Dynamic Monte Carlo renormalization-group method

Martin-D. Lacasse

*Centre for the Physics of Materials and Department of Physics, McGill University, Rutherford Building,
3600 University Street, Montréal, Québec, Canada H3A 2T8*

Jorge Viñals

Supercomputer Computations Research Institute, B-186, Florida State University, Tallahassee, Florida 32306-4052

Martin Grant

*Centre for the Physics of Materials and Department of Physics, McGill University, Rutherford Building,
3600 University Street, Montréal, Québec, Canada H3A 2T8*

The dynamical critical exponent of the two-dimensional spin-flip Ising model is evaluated by a Monte Carlo renormalization-group method involving a transformation in time. The results agree very well with a finite-size scaling analysis performed on the same data. The value of $z = 2.13 \pm 0.01$ is obtained, which is consistent with most recent estimates.

I. INTRODUCTION

The dynamics of the two-dimensional spin-flip Ising model remains a source of interest and controversy. Near the critical point, not only does the correlation length ξ diverge following $\xi \sim |T - T_c|^{-\nu}$, where T_c is the critical temperature and ν a critical exponent, the correlation time τ also diverges due to critical slowing down. This divergence can be characterized by the dynamic critical exponent z, where $\tau \sim \xi^z$, or equivalently, $\tau \sim |T - T_c|^{-\Delta}$, where $\Delta = \nu z$. The dynamic scaling hypothesis asserts that, in the long time limit, all times scale with this diverging time scale, so that a dynamical universality class is characterized by, among other things, this critical exponent z. Since the particular value of z is common to all members of a universality class, it is an important and fundamental quantity. Here we use a novel Monte Carlo renormalization-group method to estimate $z = 2.13 \pm 0.01$ for the two-dimensional spin-flip Ising model, which is in the universality class of model A (see Ref. 29), where a nonconserved scalar order parameter is the only dynamical mode.

Many authors[1–27] have attempted to evaluate z by a variety of techniques, giving values that are not always consistent with each other, even when considering the given errors. There are many possible explanations of these discrepancies, and we shall consider some of them. First, however, we shall discuss some lower bounds. For model A, mean-field theory predicts $z = 2 - \eta$, where η is the critical exponent describing the power-law decay of the correlation function. Using a generalized Langevin-equation approach, Schneider[28] showed this was a lower bound on z. Of course, the mean-field result is correct at and above the upper critical dimension $d_u = 4$, below which the $\epsilon = 4 - d$ expansion[29] gives $z = 2 + 0.01345(4 - d)^2 - 0.002268(4 - d)^3 + \mathcal{O}(4 - d)^4$. The lower critical dimension of model A is $d_\ell = 1$, and Bausch *et al.*[24] have calculated the $d = 1 + \epsilon$ expansion of the kinetic drumhead model to be $z = 2 + (d - 1) - \frac{1}{2}(d - 1)^2 + \mathcal{O}(d - 1)^3$. More recently, one of us[30] argued that the dynamic critical exponent should be larger than the reciprocal of the exponent for domain growth, yielding $z \geq 2$.

Of the different techniques used for the determination of z, no method seems to have proved better than others. Moreover, a given method does not always yield consistent results. For example, high-temperature expansions of different orders apparently converge to different values whether the expansion is computed for spin-spin time correlations[22,23] or magnetization correlations.[26,27] On the other hand, Monte Carlo techniques have systematic errors which can be quite difficult to evaluate. For example, it is generally believed[7,31,15,32] that the dynamic universality class of the spin-flip Ising model is insensitive to the algorithm used as long as the updating algorithm is local.[33,34] Some results obtained in one dimension[35,36] support this hypothesis. However, studies in three dimensions using Creutz's deterministic microcanonical dynamics[37] yield a value of z that "agrees with the Monte Carlo measurements as they agree among themselves" but is nevertheless slightly higher than most recent estimates (e.g., Refs. 37 and 38 and references therein). This discrepancy could be due to the methods of estimation of z rather than to the algorithm, but to our knowledge, there exists no systematic analysis testing the limits of validity of the dynamic universality class hypothesis. This is a potentially important issue, since nonlocal acceleration algorithms are being developed[33,34] which have exceedingly small values of z.

Besides the algorithm, another source of systematic error is from critical slowing down itself. While such effects are well known and are typically incorporated[39,40] to consistently estimate z, the existence of long time cor-

relations can potentially induce subtle couplings of correlations in pseudorandom number generators.

It has also been noted[23,41] that the linear relaxation critical exponent of the magnetization M can differ from the nonlinear one. The nonlinear relaxation time τ is defined as $\tau = \int_0^\infty [M(t) - M(\infty)]/[M(0) - M(\infty)]dt$ where the denominator is for normalization. If the integrand is written as a sum of exponentials, $\sum_i w_i e^{-t/\tau_i}$, then τ will simply be the weighted sum of the partial relaxation times. The limit when $M(0) \to M_{eq}$, i.e., as the system is left to relax from a value near its equilibrium value, defines the linear relaxation time. It characterizes a relaxation process that does not include the scaling of the order parameter itself. Rácz et al.[23,41] used scaling arguments to suggest that the nonlinear critical exponent $\Delta_A^{(nl)}$ of an observable A can be related to the linear critical exponent Δ_A by the following relation: $\Delta_A^{(nl)} = \Delta_A - \beta_A$ where β_A describes the scaling of the quantity A with respect to temperature. Mori et al.[19] in $d = 2$, and Chakrabarti et al.[42] in three dimensions, reported observations of such a relation.

Current techniques used in Monte Carlo simulations sometimes involve nonlinear response in terms of the definition given above. Some authors[12,11,16,18] have used the relaxation of the order parameter in systems prepared at zero temperature when put in contact with a heat bath at some temperature near T_c. On the other hand, other techniques[1,4-10,12,13] involve the measurement of some time correlations in critically equilibrated systems. Presumably there could be differences involving transient dynamics in these methods. However, there is no real distinction made in the literature concerning possible discrepancies between these various methods. It is not clear yet how important the distinction between linear and nonlinear relaxation times is, and further investigations should clarify this situation.

Finite-size effects can be important in simulations of critical systems, e.g., the effect of using the infinite system critical temperature can induce systematic errors in small systems. Although these effects can be exploited by finite-size scaling, very small systems may not be in the range where scaling applies. Finite systems also introduce the concept of ergodic time,[17,43] i.e., the mean lifetime of the system in one of its broken symmetry states. While infinite systems at T_c have a vanishing order parameter, finite systems of size L have nonzero values $\pm|M_c^L|$ between which the system has spontaneous transitions. Those transitions introduce a large effect in time correlations as discussed below.

Finally, it should be noted that experiments have been done on systems thought to be in the universality class of model A. The few results[44,45] of which we are aware yielded values of z well below 2. However the experiments are difficult, and the microscopic processes involved in the systems are various, so that it may be that the experiments do not probe the problem of interest herein.

II. METHOD

The Monte Carlo renormalization group (MCRG) was introduced by Ma,[46] and developed by others, espe-

cially Swendsen.[47] For critical dynamics, the method was extended by Tobochnik, Sarkar, and Cordery,[4] and others.[6,12,18,7] MCRG allows one to use the self-similarity in critically equilibrated systems by analyzing the effect of a controlled change of length scales on correlation functions. When length scales are changed by a factor of b, by some suitable blocking of b^d spins to one renormalized spin, the correlation length is changed by $\xi \to \xi/b$. This implies that time scales are changed by a factor of $\tau \to \tau/b^z$, from which the dynamic critical exponent can be estimated. Unfortunately the method is self-consistent in that there is no proof the system approaches a fixed point under the renormalization group. Thus it is essential that checks are made that, after several levels of RG, scaling is consistently observed. Here, we generalize the usual procedure of blocking in space, by blocking in time t.

Consider the Hamiltonian of an Ising-like system:

$$\mathcal{H} = \sum_\alpha K_\alpha S_\alpha, \tag{1}$$

where the K_α's are the coupling constants including temperature, the α index runs over all $i = 1, 2, \ldots, N$ spins for nearest-neighbor, next-nearest neighbor (and so on) interactions, and the S_α's are generalized spins made of specific products of spins $\sigma_i = \pm 1$ on each site. For example, the Ising model has $K_1 = -J/k_BT$, and $K_{\alpha>1} = 0$ where J is the coupling constant, k_B is Boltzmann's constant, and T is temperature and $S_1 = \sigma_i \sigma_j$ such that the sum is restricted so that i and j are nearest neighbors. Here we will consider the two-dimensional Ising model on a square lattice, and apply a renormalization-group transformation repeatedly to this evolving system. As mentioned above, a typical numerical MCRG transformation[46] is to "block" by a length rescaling factor of b: A block of b^d spins is transformed into a renormalized spin by majority rule of the spins in the block, with a random outcome on ties. The resulting renormalized Hamiltonian is assumed to be expressible in terms of another short-range Ising-like system, with more S_α terms contributing. Numerically, the approximation results from the fact that the number of spins remaining after m blockings is N/b^{md}, thus coupling constants for interactions are truncated, if they involve larger length scales than the entire system. Thus, for equilibrium properties, a suitably chosen transformation operator will change the Hamiltonian $\mathcal{H}(K)$ by moving the parameter vector K to some other point in K space.

For critical dynamics the situation is analogous. Say one begins with the Ising model again, with the dynamics of single-spin flips, where each evolving configuration depends only on the previous one, i.e., a Markov process. Under the blocking transformation mentioned above, it is expected that the original master equation which is "short range" in time is changed to a non-Markovian equation which has memory over some small time scales.

Our original contribution here is to introduce blocking in *time* as well as space. We simulate a process on a regular time scale measured in terms of Monte Carlo steps (MCS). In addition to applying a standard real-space MCRG transformation technique, we perform a

blocking of spins, by majority rule, in consecutive discrete time steps. In principle, the advantage of blocking in time can be twofold. Firstly, we expect that it will smooth out high frequency fluctuations allowing one to reach the asymptotic limit of the RG transformation more rapidly than with blocking in space alone. In the same way as blocking in space iterates away irrelevant short-length-scale behavior, we expect that blocking in time will further eliminate short-time irrelevant memory effects. Secondly, one can suitably adjust the time blocking factor b_t to balance the effects resulting from blocking

in space, by choosing, for example, $b_t = b^{z_0}$, where z_0 is some reference exponent. We choose $z_0 = 2$ for reasons that will become clear below.

Before discussing the method in more detail, we introduce the quantities that will be measured in time. Critical dynamics involves a scaling relation in which all time scales, in the long time limit, are measured in units of the diverging correlation time. Thus, one needs only to choose a convenient measure of time correlations. We shall use the time displaced correlation function for the magnetization M, as defined by

$$\varphi_M(t) = \frac{\langle M(t_0)M(t_0+t)\rangle - \langle M(t_0)\rangle\langle M(t_0+t)\rangle}{\langle M(t_0) - \langle M(t_0)\rangle^2\rangle^{1/2}\langle M(t_0+t) - \langle M(t_0+t)\rangle^2\rangle^{1/2}}, \tag{2}$$

where M is $\sum_i^N \sigma_i$ as usual. Other correlation measures are discussed below. All averages were computed from selected numerical discrete time steps δt (usually a few MCS). In principle, the time-correlation function should be fitted to a series of exponentials

$$\varphi_M(t) = \sum_i w_i e^{-t/\tau_i}, \tag{3}$$

where $\tau_i > \tau_j$ if $i < j$. However, tests made to fit the data to two exponentials showed that $\tau_1 \gg \tau_2$. Indeed, all our data were well fit to a single exponential with time constant τ_M. Data were extracted from one long simulation from which values of $\varphi_M(t)$ were computed over a time range of $t = 0$ to $t = 5\tau_M$. Further averaging was also made by running 32 systems in parallel.

To calculate z, we use a matching procedure.[4,6,7] In principle, after the irrelevant variables have been iterated away, the probability distribution function will remain invariant under further renormalization-group transformations. It is expected that, after a finite number of iterations, contributions from the irrelevant variables will be negligible. Then, any quantity determined after m blockings of an N spin system should be identical to those determined after $m + 1$ blockings of a system of Nb^d spins. In our new method, time scales after m blockings of the small lattice are also explicitly rescaled by a factor $(b_t)^m$, while the larger lattice has times explicitly rescaled by a factor $(b_t)^{m+1}$. Unless $b_t \equiv b^z$, quantities measured on the two lattices will *still* be at different times t and t'. Hence, close to the fixed point, we expect a matching condition to hold: $\varphi(N, m, t) = \varphi(Nb^d, m + 1, t')$ for a correlation function φ. From this, the time rescaling factor t'/t can be calculated, through the measurement of a suitable correlation function, φ_M in our case. The difference between the estimate of z and the correct dynamical critical exponent can then be obtained, since

$$\frac{t'}{t} = b^{z-z_0}, \tag{4}$$

where $b^{z_0} \equiv b_t$.

Our RG transformation was done in the following way.

During a simulation, every four configurations, each separated by one MCS, were "blocked" in space and time: One block spin was made by majority rule of the 16 spins coming from 4 consecutive configurations of 4 neighboring spins, ties were broken at random. This corresponds to a space blocking factor $b = 2$, and a time blocking factor of $b_t = 2^{z_0} = 4$. Such a choice would give asymptotically trivial rescaling of length and time if $z = 2$, and we expect it to make our study sensitive to the difference $(z - 2)$, which is small.

Instead of doing point to point matching, i.e., matching each discrete time step, the quality of our data is such that we have matched the entire function $\varphi_M(t)$, since it could be well fitted to one exponential. More explicitly, we have $\tau_M \sim \xi^z$ and a renormalized system for which $\tau_M' \sim \xi'^z$ where $\xi' = \xi/b$. Therefore, without blocking in time, the critical exponent is obtained from $\tau_M/\tau_M' = b^z$. Now, if time is rescaled in such a way that $\tau_M'' = \tau_M'/b_t$, then $\tau_M''/\tau_M = b^z/b_t = b^{z-z_0}$. The discrepancy $(z - 2)$ can then be obtained from

$$z - 2 = \frac{\ln[\tau_M(L, m)] - \ln[\tau_M(bL, m + 1)]}{\ln b}. \tag{5}$$

Simulations were done on two-dimensional nearest-neighbor square lattice spin-flip Ising systems with periodic boundary conditions. We used a single-flip multisystem algorithm, i.e., one running different systems in parallel instead of the more common multi-flipping one-system algorithms. The only correlation between the parallel systems is the sharing of the updating sequence history, but we expect this to be negligible. The dynamic algorithm was of *Metropolis* type, i.e., one using a flipping probability based on $\min(1, \exp^{-\Delta E/k_B T})$. Systems were initialized for 20–$50\tau_M$ at the critical temperature of the infinite system.[48] All measurements were made at the same temperature.

The results could also be interpreted using a finite-size scaling analysis. According to this approach, the correlation length of the systems should be of the order of the system size so that

$$\tau_M \sim L^z. \tag{6}$$

Therefore, the correlation time for different system sizes directly yields the critical dynamic exponent. Consistent results from both methods will be presented in the next section.

III. RESULTS

From each of the simulations detailed in Table I a correlation time was extracted, as listed in Table II. Figures 1 and 2 show a typical decay of $\varphi_M(t)$, demonstrating that the time correlations for finite systems can be well described by an exponential. All the fits were done using a least-squares fit algorithm. The dynamic critical exponent could then be obtained by comparing the values of τ_M for different systems. Values of z thus obtained are listed in Table III. The first striking fact is that a point to point finite-size scaling yields a value that compares very well with the one obtained from the dynamic MCRG we propose. This suggests that the discrepancies in the values of z as obtained from systems of different sizes are not systematic errors in the evaluation methods.

Although our study involves more accumulated averages than any previous work, it is still difficult for us to uniquely extract errors. We have found that the "instantaneous" values of τ_M contains large fluctuations. Figure 3 shows that even when binned and averaged over $\sim 75\tau_M$, the value of τ_M averaged for 32 systems still contains a fair amount of fluctuations. Therefore, as is well known,[39,40] very long simulations are required to get a representative value of time correlations. Furthermore, the regimes of fitting of $\varphi_M(t)$ have been chosen as well as possible, but it should be noted that a logarithmic scale applied to small numbers can introduce large fluctuations. Nevertheless, we found that our data was well represented by simple exponential decay over the long times we considered ($t \leq 5\tau_M$).

If one computes the same time correlations with the

TABLE I. Simulation details for the various systems. The range is the amount of Monte Carlo steps per spin (mcs) for which the function $\varphi_M(t)$ has been extracted. It can be thought of as an observation window over one simulation running in time. The total mcs for one system can be obtained by multiplying columns 2 and 4. All the systems were first equilibrated for 10 times the value of column 2, which in turn is of the order of 2–5 τ_M.

L	Range (mcs)	δt (mcs)	Average No.	m_{max}
8	1024	4	32 000	2
12	2048	8	32 000	2
16	8192	16	64 000	3
16	4096	16	32 000	2
20	8192	16	32 000	2
24	8192	16	26 400	3
24	16 384	16	32 000	3
32	16 384	16	64 000	4
48	32 768	16	4832	4
64	65 536	64	18 016	4
96	98 304	64	2336	4

absolute value of the magnetization, then one finds much smaller correlation times, thus showing that the ergodic time is for the most part responsible for the large value of τ_M. Since the ergodic time is due to a finite-size effect, it is not surprising to find such a good agreement between our results and finite-size scaling. Also, comparison with other kinds of time correlations,[7] e.g.,

$$C(t) = \sum_i \sigma_i(t_0)\sigma_i(t_0 + t)$$

or

$$E(t) = \sum_{ij} \sigma_i(t_0)\sigma_j(t_0 + t),$$

where i and j are nearest neighbors, showed that $\varphi_M(t)$

TABLE II. The values of τ_M as estimated from a least-squares fit of the time-time correlation function $\varphi_M(t)$ to a simple exponential. The values are in mcs and the simulation characteristics can be read from the respective entry in Table I. The errors indicated in parentheses are those obtained from the fit. The last line represents the value of z obtained from finite-size scaling analysis applied to each column.

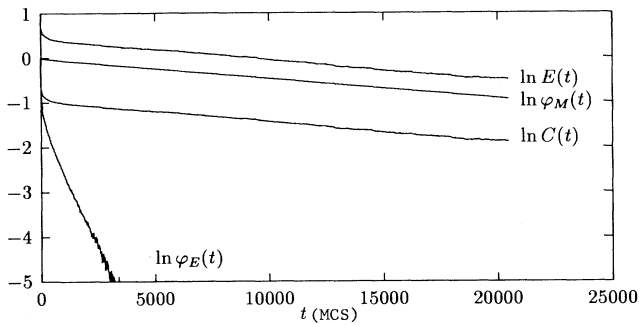| L	MCRG iteration number				
	0	1	2	3	4
8	261.41(6)	64.31(4)	16.34(4)		
12	631.8(2)	157.9(1)	39.5(1)		
16	1186.6(3)	296.5(1)	74.0(1)	18.6(1)	
16	1189.1(5)	296.9(3)	74.3(2)		
20	1930.7(3)	482.9(1)	120.5(2)		
24	2853.9(3)	716.0(4)	179.0(3)	44.8(2)	
24	2837.9(3)	713.3(6)	178.3(3)	44.5(1)	
32	5355(2)	1338.8(3)	334.6(2)	83.7(1)	20.8(1)
48	12528(2)	3130.4(5)	782.8(3)	195.6(1)	49.4(2)
64	23316(4)	5814(2)	1453(1)	363.3(8)	92(1)
96	54620(20)	13660(10)	3415(5)	852(3)	214(2)
z	2.153	2.145	2.142	2.125	2.128

FIG. 1. Critical dynamics MCRG on a 64×64 system. Curves are for $m = 0, 1, 2, 3, 4$, from top to bottom. Averaged over 32 independent systems observed for 11 468 800 mcs. The equilibrating time of 204 800 mcs and φ_M calculated every 16 mcs.
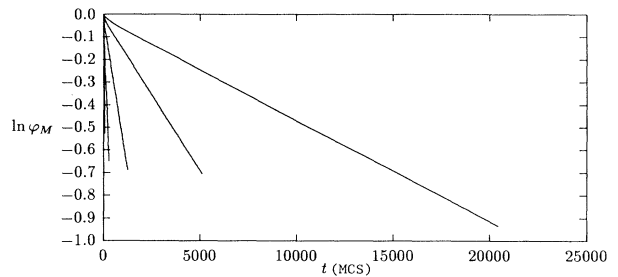

FIG. 2. Critical dynamics MCRG on a 32×32 system. Curves are for $m = 0, 1, 2, 3$, from top to bottom. Averaged over 32 independent systems each observed for 8 192 000 mcs. Equilibrating time of 81 920 mcs and φ_M calculated every 16 mcs.

is by far less noisy. See Fig. 4.

Evaluation of the data with standard finite-size scaling gives a result of $z = 2.14 \pm 0.01$, consistent with recent works which used this technique[5,10,13] on systems of comparable size. However, pointwise scaling shows that small systems tend to show a larger value of z and that this tendency seems to disappear for L larger than ~ 32. This result is somewhat surprising since a previous MCRG study[7] observed a small $z \approx 2$ from matching systems of size $L = 8$ and 16, and obtained a larger value when matching larger systems. On the other hand, a numerical study of very large systems[19] gave a low value of $z = 2.076 \pm 0.005$. Therefore, there is still some reason for concern on z's dependence on system size.

Some authors[25] have argued that the smallness of the dynamic critical region could be held responsible for the difficulties encountered in evaluating z. However, the scaling relations obtained near the critical point[17] do not seem to show such a sharp region, and those effects are thought to be strong finite-size effects. Moreover, our MCRG results are quite consistent from the first level of RG, as the level of iteration of RG is increased. This self-consistently shows that the system is in the critical regime.

Finally, by considering that small systems have a sys-

tematic error and do not seem to be in the asymptotic scaling regime, we obtain an estimate of $z = 2.13 \pm 0.01$ from the MCRG method we propose. This value is consistent with most of the recent work,[5,18,7,9,10,12,13] as well as our finite-size scaling study herein.

IV. CONCLUSION

We showed that time can be used as a renormalizable variable in a MCRG method. Combined with standard real-space MCRG techniques, we extracted a value for the dynamic critical exponent that was consistent with values extracted from the same data by finite-size scaling. Our estimated value of $z = 2.13 \pm 0.01$ is also consistent with most recent estimates.

The motivation for introducing this method was the possibility of obtaining a more accurate value of z. Unfortunately, we found that the method was not superior to conventional finite-size scaling or real-space MCRG techniques for this problem, although it proved to be at least equivalent. Further studies would be required to see if this new MCRG method would be of use for other related dynamic problems, such as spinodal decomposition.

TABLE III. Values of z as estimated from point to point finite-size scaling (FSS) and by matching the correlation times according to relation (5).

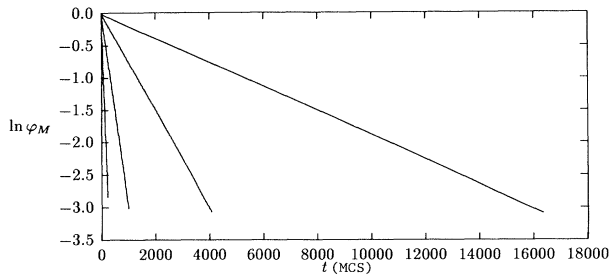| L	MCRG iteration number				
	FSS	1	2	3	4
8–16	2.183	2.182	2.182	2.182	
12–24	2.171	2.178	2.178	2.179	
16–32	2.172	2.173	2.174	2.176	2.167
24–48	2.139	2.138	2.132	2.131	2.144
32–64	2.124	2.120	2.118	2.119	2.137
48–96	2.124	2.125	2.126	2.122	2.130

FIG. 3. The evolution of the value of the cumulated average of the time-displaced correlation functions for a system of 32 × 32 sites. Even if we accumulated a large amount of data, we see that the cumulative average still contains a fair amount of fluctuations.
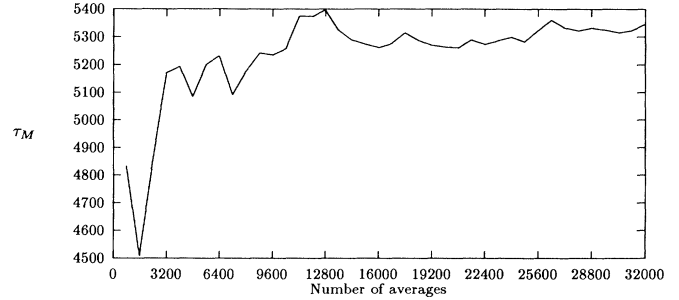

FIG. 4. Different time-displaced correlation functions for a system of 64 × 64 sites. Note the large difference between $\varphi_E(t)$ and $\varphi_M(t)$ showing that the energy relaxes much more rapidly than the order parameter. Also note the noise common to $C(t)$ and $E(t)$. We used $\varphi_M(t)$ in our estimations.

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