Wilson’s Momentum Shell Renormalization Group from Fourier Monte Carlo Simulations

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Abstract

Previous attempts to accurately compute critical exponents from Wilson’s momentum shell renormalization prescription suffered from the difficulties posed by the presence of an infinite number of irrelevant couplings. Taking the example of the 1d long-ranged Ising model, we calculate the momentum shell renormalization flow in the plane spanned by the coupling constants \((t_0, r_0)\) for different values of the momentum shell thickness parameter \(b\) by simulation using our recently developed Fourier Monte Carlo algorithm. We report strong anomalies in the \(b\)-dependence of the fixed point couplings and the resulting exponents \(\gamma\) and \(\omega\) in the vicinity of a shell parameter \(b^* < 1\) characterizing a thin but finite momentum shell. Evaluation of the exponents for this value of \(b\) yields a dramatic improvement of their numerical accuracy, indicating a strong damping of the influence of irrelevant couplings for \(b = b^*\).

1. Wilson’s Momentum Shell Renormalization Group: A Reminder

Recall that – in a nutshell – a general momentum shell renormalization group (MSRG) transformation is a mapping \(R(t,b) : \mathcal{K} \to \mathcal{K}\) induced by [1, 2]

1. coarse graining,
2. rescaling of lengths/momenta, and
3. renormalization of field(s),

on the infinite-dimensional space \(\mathcal{K} = (K_0, K_1, K_2, \ldots)\) of coupling constants of a given model. In the following we will frequently deal with the parameter \(b > 1\) measuring the “thickness” of the “momentum shell” \(\Lambda/b < |k| < \Lambda\) at fixed cutoff \(\Lambda\), which is therefore indicated explicitly in our notation.

Nontrivial critical behavior is connected to fixed points (FPs) \(\mathcal{K}^0 \equiv \mathcal{K}^*\) of \(\mathcal{R}(t,b)\) corresponding to a correlation length \(\xi(K^*) = \infty\). Linearizing around such an FP, one obtains a matrix equation \(\delta K_i = \sum_j M_{ij}[K] \delta K_j + O(\delta K^2)\) where \(\delta K = K - K^*\), and the eigenvalues \(\lambda_i\) of \(M_{ij}[K^*] = \frac{\partial R(k,b)}{\partial \bar{K}_i} \bigg|_{K=K^*}\), are related to universal critical exponents \(y_i\) by \(\lambda_i \equiv b^{y_i}\). These are termed relevant, irrelevant and marginal if \(y_i > 0, y_i < 0\) or \(y_i = 0\), respectively.

In what follows, we will focus on a subject which is usually not regarded to be of any importance, namely the effect of choosing a particular value for the parameter \(b\). In fact, all universal quantities as well as \(K^*\) should be independent of such a choice in a (hypothetical) exact calculation. In analytical \(\epsilon\)-expansion calculations, choosing \(b \sim 1 + \delta\) for infinitesimal \(\delta > 0\) is usually computationally convenient. However, what is usually swept under the rug is that in a real world computation, where truncations and approximations are unavoidable, exact invariance with respect to the choice of \(b\) may be broken (cf. an early analysis of this situation in Ref. [3, 4]). We thus raise the following question: “What is the qualitative as well as the quantitative influence of a concrete choice of \(b\) on the results obtained from the MSRG?”

In an analytic approach, there is little hope to answer this question. To make progress, we thus have to resort to simulations.

2. RG Flows From Fourier Monte Carlo Simulations

In recent papers [5, 6] we presented a new simulation method that in principle allows to non-perturbatively calculate renormalization group (RG) flows and its fixed points in the space \(\mathcal{K}\) for Wilson’s MSRG scheme. These as well as the present simulations are based on our recently developed Fourier Monte Carlo (FMC) algorithm. This method, which allows to work exclusively in reciprocal space and thus avoid any reference to real space, is tailor-made for studying coarse graining and criticality for \(\varphi^4\) type models. It is based on the following observations and ideas (see [7, 8, 9, 10] for details):

In FMC, the real and imaginary parts of the discrete Fourier amplitudes \(\tilde{\varphi}(k) = N^{-1/2} \sum_x \varphi(x) e^{-ikx}\) of lattice fields \(\varphi(x)\) act as the basic MC variables. MC moves are constructed by picking a particular wave vector \(k_0\) at random and shifting the associated Fourier amplitude according to

\[
\tilde{\eta}(k) \to \tilde{\eta}(k) + \xi \tilde{\varphi}_k \xi_{-k} \tilde{\varphi}_0
\]

As the harmonic part is always diagonalized by Fourier transform, it is easy to keep track of the change of this contribution to any \(\varphi^4\) type of Hamiltonian under this move. The central observation [11] leading to an efficient and manageable MC algorithm for \(\varphi^4\) type models is that the remaining anharmonic part \(- \sum_x \varphi^3(x) = \sum_x (\varphi^2(x))^2\) can also be diagonalized – not in terms of the original Fourier amplitudes, but in terms of the Fourier amplitudes \(\tilde{\varphi}^2(k) = N^{-1/2} \sum_p \tilde{\varphi}(p) \tilde{\varphi}(k-p)\) of the squared field \(\varphi^2(x)!\) Additional recording and smart bookkeeping of these quadratic modes and their changes under shifts...
of type (1) of the basic modes \( \tilde{\eta}(k) \) during the course of the simulation thus leads to a manageable algorithm that succeeds in avoiding any reference to the original lattice.

While this strategy may be quite inefficient for studying problems in lattice systems for which all Fourier modes of fields have to be fully included, it can out–power other approaches in situations where one concentrates on a small subset of Fourier modes, while all others can be put to zero. Such cases include coarse graining problems [11] like the MSRG, in which one sums over modes belonging to comparatively thin shells of momenta inside the Brillouin zone, or problems based on a given effective Hamiltonian defined with respect to a small wave vector cutoff \( \Lambda \ll \pi/a \), where \( a \) is a measure of the microscopic lattice spacing. In particular, the FMC is tailor-made to study the critical behavior of lattice models of the \( \varphi^4 \) type. Other situations in which FMC will be advantageous include problems with a complicated anharmonic coupling structure ([7, 12]) or models involving long-range lattice interactions, as these are conveniently diagonalized by Fourier transform [13].

A representative of the latter class is the long-range \( \varphi^4 \) model defined by the dimensionless lattice Hamiltonian

\[
\beta H[s] = \frac{1}{2} \sum_{x,y} \frac{\varphi(x)\varphi(y)}{|x-y|^{d-\sigma}} + \sum_{x} \left[ r_0 \phi^2(x) + u_0 \phi^4(x) \right]
\]

for non–integer \( \sigma > 0 \), whose critical properties have been studied theoretically at length [14, 15, 16]. For our present purposes this model is particularly convenient. In fact, its dispersion term \( k^2 \) is non-analytic and therefore left invariant under the RG, which only generates analytic corrections in each consecutive iteration. Thus, it follows from the analysis of the MSRG that for this model the critical exponent \( \eta = 2 - \sigma \) and its RG field rescaling factor \( z(b) = b^{d+\sigma}/2 \) are known exactly to all orders of perturbation theory [14]. In addition, the model’s upper critical dimension \( d_c(\sigma) \geq 2\sigma \) is found to manifestly depend on \( \sigma \); defining \( \tilde{\sigma} \equiv d_c(\sigma) - d = 2\sigma - d \), thus allows to reinterpret the \( \epsilon \)-expansion as an expansion in \( \tilde{\sigma} \) for variable \( \sigma \) at fixed integer dimension \( d \). Of course, in computer simulations only integer dimensions \( d \) are at our disposal. Thus, the model offers the rather unique possibility to test predictions derived from analytical \( \epsilon \)-expansions by simulation. Moreover, for the model defined by the Hamiltonian (2), state-of-the-art computer simulation results utilizing modern cluster algorithms combined with finite size scaling analysis are available in dimensions \( d = 1, 2, 3 \) for comparison [17].

To mimic the steps defining a MSRG, we consider the above model on a cubic \( d \)-dimensional lattice of size \( L^d \) with spacing \( a = 1 \). Wave vector components are parametrized by integers \( n_i \) as \( k_i = 2\pi n_i/L \) and cutoffs by \( \Lambda = \Lambda(l) = 2\pi l/L \). Inside this cutoff, the dispersion \( |x-y|^{d-\sigma} \) is represented by its Fourier transform \( k' \), \( k = ||k|| \) being approximated by the lattice-periodic expression \( \left[ 2 \sum_{n=0}^{N} \sin(k_n/2)^{1/2} \right]^{1/2} \) for wave vectors below some sufficiently small cutoff \( \Lambda \). Using the full Fourier-transformed effective Hamiltonian with the above momentum cutoff and dispersion, we compute the probability distribution of the zero mode \( \tilde{\eta}(0) \), which is of course proportional to the system’s “magnetization”, upon averaging out the “fast”

\[
\begin{align*}
\frac{\mu'_0}{r'_0} &= \left( \frac{\mu_0}{r_0} \right) + \left( M_u \frac{\mu_0}{M_a} \frac{\mu_r}{M_r} \right) \left( \frac{u_0 - u'_0}{r_0 - r'_0} \right)
\end{align*}
\]

in a neighborhood of \( \pm8\% \) around the FP, treating the matrix entries \( M_{ij} \) as well as the exact fixed point values \( (\mu_0', r_0') \) as fit parameters. The critical exponents \( \nu \) and \( \omega \) are then identified from the RG relations \( \nu = 1/r_c \) and \( \omega = -\tau_a \), where \( r_c \equiv b^{r_c} > 1 \) and \( \tau_a \equiv b^{r_a} < 1 \) denote the two eigenvalues of the above \( 2 \times 2 \)-matrix corresponding to the only relevant and the least irrelevant direction in the projection of the full space of coupling constants onto the \((r_0, u_0)\)-sub-plane.

Figure 1: Typical RG flow pattern emerging for model (2) for \( d = 3 \). Parameters \( L = 36, \sigma = 1.65, l = 9, b = 9/7 \)
3. Results for Fixed Shell Thickness

In Ref. [6], we compare the results obtained in $d = 3$ by the above procedure to

- high-precision simulation results [17]
- the analytic $\epsilon$-expansion results [14, 17]

$$\gamma_r = \sigma - \frac{\tilde{\epsilon}}{3} - \frac{1}{6} \frac{\mathcal{A}(\sigma)}{\sigma} \tilde{\epsilon}^2 + O(\tilde{\epsilon}^3) \quad (4)$$

$$\omega = 2\sigma - 3 + O(\tilde{\epsilon}^2) \quad (5)$$

where, denoting the Digamma function by $\psi(z) : = \Gamma'(z)/\Gamma(z)$, we abbreviate

$$\frac{\mathcal{A}(\sigma)}{\sigma} = \psi(1) - 2\psi(\sigma/2) + \psi(\sigma) \quad (6)$$

- straightforward numerical perturbation theory

Despite the intrinsic non–perturbative nature of our Monte Carlo approach, our findings, which are gathered in Fig. 2, turn out to be only of an accuracy comparable to an $O(\tilde{\epsilon})$ calculation. It is easy to understand the cause of this rather sobering fact. In evaluating the simulation data, we were forced to project the full RG flow is onto the two-dimensional $(\tilde{\epsilon}_0, r_0)$-plane, thus implicitly erasing the information encoded in the flow components along the infinitely many remaining directions of full coupling space. Now, recall that in a standard $\epsilon$ expansion calculation, both fixed point values $r_0^*$ and $u_0^*$ are found to be of order $\tilde{\epsilon}$, while the fixed point values taken on by all other couplings are at least of order $O(\tilde{\epsilon}^2)$.

4. Optimization in the Parameter $b$

It seems prohibitively difficult at first sight to improve the above method significantly and promote it from just an illustrative approach further to one that is also numerically accurate. In fact, any inclusion of a finite (but certainly small) number of additional irrelevant couplings immediately leads to an enormous increase of complexity of both the simulation as well as the evaluation of its results, probably without gaining much in accuracy. In this respect, the situation seems to be just as hopeless as that had been historically encountered in analytical calculations, in which the MSRG approach was finally more or less completely abandoned in favor of the field-theoretic RG or other calculation schemes of superior efficiency. In an attempt to overcome these difficulties, the authors of Ref. [4] put forward the idea of taking the limit $b \to \infty$, as their analysis of the $b$-dependence of the Feynman diagrams contributing in second order perturbation theory indicated a strong damping of the influence of irrelevant couplings in this limit. Of course, neither the large $b$ limit nor the limit $b \to 1$ are directly accessible in FMC, since simulations are always based on a necessarily finite system. However, one can still study the behavior of results with respect to different choices of $b$ with the hope to extract some systematic trends.

Nevertheless, to provide a reasonably large range of choices for $b$ clearly requires a rather large linear system size $L$. To keep the computational costs a reasonable level, we thus chose to study the problem in $d = 1$. In addition, rather than focusing on the large $b$ region, we started our investigations looking at systems with $b$ values close to 1, frankly because such $b$-values imply a thin momentum shell and thus only require to operate on a small number of shell modes in the FMC algorithm. A bit to our surprise, for a one-dimensional lattice with $L = N = 8192$ and fixed cutoff $A = \pi/4$, we observe [5] a pronounced anomalous $b$-dependence of the FP values $u_0^*, r_0^*$ with a “critical” value $1/b^* < 1$, which extremizes both $r_0^* (b)$ and $u_0^* (b)$. Even more to our surprise, this distinct value $1/b^*$ of the parameter $1/b$ is found to be quite close but still markedly smaller than 1 (see Fig. 3). The obtained critical exponents also show corresponding anomalies around $b^*$ for all observed values of $\sigma$ (see Fig. 4). In detail, $y_r^*(b)$ is close to a minimum near $b^*$, while $\omega(b) = -y_\omega(b)$ shows a sharp variation in this $b$-region. Most interestingly, however, we note the striking fact that the values $y_r^* := y_r(b^*)$ and $\omega^* := -y_\omega(b^*)$ appear to be in excellent agreement with the high-precision FSS results of Ref. [17]!

But does the gap between the critical value $b^* < 1$ and 1 eventually close in the thermodynamic limit? Fig. 5 shows that this gap persists and saturates for $L \to \infty$ and thus is not a finite size effect. In fact, a critical value $1/b^* < 1$ only ceases to exist for system sizes smaller than a certain $\sigma$-dependent lower bound $L_\ast (\sigma)$ due to the discreteness of the Brillouin zone of a finite system, but could be detected for all larger accessible $L$ values. As is illustrated in Fig. 5, $1/b^*$ clearly tends to a finite limit distinctly different from 1 in the limit $L \to \infty$.
Discussion

At this point, the alert reader should – as we did – feel quite uneasy about the reported behavior. Why? Well, simply because the observed $b$-dependent anomalies, i.e. the pronounced $b$-dependence of the fixed point location and exponents (and even the clearly visible “hysteresis” of the corresponding trajectory of fixed point locations, cf. Fig. 3) appear to be in violent conflict with the *semi-group property* of the RG, according to which neither the fixed point location nor the observed exponents should show any dependence on $b$! The reason for the observed seemingly paradoxical behavior can, however, be easily understood.

Recall that in order to perform the coarse graining step of our RG prescription, we had to fit the potential produced by Wang-Landau FMC simulation to a $\varphi^4$ type of potential to obtain the coefficients $b_1, b_0$, which are then subjected to the rescaling steps of the MSRG prescription. Implicitly, however, this fitting procedure amounts to boldly projecting out an infinite number of RG-irrelevant contributions that were generated by integrating out the “fast” modes. From this perspective, it is immediately clear that performing two such RG steps – both with parameter $b$ – in a consecutive manner is usually bound to fail to produce the same results as a single RG step carried out with parameter $b^2$, in which the unnecessary “intermediate” projection onto the $(r_0, u_0)$-plane is absent. The inevitable conclusion is that the operation $\mathcal{R}^{\text{FMC}}(\cdot, b)$ does not resemble a meaningful RG transformation for arbitrary $b$, and that this failure is of course due to the unavoidable implicit influence of higher irrelevant couplings. It goes without saying that this fact also explains all other “paradoxical” observations we encountered for transformations at $b \neq b^r$.

Nevertheless, for varying $b$ our results strongly suggest that around $b = b^r$ the influence of irrelevant terms seems to be minimized. On the one hand, our simple theoretical argument explaining the violation of the RG semi-group property for arbitrary $b$ that we presented above in qualitative accordance with this conclusion. Also, the fact that the location $(u_0^*(b), r_0^*(b))$ of the fixed point shows a stationary behavior around $b^r$ can be understood (and should even have been expected) on this basis. Finally, the exponents $y_r(b)$ and $\omega(b^r)$ are also numerically found to approach their “true” values at $b = b^r$.

To sharpen our theoretic predictions further, we assert that our simulations indicate that only $\mathcal{R}^{\text{FMC}}(\cdot, b^r)$ qualifies as a “true” RG transformation. In other words, we are led to define

$$\mathcal{R}((u_0, r_0), (b^r)^n) := (\mathcal{R}^{\text{FMC}}((u_0, r_0), b^r))^n, \quad n \in \mathbb{N}$$

(7) for all integer powers of $b^r$. Numerical interpolation then even allows to give a corresponding definition of $\mathcal{R}((u_0, r_0), (b^r)^r)$ for non-integer exponents $r$. In other words, we can numerically compute $\mathcal{R}((u_0, r_0), b)$ for arbitrary $b \in \mathbb{R}$! Thus, our observations finally even indicate the unexpected possibility to investigate the accompanying differential RG flow equations using results from FMC simulations. We hope to present some interesting applications of this idea in the near future.

In closing, we note that for all accessible system sizes we were unable to observe any anomalies in the FP locations or exponents on the large $b$ side i.e. for $b \gg 1$. However, we would not go so far as to regard this failure as a contradiction to the predictions of Ref. [4], since the lattice interaction considered in [4] was of short range.

Figure 5: $L$-dependence of $b^*$ for system sizes $L = 2560$ (filled circle), 4096 (open square), 6144 (filled diamond) and 8192 (open triangle) at $\sigma = 0.75$. A fit with the heuristic function $1/b^*(L) = 1/b^*(\infty) + c/L$ gives excellent agreement, indicating a limiting value $1/b^*(\infty) = 0.9843 < 1$. Insets: Locations of $u^*_0$ and $r^*_0$ as functions of $1/b$ for the same system sizes at $\sigma = 0.75$. Extrema of $u^*_0$ and $r^*_0$ as functions of $b$ cease to exist for sizes $L = 1024$ and smaller due to the discreteness of the Brillouin zone.