delta^{2s}(0)\phi^{-2}(x)/2 + \delta_{\phi(x)}^2\} \\ &= \hbar^2(3/4)\delta^{2s}(0)\phi^{-2}(x) - \hbar^2\delta_{\phi(x)}^2 \\ &= \hbar^2(3/4)\delta^{2s}(0)\phi^{-2}(x) + \widehat{\pi}^2(x). \end{aligned} \tag{A1}$$

We then see the appearance of an extra ‘3/4’ potential term. The lattice version of such a term will then be

$$\hbar^2(3/4)a^{-2s}\phi^{-2}(x) \tag{A2}$$

where a is the lattice spacing.

Appendix B. Error analysis in the simulation

Let F be a given property and let its value at step k of the random walk be F_k . Let the mean and intrinsic variance of F be denoted by

$$\bar{F} = \langle F_k \rangle = \frac{1}{P} \sum_{k=1}^P F_k \tag{B1}$$

and

$$\sigma_F^2 = \langle (F_k - \bar{F})^2 \rangle. \tag{B2}$$

These quantities depend only on the distribution $e^{-S}/\int e^{-S}$, not on the MC procedure. We can show that the standard error of the estimate of the average, \bar{F} , over a Markov chain with P steps, is

$$\text{error}[\bar{F}] = \sqrt{\left\langle \left(\frac{1}{P} \sum_{k=1}^P F_k - \frac{1}{P} \sum_{k=1}^P \bar{F} \right)^2 \right\rangle} = \sqrt{\frac{\sigma_F^2 \tau_F}{P}}, \tag{B3}$$

where τ_F is the correlation time that can be estimated as follows:

$$\tau_F \approx 1 + 2 \sum_{k=1}^P \frac{\langle (F_0 - \bar{F})(F_k - \bar{F}) \rangle}{\sigma_F^2}, \tag{B4}$$

and it gives the average number of steps to decorrelate the property F . The correlation time will depend crucially on the transition rule and has a minimum value of 1 if one can move so far in the configuration space that successive values are uncorrelated. In general, the number of independent steps that contribute to reducing the error bar from equation (B3) is not P but P/τ .

Hence, to determine the true statistical error in a random walk, one needs to estimate the correlation time. To do this, it is very important that the total length of the random walk be much greater than τ_F . Otherwise, the result and the error will be unreliable. Runs in which the number of steps is $P \gg \tau_F$ are called well-converged. In general, there is no mathematically rigorous procedure to determine τ . Usually one must determine it from the random walk. It is a good practice occasionally to run very long runs to test that the results are well-converged.

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