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Kinetic factors in affine quantization and their role in field theory Monte Carlo

Riccardo Fantoni*

Università di Trieste, Dipartimento di Fisica,
Strada Costiera 11, 34151 Grignano (Trieste), Italy
riccardo.fantoni@posta.istruzione.it

John R. Klauder

Department of Physics and Department of Mathematics
University of Florida, Gainesville, FL 32611-8440, US
klauder@ufl.edu

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Affine quantization, which is a parallel procedure with canonical quantization, needs to use its principal quantum operators, most simply $D = (PQ + QP)/2$ and $Q \neq 0$, to represent appropriate kinetic factors, normally P^2, which involve only one canonical quantum operator. The need for this requirement stems from the quantization of selected problems that require affine quantization to achieve valid Monte Carlo results. This task is resolved for introductory examples as well as examples that involve scalar quantum field theories.

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1. Introduction

In our previous papers, where some suitable Monte Carlo (MC) calculations have been reported, it was established that the quantum procedure called affine quantization (AQ) finds "nonfree" results for the model φ_4^4,[1,2] while identical studies, which used canonical quantization (CQ), have only found "free" results, as if the coupling constant had been zero.[3–7] After a careful comparison between the procedures of both CQ and AQ, a detailed MC study of the model $(\varphi^2 - \Phi^2)_4^2$ is

*Corresponding author.

presented. While the differences between AQ and CQ for the first model are significant, the differences between AQ and CQ for the second model are much smaller, and a detailed study has found the reason why that could happen. Even if the AQ and CQ results for the second model are rather close, only one of those results can be physically correct.

A general effort to transform a variety of affine expressions opens up a variety of problems regarding their interaction terms and our present work was designed to do just that.

MC studies are greatly simplified by transforming affine variables back into canonical variables, so the π^2 can join $(\sum_j d\varphi/dx_j)^2$ and imaginary time, to ensure a vast simplification of the MC work. Such a transformation from affine to equivalent canonical variables being required to achieve nontrivial results.

2. Some Relations Involving the Quantum Operators P, Q, and D

We need $[Q,P] = i\hbar\mathbb{1}$, $F = F(Q) \neq 0$, and we define $D = [PF + FP]/2$, so that $P^\dagger F = PF$.[a] Then we examine

$$\begin{aligned} 2[F,D] &= F(PF+FP) - (PF+FP)F \\ &= FPF + FFP - PFF - FPF = FFP - PFF = [F^2, P]. \end{aligned} \tag{1}$$

This leads to $[F,D] = [F^2,P]/2 = i\hbar(F^2)'/2$, where the prime denotes a derivative with respect to Q. As a familiar example, choose $F(Q) = Q$, then $[Q,D] = [Q^2,P]/2 = i\hbar\,(Q^2)'/2 = i\hbar\,Q$, analogues to the Lie algebra of the affine group,[8] and from which AQ got its name.

3. The Kinetic Factor in Hamiltonians

In simple problems, the most commonly chosen classical kinetic factor is p^2. In that realm, we can choose $f(q) = 1/g(q) \neq 0$ ($g(q) \neq 0$ is added because $1/f(q)$ is very often used). Now we define $d = pf(q)$ and we then recover p^2 from $d^2g^2 = d^2/f^2 = p^2$. Admittedly, this is utterly trivial. However, when we quantize these variables to P, $D = (PF+FP)/2$, $F = F(Q) \neq 0$ and $G = G(Q) = 1/F(Q) \neq 0$, difficulties can arise.

The quantum kinetic term (with $\hbar = 1$) in affine variables is DG^2D. This expression, helped by $FP - PF = i\,F'$ and $GP - PG = i\,G'$, leads to

$$\begin{aligned} 4DG^2D &= (PF+FP)GG(PF+FP) \\ &= PP + FPGGPF + FPGP + PGPF \\ &= PP + (PF+iF')GG(FP-iF') + (PF+iF')GP + PG(FP-iF') \end{aligned}$$

[a]As AQ permits, the dilation operator, D, may take different forms, namely, $D = [PF(Q) + F(Q)P]/2$, for a variety of $F(Q) \neq 0$ functions — chosen such that $P^\dagger F(Q) = PF(Q)$ — and which are of assistance in solving various problems.

$$= 4PP + 2i(F'GP - PGF') + F'GGF'$$
$$= 4PP - 2(F'G)' + (F')^2G^2. \tag{2}$$

Restoring $\hbar$, it follows that

$$DG^2D = P^2 + (1/4)\hbar^2[(F')^2G^2 - 2(F'G)']. \tag{3}$$

As a check on this expression, the example in which $F(Q) = Q$ and thus $G(Q) = 1/Q$, leads to $P^2 + (3/4)\hbar^2/Q^2$, which is the result previously found when $F(Q) = Q$. There is every reason to accept this latter equation as the proper kinematical operator for the half-harmonic oscillator.[9–11]

4. Application to Some Field Theory Examples

4.1. *A straightforward example for φ_n^p*

Regarding our field theory examples, our procedures will naturally encounter $\delta(0)$ divergences. A scaling procedure that eliminates such divergences will be introduced as well as illustrated. As our fist example, we choose the classical canonical kinematic field $\pi(x)^2$, for which we choose the dilation field $\kappa(x) = \pi(x)\varphi(x)$, with $\varphi(x) \neq 0$. The classical Hamiltonian in affine variables is

$$H_1 = \int \left\{ \frac{1}{2}[\kappa(x)^2/\varphi(x)^2 + (\nabla\varphi(x))^2 + m^2\varphi(x)^2] + g\,\varphi(x)^p \right\} d^s x, \tag{4}$$

where $p = 4, 6, 8, \ldots$ is the interaction power and $n = s + 1$ is the number of space–time dimensions. The advantage of this pair of variables is that $0 < \varphi(x)^{-2} < \infty$ which implies that $0 < \varphi(x)^p < \infty$, for all p, and thus the Hamiltonian does not experience any non-renormalizability.

Adopting the message from the half-harmonic oscillator, the affine quantum Hamiltonian for this model is

$$\mathcal{H}_1 = \int \left\{ \frac{1}{2}[\hat{\kappa}(x)(\hat{\varphi}(x))^{-2}\hat{\kappa}(x) + (\nabla\hat{\varphi}(x))^2 + m^2\hat{\varphi}(x)^2] + g\,\hat{\varphi}(x)^p \right\} d^s x, \tag{5}$$

where

$$\hat{\kappa}(x)(\hat{\varphi}(x)^{-2})\hat{\kappa}(x) = \hat{\pi}(x)^2 + (3/4)\hbar^2\delta(0)^{2s}/\varphi(x)^2. \tag{6}$$

The origin of $\delta^s(0) = \infty$ is simply the fact that $[\hat{\varphi}(x), \hat{\pi}(x)] = i\hbar\,\delta^s(0)\mathbb{1}$.

In a sense, this result is strange. For example, for a single classical variable $(pq)^2 < \infty$ and $|QP - PQ|^2 = \hbar^2\mathbb{1}$. However, for a classical field $(\pi(x)\,\varphi(x))^2 < \infty$ while $|\hat{\varphi}(x)\,\hat{\pi}(x) - \hat{\pi}(x)\,\hat{\varphi}(x)|^2 = \infty\,\hbar^2\mathbb{1}$. When approximated, as for an integration, then $\hat{\varphi}(x) \to \hat{\varphi}_k$ and $\hat{\pi}(x) \to \hat{\pi}_k$, where instead of the continuum that x represents, k identifies different points on a discrete lattice. This leads to $[\hat{\varphi}_k, \hat{\pi}_k] = i\hbar\,a^{-s}\mathbb{1}$, where a is a tiny spatial distance between neighboring lattice points. In preparation for our integration, just as every integral involves a continuum limit of an appropriate summation, these expressions are used in MC calculations which involve proper sums for their "integrals". All of these are designed to provide a path integral

quantization, and, when necessary, their sums need to be regularized. In our case, the regularized version becomes appropriately "scaled": specifically $\varphi_k \to a^{-s/2}\varphi_k$, $\pi_k \to a^{-s/2}\pi_k$, $\kappa_k \to a^{-s}\kappa_k$, $g \to a^{s(p-2)/2}\, g$, and the regularized $d^s x \to a^s$ may also be scaled as $a^s \to a^{2s}$.

Using such scaling, in an AQ formulation with MC, has led to a "nonfree" result for the scalar field φ^4_4.[1] However, a CQ formulation with MC, along with analytic studies, has led to a "free" result.[1,3–7]

4.2. *A less common example using CQ and AQ*

With first using CQ for the next example, our next classical Hamiltonian is given by

$$H_2 = \int \left\{ \frac{1}{2}[\pi(x)^2 + (\nabla\varphi(x))^2 + m^2\varphi(x)^2] + g\,(\varphi(x)^2 - \Phi^2)^r \right\} d^s x, \tag{7}$$

where the interaction power has been changed to $r = 2, 4, 6, \ldots$, and $n = s + 1$ is the same as before. This unusual interaction term deserves a new dilation variable,[b] and in this section we choose $\kappa(x) = \pi(x)\,(\varphi(x)^2 - \Phi^2)$, where $(\varphi(x)^2 - \Phi^2) \neq 0$. In this case, the classical Hamiltonian in affine variables becomes

$$\begin{aligned} H_3 = \int \Big\{ & \frac{1}{2}[\kappa(x)^2/(\varphi(x)^2 - \Phi^2)^2 + (\nabla\varphi(x))^2 + m^2\varphi(x)^2] \\ & + g\,(\varphi(x)^2 - \Phi^2)^r \Big\} d^s x. \end{aligned} \tag{8}$$

In these variables, $0 < (\varphi(x)^2 - \Phi^2)^{-2} < \infty$, which implies that $0 < (\varphi(x)^2 - \Phi^2)^r < \infty$, for all r, thereby eliminating any non-renormalizablity.

Next we find that the quantum Hamiltonian, using affine variables and Schrödinger's representation, is given by

$$\begin{aligned} \mathcal{H}_3 = \int \Big\{ & \frac{1}{2}[\hat{\kappa}(x)(\varphi(x)^2 - \Phi^2)^{-2}\hat{\kappa}(x) + (\nabla\varphi(x))^2 + m^2\varphi(x)^2] \\ & + g\,(\varphi(x)^2 - \Phi^2)^r \Big\} d^s x, \end{aligned} \tag{9}$$

and this expression will become more useful after the kinetic term is fully analyzed. In order to obtain a valid quantum Hamiltonian for this model, we are first drawn back to Eq. (3) in Sec. 2, which reads $DG^2D = P^2 + (1/4)\hbar^2[(F')^2G^2 - 2(F'G)']$. In the present case, temporally ignoring (x) and still using Schrödinger's representation, $F = (\varphi^2 - \Phi^2)$ and $G = 1/F$. It follows, that $F' = 2\varphi$ and $G' = -2\varphi/(\varphi^2 - \Phi^2)^2$. We also need $(F')^2G^2 = 4\varphi^2/(\varphi^2 - \Phi^2)^2$ and $-2(F'G)' = -4/(\varphi^2 - \Phi^2) + 8\varphi^2/(\varphi^2 - \Phi^2)^2 = 4(\varphi^2 + \Phi^2)/(\varphi^2 - \Phi^2)^2$. Hence, for this model, the kinematic factor is

$$\begin{aligned} & \hat{\kappa}(x)(\varphi(x)^2 - \Phi^2)^{-2}\hat{\kappa}(x) \\ & \quad = \hat{\pi}(x)^2 + \hbar^2\delta^{2s}(0)(2\varphi(x)^2 + \Phi^2)/(\varphi(x)^2 - \Phi^2)^2. \end{aligned} \tag{10}$$

[b]Being able to change the dilation variable is an important feature of AQ.

As was the case in Sec. 3.1, scaling can eliminate the $\delta^{2s}(0)$ factor by including the additional scaling factor $\Phi^2 \to a^{-s}\Phi^2$, and changing the scaling of g to $g \to a^{s(r-1)}g$.

5. Lattice Formulation of the Field Theory

We used a lattice formulation of the AQ field theory stemming from the Hamiltonian of Eq. (9) for $r = 2$ and $s = 3$ using the scaling $\varphi \to a^{-s/2}\varphi, \Phi \to a^{-s/2}\Phi, g \to a^s g$ already employed in Refs. 2, 12, 13. The theory considers a real scalar field φ taking the value φ_k on each site of a periodic, hypercubic, n-dimensional lattice of lattice spacing a, our ultraviolet cutoff, and periodicity $L = Na$. Using the usual classical expression $\pi = d\varphi/dt$, where t is imaginary time, for the momentum field, the affine action, $S = \int \mathcal{H}_3\, dx_0$, with $x_0 = ct$ where c is the speed of light constant, is then approximated on the lattice by

$$S[\varphi]/a^{n-s} \approx \frac{1}{2}\left\{\sum_{k,\mu} a^{-2}(\varphi_k - \varphi_{k+e_\mu})^2 + m^2 \sum_k \varphi_k^2\right\} + \sum_k g\,(\varphi_k^2 - \Phi^2)^2 + \frac{1}{2}\sum_k \hbar^2 \frac{2\varphi_k^2 + \Phi^2}{(\varphi_k^2 - \Phi^2)^2}, \tag{11}$$

where e_μ is 1 in the $+\mu$ direction and 0 else. This is known as the *primitive approximation* for the action and could be improved in various ways.[14] For the CQ field theory, the last term in (11), proportional to $\hbar^2$ should be dropped.

In this work, we are interested in reaching the continuum limit by taking Na fixed and letting $N \to \infty$ at fixed volume L^s and absolute temperature $T = 1/k_B L$ with k_B the Boltzmann's constant. We will always work in natural units $c = \hbar = k_B = 1$.

6. PIMC Results

We performed path integral MC[14–17] calculation for the AQ field theory described by Eq. (11) for $n = 3 + 1$ and $\Phi = 1$, and compared it with the corresponding CQ field theory. In particular, we calculated the renormalized coupling constant g_R (which must be non-negative due to Lebowitz inequality) and mass m_R defined in Eqs. (4.3) and (4.5) of,[18] respectively. This will allow us to explore the behavior of the renormalized system, for a given set of parameters m, g, as a function of N at fixed volume and temperature.

Following Freedman *et al.*,[3] for each N and g, we adjusted the bare mass m in such a way to maintain the renormalized mass approximately constant $m_R \approx 3$ to within a few percent (in all cases less than 25%). Differently from our previous study[1] with the unscaled version of the affine field theory we did not need to choose complex m in order to fulfill this constraint, as shown in Table 1. In fact, our present CQ model can be obtained from the φ_4^4 model studied in Ref. 1 by changing $m^2 \to m^2 - 4g\Phi^2 \equiv M^2$ which will become negative for g big enough. From the

Table 1. Choice of the bare mass m in the simulations for CQ and AQ cases. Also shown is $M^2 = m^2 - 4g\Phi^2$ and $m^2/4g\Phi^2$.

		CQ			AQ		
N	g	m	M^2	$m^2/4g\Phi^2$	m	M^2	$m^2/4g\Phi^2$
4	12	7.00	1.000	1.021	6.65	−3.777	0.921
	50	13.70	−12.31	0.938	13.55	−16.397	0.918
	200	27.20	−60.16	0.925	27.10	−65.590	0.918
	1000	61.25	−248.438	0.938	61.20	−254.56	0.936
6	12	7.20	3.840	1.080	6.80	−1.76	0.963
	50	14.00	−4.000	0.980	13.75	−10.937	0.945
	200	27.50	−43.750	0.945	27.40	−49.240	0.938
	1000	61.57	−209.135	0.948	61.53	−214.059	0.946
10	12	7.40	6.760	1.141	7.00	1.000	1.021
	50	14.20	1.640	1.008	14.00	−4.000	0.980
	200	27.80	−27.160	0.960	27.80	−27.160	0.960
	1000	62.10	−143.590	0.964	62.00	−156.000	0.961
12	12	7.40	6.760	1.141	7.30	5.29	1.110
	50	14.20	1.640	1.008	14.20	1.640	1.008
	200	27.90	−21.590	0.973	27.90	−21.590	0.973
	1000	62.20	−131.160	0.936	62.20	−131.160	0.936
15	12	7.40	6.760	1.141	7.40	6.760	1.141
	50	14.40	7.36	1.037	14.20	1.640	1.008
	200	28.10	−10.390	0.987	27.90	−21.590	0.973
	1000	62.40	−106.240	0.973	62.40	−106.240	0.973

table, we can see how for the chosen cases $m^2/4g \sim \Phi^2$, meaning that the minima $\varphi_\pm = \pm\sqrt{-M^2/4g}$ of the potential profile $\mathcal{V}[\phi] = m^2\varphi^2/2 + g\,(\varphi^2 - \Phi^2)^2$ are far from $\pm\Phi$, where the effective potential term, $(2\varphi^2 + \Phi^2)/2(\varphi^2 - \Phi^2)^2$, stemming from the kinetic part of the action (the last term in Eq. (11) proportional to $\hbar^2$) diverges. As a consequence, CQ will be very similar to AQ, which means that the required bare masses to reach a given renormalized mass in the two cases are very close. Then we measured the renormalized coupling constant g_R defined in Refs. 1, 18 for various values of the bare coupling constant g at a given small value of the lattice spacing $a = 1/N$ (this corresponds to choosing a fixed absolute temperature $k_BT = 1$ and a fixed volume $L^3 = 1$) as already explained for example in Refs. 1, 18. With Na and m_R fixed, as a was made smaller, whatever change we found in $g_R m_R^n$ 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 Fig. 1 for the scaled affine action (AQ case) (11), where, following Freedman *et al.*[3] we decided to compress the range of g for display, by choosing the horizontal axis to be $g/(50 + g)$. For comparison we also show in Fig. 2 the results for canonical quantized action (CQ case) which is given by Eq. (11) without the last term proportional to $\hbar^2$. The constraint $m_R \approx 3$ 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 in order to determine

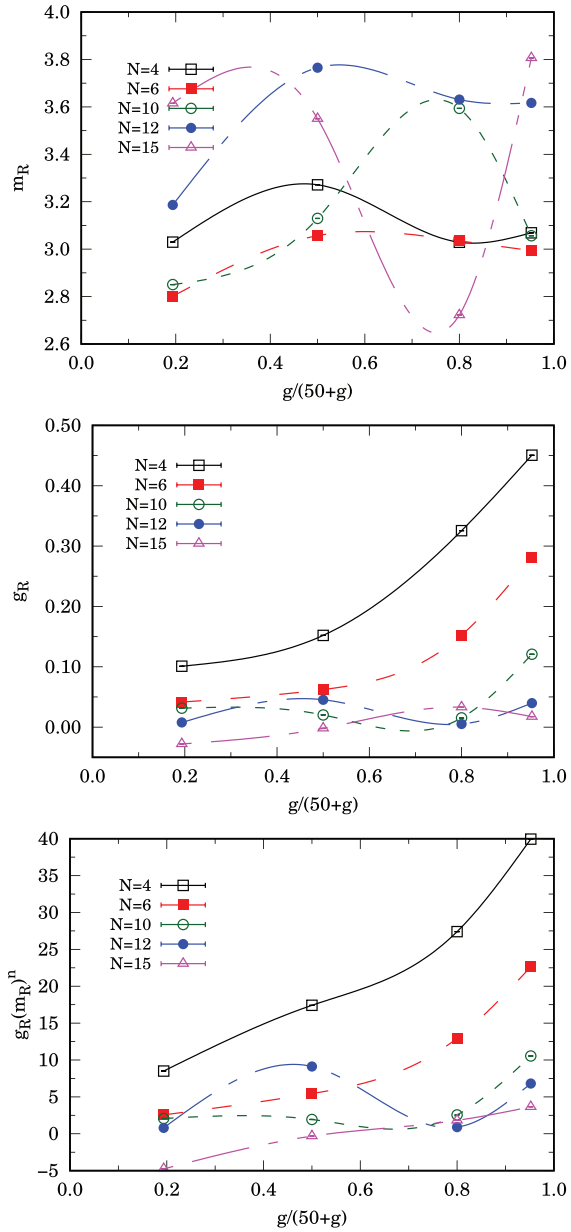

Fig. 1. AQ case. We show the renormalized mass $m_R \approx 3$ (top panel), the renormalized coupling constants g_R (central panel), and $g_R m_R^n$ (bottom panel) for various values of the bare coupling constant g at decreasing values of the lattice spacing $a = 1/N$ ($N \to \infty$ continuum limit) for the *scaled affine* covariant Euclidean scalar field theory described by the lattice action of Eq. (11) for $n = 3 + 1$ and $\Phi = 1$. The lines connecting the simulation points are just a guide for the eye. The lack of error bars in the data presented is justified by the fact that the errors are dominated not from the statistical ones but rather from the ones due to the adjustments in the bare mass required by the trial and error procedure suggested by Freedman *et al.*[3] This error is very hard to be estimated.

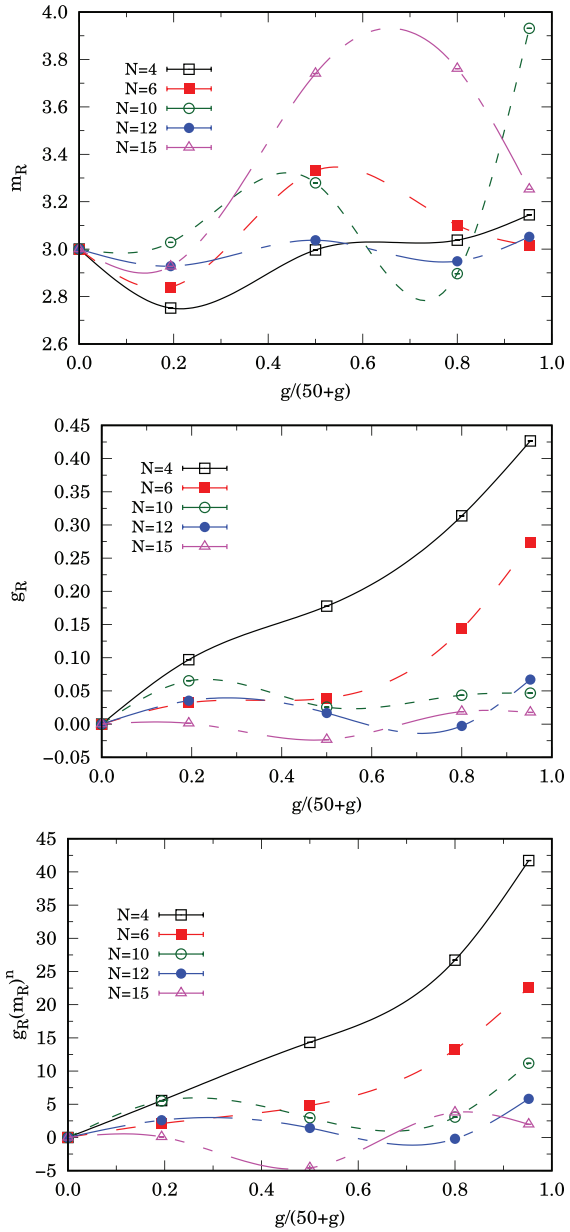

Fig. 2. CQ case. We show the renormalized mass $m_R \approx 3$ (top panel), the renormalized coupling constants g_R (central panel), and $g_R m_R^n$ (bottom panel) for various values of the bare coupling constant g at decreasing values of the lattice spacing $a = 1/N$ ($N \to \infty$ continuum limit) for the *canonical* covariant Euclidean scalar field theory described by the lattice action of Eq. (11) without the last term proportional to $\hbar^2$, for $n = 3 + 1$ and $\Phi = 1$. The lines connecting the simulation points are just a guide for the eye. The lack of error bars in the data presented is justified by the fact that the errors are dominated not from the statistical ones but rather from the ones due to the adjustments in the bare mass required by the trial and error procedure suggested by Freedman *et al.*[3] This error is very hard to be estimated.

the value which would satisfy the constraint $m_R \approx 3$. In our simulations we always used 3×10^7 MC sweeps (where one sweep moves all the N^n field points which took about one week of computer time for the $N = 15$ case). We estimated that it took roughly 10% of each run in order to reach equilibrium from the arbitrarily chosen initial field configuration, for each set of parameters.

As we can see from our figures, the renormalized coupling constant $g_R(m_R)^4$ of the scaled affine version (AQ of Fig. 1) behaves very similarly to the one of the canonical version (CQ of Fig. 2) going toward the continuum limit, taken at fixed volume and temperature, when the ultraviolet cutoff is gradually removed ($Na = 1$ and $N \to \infty$). The only difference is at $g = 50 - 100$ where in the AQ case the $N = 12$ results for the renormalized coupling fall above the ones for $N = 10$, unlike what happens in the CQ case. Note that for the CQ case the results at $N = 12, 15$ are new, since Freedman *et al.*[3] and ourselves[1] only previously studied up to $N = 10$ discretization points.

During our simulations, we kept under control also the vacuum expectation value of the field which is not diverging going toward the continuum limit, like what was happening in Ref. 12 but not in Ref. 19. Choosing the initial configuration with $\varphi = 0$ at all lattice points, when M^2 is not too negative the symmetry $\varphi \to -\varphi$ is not broken and we find $\langle\varphi\rangle \sim 0$.

We also studied the behavior of the AQ case when choosing a much lower renormalized mass $m_R \sim 1/10$. In this case, the necessary bare mass is such that $m^2/4g \ll \Phi^2$, at all studied values of the bare coupling $g = 12, 50, 200, 1000$. In particular, the potential profile $\mathcal{V}$ becomes a symmetric double well with the two minima, at $\varphi_\pm$, near the two repulsive spikes localized at $\varphi = \pm\Phi$ and forbidding paths to access the minima of the double well.[c] In this case, we found that the paths tend to be very localized just outside of the forbidden region due to the repulsive spikes. As a consequence, we found $g_R \sim 2$ for all N. So in this case, AQ is very different from CQ and the bare masses necessary to reach the same renormalized mass are very different. Note that when $M^2 > 0$ the two repulsive spikes do not forbid the path from sitting at the minimum of the potential profile at $\varphi = 0$ and as a consequence AQ and CQ are very similar. Note also that in the limit $\Phi \to 0$ the situation is inverted and for m^2 positive, AQ is very different from CQ, whereas for m^2 negative, AQ is very similar to CQ.

7. Conclusions

We studied through path integral MC a plausible kinetic factor in AQ of a scalar covariant Euclidean field theory of mass m subject to a potential energy of the form $g(\varphi^2 - \Phi^2)^2$ in $3 + 1$ space–time dimensions, which is known to suffer from asymptotic freedom in the continuum limit when it is quantized through CQ. This

[c]The case when the classical minima of the potential and the extra spikes in the potential of the affine Hamiltonian are close together has been already studied in several of our previously published papers.[1,2,13,18,20]

kinetic factor reduces to the usual one previously introduced in Refs. 1, 2, 12, 13, 18, 19 in the limit $\Phi \to 0$, apart from the multiplicative coefficient. Moreover, its behavior is similar to the one found in the $\Phi \to 0$ limit in the sense that it gives rise to an additive effective potential term which diverges in a neighborhood of the minima in the potential therefore producing a forbidden region for the field paths exactly where it would naturally sit in a CQ framework. This exclusion of the field path from the minima of the potential renders the AQ version of the field theory asymptotically non-free in the continuum limit.

Our numerical results clearly show how the two field theories obtained through CQ and AQ behave very differently whenever $m^2/4g \ll \Phi^2$. Otherwise they are very similar.

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