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OPEN PROBLEMS IN MONTE CARLO RENORMALIZATION GROUP APPLICATION TO CRITICAL PHENOMENON‡

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ABSTRACT

The Monte Carlo Renormalization Group (*MCRG*) methods and the theory behind them are reviewed. The Gupta-Cordery improved *MCRG* method is described and compared with the standard one. The emphasis is on the progress made in understanding the truncation errors in the Linearized Transformation Matrix and on open problems. Lastly, some of the existing methods for calculating the renormalized Hamiltonian are reviewed and evaluated.

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The development of Monte Carlo Renormalization group method (*MCRG*) was essentially complete in 1979 with the work of Wilson[1], Swendsen[2] and Shenker and Tobochnik[3]. Prior to this Ma[4] and Kadanoff[5] had provided key ingredients. There already exists extensive literature on *MCRG* and I direct the reader to it [1,3,6,7,8] for details and for a wider exposure. Similarly, the reviews [9,10] are a good starting point for background on spin systems. The topics I shall cover are

1) Introduction to *MCRG* and its methodology.
2) Improved Monte Carlo Renormalization Group.
3) Comparison of the standard MCRG method and IMCRG with emphasis on the truncation errors.
4) Renormalized Hamiltonians and Methods to calculate them.
5) Open problems.

1) INTRODUCTION TO *MCRG*

Renormalization Group[10,11,12,13] (RG) is a general framework for studying systems near the critical surface (defined by a divergent correlation length) where singularities in thermodynamic functions arise from coherence at all length scales. The *MCRG* method was developed to handle this problem of infinitely many coupled degrees of freedom so that sensible results can be obtained from finite computers. There are two central ideas behind *MCRG*: The first is to average over the infinitely many degrees of freedom in discreet steps. The block degrees of freedom on the coarse lattice are the ones relevant to the description of the physical quantities of interest. The interaction between these averaged (block) fields is described by an infinite set of couplings that get renormalized at each blocking step. The second point is that there are no singularities in the coupling constant space even though the correlation length and thermodynamic quantities diverge on the critical surface.

The MCRG methods discussed here have a fundamental assumption: the fixed point is short ranged. Thus even though an infinite number of couplings are generated under renormalization, we shall assume that only a few short range ones are sufficient to simulate the system at a given scale and preserve the long distance physics.

1.1) Standard Monte Carlo:

Consider a magnetic system consisting of spins $\{s\}$ on the sites of a *d-dimensional* lattice L described by a Hamiltonian H. From the outset, H will include all possible couplings $\{K_\alpha\}$. The behavior of all thermodynamic quantities can be determined from a detailed knowledge of the partition function

$$Z = \sum e^{-H} = \sum e^{K_\alpha S_\alpha} \tag{1.1}$$

where S_α are the interactions. In Monte Carlo, configurations of spins on the original lattice are generated by the Metropolis[14], heat bath[15], molecular dynamics alias Microcanonical[16] or the Langevin[17,18] algorithm with a Boltzmann distribution $e^{-H} = e^{K_\alpha S_\alpha}$. All thermodynamic quantities are given as simple averages of correlation functions over these 'importance sampled' configurations. The accuracy of the calculations depend on the size of the

statistical sample and the lattice size L used. Both these quantities depend on the largest correlation length ξ in the system. Near the critical temperature, T_c, associated with second order phase transitions, the correlation length and consequently thermodynamic quantities like the specific heat *etc* diverge as functions of $(T - T_c)$ with universal critical exponents. These have been calculated for many systems analytically or by Monte-Carlo using finite size scaling or by the $MCRG$ method. Because ξ diverges at T_c, long runs are needed to counter the critical slowing down. Also, to control finite size effects the lattice size has to be maintained at a few times ξ. The problem of critical slowing down is addressed by analyzing update algorithms (Metropolis vs. heat bath vs. Microcanonical vs. Langevin with acceleration techniques like multi-grid[19], fourier acceleration[18,20] etc). The optimum method is, of course, model dependent and has to take care of metastability (local versus global minima) and global excitations like vortices, instantons etc that are not efficiently handled by local changes. This last feature has not received adequate attention. To control the second problem in standard Monte Carlo, effects of a finite lattice especially as $\xi \to \infty$, finite size scaling[10] has been used with success. In this review I shall concentrate on $MCRG$. First I shall describe how universality and scaling are explained by the renormalization group.

The renormalization group transformation (RGT) is an operator R defined on the space of coupling constants, $\{K_\alpha\}$. In practice the RGT is a prescription to average spins over a region of size b, the scale factor of the RGT, to produce the block spin which interacts with an effective theory $H^1 = R(H)$. The two theories H and H^1 describe the same long distance physics but the correlation length in lattice units $\xi \to \frac{\xi}{b}$. If this RGT has a fixed point H^* such that $H^* = R(H^*)$, then clearly the theory is scale invariant at that point and ξ is either 0 or ∞. An example of a fixed point with $\xi = 0$ is $T = \infty$ and these are trivial. The interesting case is $\xi = \infty$ about which the theory is governed by a single scale ξ. I will discuss this assumption of hyperscaling, *i.e.* a single scale controlling all physics, later. If this fixed point is unstable in 1 direction only (this direction is called the Renormalized Trajectory (RT)), then non-critical H will flow away from H^* along trajectories that asymptotically converge to the RT. Thus the long distance physics of all the trajectories that converge is identical and is controlled by the RT. Similarly, points ϵ away from H^* on the $\infty - 1$ dimension hypersurface at which $\xi = \infty$ (the critical surface) will converge to H^*. The fact that the fixed point with its associated RT control the behavior of all H in the neighborhood of H^* is universality.

Next, consider a non-critical H that approaches H^* along the RT. Thermodynamic quantities depend on a single variable *i.e.* distance along the RT. This is scaling. Corrections to scaling occur when H does not lie on the RT. These are governed by the irrelevant eigenvalues of the RGT which give the rate of flow along the critical surface towards H^* and for H not on the RT, the rate of convergence towards it. The relevant eigenvalue gives the rate of flow away from the fixed point along the unstable direction RT and is related to the critical exponent ν. This terse exposé ends with a word of caution; all these statements have validity close to H^*.

1.2) Standard MCRG method

In the $MCRG$ method, configurations are generated with the Boltzmann factor $e^{K_\alpha S_\alpha}$ as in standard Monte Carlo. The RGT, $P(s^1, s)$, is a prescription for averaging variables over a cell of dimension b. The blocked variables $\{s^1\}$ are defined on the sites of a sublattice

L^1 with lattice spacing b times that of L. They interact with apriori undetermined couplings $\{K^1_\alpha\}$, and the configurations are distributed according to the Boltzmann factor e^{-H^1} *i.e.*

$$e^{-H^1(s^1)} = \sum P(s^1, s)\, e^{-H(s)} \quad . \tag{1.2}$$

All expectation values, with respect to the Hamiltonian H^1, can be calculated as simple averages on the blocked configurations. The blocking is done n times to produce a sequence of configurations distributed according to the hamiltonians H^n. They all describe the same long distance physics but on increasingly coarse lattices. The fixed point H^*, the RT and the sequence of theories, H^n, generated from a given starting H depend on the RGT.

The RGT should satisfy the Kadanoff constraint

$$\sum^{1} P(s^1, s) = 1 \tag{1.3}$$

independent of the state $\{s\}$. This guarantees that the two theories H and H^1 have the same partition function. The RGT should also incorporate the model's symmetry properties; a notable example is the choice of the block cell in the anti-ferromagnetic Ising model. Usually, there exists considerable freedom in the choice of the RGT. In fact many different RGT can be used to analyze a given model. In such cases a comparison of the universal properties should be made and the RGT dependent quantities isolated. I defer discussion on how to evaluate the efficiency of a RGT to section 1.5.

1.3) Methods to calculate the critical exponents

There are two methods to calculate the critical exponents from expectation values calculated as simple averages over configurations. In both there is an implicit assumption that the sequence H^n stays close to H^*. The more popular method is due to Swendsen[2,7] in which the critical exponents are calculated from the eigenvalues of the linearized transformation matrix $T^n_{\alpha\beta}$ which is defined as

$$T^n_{\alpha\beta} = \frac{\partial K^n_\alpha}{\partial K^{n-1}_\beta} = \frac{\partial K^n_\alpha}{\partial \langle S^n_\sigma \rangle} \frac{\partial \langle S^n_\sigma \rangle}{\partial K^{n-1}_\beta} \quad . \tag{1.4}$$

Each of the two terms on the right is a connected 2-point correlation matrix

$$U^n_{\sigma\beta} = \frac{\partial \langle S^n_\sigma \rangle}{\partial K^{n-1}_\beta} = \langle S^n_\sigma S^{n-1}_\beta \rangle - \langle S^n_\sigma \rangle \langle S^{n-1}_\beta \rangle \,. \tag{1.5}$$

and

$$D^n_{\sigma\beta} = \frac{\partial \langle S^n_\sigma \rangle}{\partial K^n_\beta} = \langle S^n_\sigma S^n_\beta \rangle - \langle S^n_\sigma \rangle \langle S^n_\beta \rangle \,. \tag{1.6}$$

Here $\langle S^n_\sigma \rangle$ are the expectation values on the n^{th} renormalized lattice and K^n_σ are the corresponding couplings. The relevant exponent ν is found from the leading eigenvalue λ_t of $T^n_{\alpha\beta}$ as

$$\nu = \frac{\ln b}{\ln \lambda_t} \tag{1.7}$$

where b is the scale factor of the RGT. I have restricted the discussion to the special case of one relevant eigenvalue. In general, systems can have multi-critical points with more than one relevant interaction. The eigenvalues which are smaller than one (called irrelevant) yield exponents that control corrections to scaling. An eigenvalue of exactly one is called marginal. There is an additional class of eigenvalues, the redundant eigenvalues, that are not physical. Their value depends on the RGT, so one way to isolate them is to repeat the calculation with a different RGT. I shall return to these in section 1.5

The accuracy of the calculated exponents improves when they are evaluated close to the fixed point. This can be achieved by starting from a critical point and blocking the lattice a sufficient number of times *i.e.* H^n for large n. In this case the convergence is limited by the starting lattice size and how close the starting H^c is to H^*. This method can be improved if the renormalized couplings $\{K^n\}$ are determined starting from a known critical Hamiltonian. We assume that the couplings fall off exponentially with the range, so that H^* can be approximated by a small number of short range couplings. An approximate critical point in this subspace should then be used in the update. Models for which the critical coupling is not known exactly, this improvement has no disadvantage. Otherwise one has to optimize between moving closer to H^* and flowing away from it under blocking. This flow away from the critical surface can be corrected for by Wilson's 2-lattice method described in section 1.4. Later, I will also describe a few methods to calculate the renormalized couplings.

A second possible improvement is to tune the RGT so that the convergence to H^* from a starting H^c takes fewer blocking steps. This is discussed in section 1.5

The practical limitation in Monte Carlo simulations is that the two matrices U and D can only be determined in a truncated subspace. Further, in order to set up T, the matrix D has to be inverted. Thus the determination of exponents has two types of truncation errors: The elements of the truncated T differ from the true T due to the inversion of a truncated D and the second come from diagonalizing a truncated T. These errors will be analysed in detail in section 3.

The second method to calculate the leading relevant exponent is due to Wilson[6]. Consider once again the 2-point connected correlation function (the derivative of an expectation value) $\langle S^i_\alpha S^j_\beta \rangle_c$ with $j > i$. Expand S^i_α in term of the eigenoperators O^i_α of the RGT. Close to H^* the level dependence in O^i_α (equivalently in the expansion coefficients $c^i_{\alpha\beta}$) can be neglected. Then to the leading order

$$\langle S^i_\alpha S^j_\beta \rangle \sim \lambda_t^{j-i} c_{\alpha,t} \langle O_t S^j_\beta \rangle \tag{1.8}$$

where λ_t is the leading relevant eigenvalue and corrections are suppressed by $(\frac{\lambda}{\lambda_t})^{j-i}$. Thus for each α and β, the ratio $\frac{\langle S^i_\alpha S^j_\beta \rangle}{\langle S^{i+1}_\alpha S^j_\beta \rangle}$ gives an estimate for the leading eigenvalue λ_t. The accuracy of the method improves if $j - i$ is large since non-leading terms are suppressed geometrically. So far this method has not been used extensively so its practical accuracy cannot be evaluated.

The calculation of ν from the leading eigenvalue does not assume hyperscaling. The relation between ν and the specific heat index α *i.e.* $\alpha = 2 - \nu d$ does. If hyperscaling is violated, then MCRG has no predictions for α, but it can be determined from a finite size scaling analysis (with an enhanced definition of the scaling functions) of the specific heat

data. Also, the interpretation of ν as the correlation length exponent becomes unreliable away from the fixed point. To the best of my knowledge, there does not exist a calculation in a model with known hyperscaling violations, so we cannot really judge how it would effect MCRG results. This is an open problem.

On the critical surface the 2-point correlation functions (like in Eq. (1.5) and (1.6)) diverge in the thermodynamic limit. However, their ratio is the rate of change of couplings and these are well behaved provided one considers only short ranged correlation functions as will be shown later. The reason that *MCRG* is assumed to have better control over finite size effects is that if H^* is short ranged then a truncated $T^n_{\alpha\beta}$ is sufficient to determine the leading eigenvalue. Also, the finite size contributions to the elements $T^n_{\alpha\beta}$ fall off like the couplings *i.e.* exponentially. Thus reliable estimates may be obtained from small lattices.

1.4) Wilson's 2-lattice method to find a critical point:

Consider *MCRG* simulations L and S with the same starting couplings K^0_α but on lattice sizes $L = b^n$ and $S = b^{n-1}$. If K^0_α is critical and after a few blockings the 2 theories are close to H^*, then all correlation functions attain their fixed point values. For non-critical starting H, expand about H^* in the linear approximation

$$\langle L^m_\alpha \rangle - \langle S^{m-1}_\alpha \rangle = \frac{\partial}{\partial K^0_\beta} \{\langle L^m_\alpha \rangle - \langle S^{m-1}_\alpha \rangle\} \Delta K^0_\beta$$

$$= \{\langle L^m_\alpha L^0_\beta \rangle_c - \langle S^{m-1}_\alpha S^0_\beta \rangle_c\} \Delta K^0_\beta \tag{1.9}$$

to determine ΔK^0_α. To reduce finite size effects the compared expectation values are calculated on the same size lattices. The critical coupling is given by

$$K^c_\alpha = K^0_\alpha - \Delta K^0_\alpha \tag{1.10}$$

and this estimate should be improved iteratively.

1.5) Optimization of the RGT

The freedom to choose the *RGT* leads to the question. What are the criteria by which to decide what is the best *RGT*. I will first address the question -- what is the effect of changing the *RGT* on the fixed point and on the RT. The answer is a Conjecture: Changing the *RGT* moves the fixed point on the critical surface but only along redundant directions. A simple argument is as follows[21]: Consider two different *RGT*, R_1 and R_2, and their associated fixed points H^*_1 and H^*_2. There are no non-analytic corrections to scaling at either fixed points and the associated *RT*. If these two points are distinct, then under R_1 H^*_2 flows to H^*_1. Consequently there are no scaling violations along the flow. This is by definition a redundant direction. This implies that the associated *RT* differ by redundant operators.

The presence of redundant operators does not effect the physics, however it can obscure the results[22]. The redundant eigenvalues are not physical, depend on the *RGT*, and can

be relevant or irrelevant. If a relevant redundant operator is present then the flows will not converge to the H^* or to the RT. Thus the first criterion in picking a RGT is that the redundant eigenvalues be small.

We desire the convergence to H^* be fast. This gives the second criterion: the coefficients of the leading irrelevant operators in $(H^* - H_c)$ should be small. The basis vectors corresponding to irrelevant eigenvalues are a function of the position of H^* on the critical surface. Consequently, even though changing the RGT only moves H^* along redundant directions, it is possible to reduce the coefficient of the irrelevant operators.

Swendsen[22] has conjectured that the fixed point can be moved anywhere on the critical surface by tuning the RGT. In particular, if the simulation point is made H^*, then that RGT is optimal. There is some support for this in spin systems, where by adding terms to the RGT, one can successively kill terms in the renormalized hamiltonian. Swendsen[23] found that the eigenvalues for the $d = 3$ Ising model are significantly improved with a tuned 10 term RGT. He also found that on using a 10 term truncated renormalized hamiltonian closer to H^* for a simple RGT, the improvement was not as good. Since his determination of renormalized couplings have large truncation errors, the comparison is not complete. Tests with the $d = 2$ Ising model confirm that H^* can indeed be brought close to the nearest neighbour critical point[24]. However, the improvement in the thermal exponent is not systematic. In all cases we have tried, the value of ν increases and in most cases it overshoots the known exact result. This might explain the improvement seen by Swendsen in $d = 3$ where the simple majority rule RGT gives too low a value.

The central problem in this approach is that in all cases tuning the RGT causes the results for the magnetic exponent to deteriorate. The magnetic eigenvalue at first blocking with the majority rule is[24] 3.683(2) which agrees with the earlier result of Swendsen[7]. Gausterer and Lang[25] find 3.692(3) with a 3 parameter RGT of slightly larger range. Umrigar and I[24] find 3.713(2) with a 21 parameter RGT. Since the exact result is 3.668, we conclude that the eigenvalue increases as the range of the RGT increases. This is surprising because the fixed point is at zero odd couplings and these remain unchanged in tuning the RGT.

There are two additional things to check in this approach: first whether the coefficients of the RGT terms fall off like the couplings with the range, i.e. exponentially, and second whether the long range untuned couplings continue to fall off at least as fast as before. Finally, the quantity to optimize is the update complexity (embodied in the RGT or the hamiltonian) versus the decrease in the coefficient of the leading irrelevant operator.

To summarize, the criterion for an optimum RGT is to make the H^* and the RT as short ranged as possible and to have small redundant eigenvalues. In critical phenomena, the improvement can be quantified by measuring the convergence of the exponents as a function of the blocking level. I feel that the present status of understanding is ambiguious. For the moment let me conclude this section by: The the question of how best to optimize $MCRG$ has not been adequately answered and should be investigated further.

2: IMPROVED MONTE CARLO RENORMALIZATION GROUP[26]

I shall describe the Gupta-Cordery MCRG method ($IMCRG$) in some detail. In

this method too the Renormalized Hamiltonian and the Linearized Transformation Matrix, LTM, are determined in some truncated space of interactions. However, in this sub-space they have no additional truncation errors *i.e.* the determined quantities have their infinite component values. Next, there are no long time correlations even on the critical surface and the block n-point correlation functions like $\langle S^1_\alpha S^1_\beta\rangle - \langle S^1_\alpha\rangle\langle S^1_\beta\rangle$ are calculable numbers. Because of these properties, the method allows a careful error analysis in the determination of the exponents from a truncated LTM.

In the $IMCRG$ method the configurations $\{s\}$ are generated with the weight

$$P(s^1, s)e^{-H(s)+H^g(s^1)} \tag{2.1}$$

where H^g is a guess for H^1. Note that both the site and block spins are used in the update of the site spins. In analogue to Eq. (1.2), the distribution of the block spins is given by

$$e^{-H^1(s^1)+H^g(s^1)} \;=\; \sum P(s^1, s)e^{-H(s)+H^g(s^1)} \quad . \tag{2.2}$$

If $H^g = H^1$, then the block spins are completely uncorrelated and the calculation of the n-point functions on the block lattice is trivial.

$$\langle S^1_\alpha\rangle = 0 \qquad \langle S^1_\alpha S^1_\beta\rangle \;=\; n_\alpha\delta_{\alpha\beta} \qquad \ldots \tag{2.3}$$

where for the Ising model (and most other models) the integer n_α is simply a product of the number of sites times the multiplicity of the interaction type S_α. When $H^g \neq H^1$, then to first order

$$\langle S^1_\alpha\rangle \;=\; \langle S^1_\alpha S^1_\beta\rangle_{H^g=H^1}\,(K^1 - K^g)_\beta \quad . \tag{2.4}$$

Using Eqs. (2.3,2.4), the renormalized couplings $\{K^1_\alpha\}$ are determined with no truncation errors

$$K^1_\alpha \;=\; K^g_\alpha \;+\; \frac{\langle S^1_\alpha\rangle}{n_\alpha} \quad . \tag{2.5}$$

This procedure can be iterated —— use H^{n-1} as the spin H in Eq. (2.1) to find H^n. If the irrelevant eigenvalues are small, then after two or three repetitions of the RGT, the sequence H^n converges to the fixed point Hamiltonian H^* which is assumed to be short ranged. For the $d = 2$ Ising model, the method has been shown to be extremely stable[27]. The linearity approximation, Eq. (2.4), is under control. An iteration process using a few thousand sweeps suffices to determine successively improved H^g upto an accuracy of $O(10^{-4})$. Beyond that the errors fall as $\sqrt{N}$ and the number of interactions that have to be included grow rapidly.

The one remaining approximation is in the use of a truncated H^{n-1} for the spin Hamiltonian in the update to find H^n. This is solved formally in a straightforward manner: In Eq. (2.1) use H^g as the guess for H^n. The update now involves the original spins and all block spins up to the n^{th} *level* in the Boltzmann weight

$$P(s^n, s^{n-1}) \;\ldots\ldots\; P(s^1, s)e^{-H(s)+H^g(s^n)} \quad . \tag{2.6}$$

The four Eqs. (2.2-2.5) are unchanged except that the *level* superscipt is replaced by n, *i.e.* the n^{th} *level* block-block correlation matrix .s diagonal and given by Eq. (2.3). With this modification, the H^n is calculated directly. The limitation on n is the size of the starting lattice. The other practical limitation is the complexity of the computer program. I have made the following comparison in the $d = 2$ Ising model[28]: H^2 was calculated using (2.2) and by iterating *i.e.* $H_c \rightarrow H^1 \rightarrow H^2$ in which case all interactions of strength $> 5\times10^{-4}$ are retained in H^1. The statistical accuracy in both cases is $O(10^{-5})$. I find that the iterated answer is good to only 10^{-4}. Thus the truncation errors do conspire and get magnified. The lesson learnt from the simple case of $d = 2$ Ising model is that in order to get couplings correct to one part in 10^{-5} at $n = 2$, it is necessary to include all couplings of strength $\geq 10^{-5}$ in H^1.

The calculation of the LTM proceeds exactly as in the standard $MCRG$ *i.e.* Eqs. (1.4) to (1.6). However, in the limit $H^g = H^1$, the block-block correlation matrix D is diagonal and given by Eq. (2.3). Thus it has no truncation errors, can be inverted with impunity and the final LTM elements are free of all truncation errors. This is the key feature of IMCRG. The only error comes from finding the eigenvalues from a truncated T matrix. These errors can be estimated and the results improved perturbatively as explained in section 3.

In addition to the advantages mentioned above, simulating with $IMCRG$, the system does not have critical slowing down. Second, the correlation length ξ can always be made of $O(1)$, so finite size effects are dominated by the range of interactions, which by assumption of a short range H^* fall off exponentially. Thus, critical phenomenon can be studied on small lattices and with no hidden sweep to sweep correlations that invalidate the statistical accuracy of the results. Using H^0 as the known nearest-neighbor critical point $K^c_{nn} = 0.4406868$, we[24] find that the $IMCRG$ results[27] for H^1 are independent (within the statistical accuracy $\approx 10^{-5}$) of finite size effects for lattice sizes 16, 32, 64 and 128. Again only couplings that fit into a 3×3 square were included.

$IMCRG$ is in practice very similar to $MCRG$ though a little more complicated because it requires a simultaneous calculation of a many term $H(s)$ and H^g at update. However, conceptually it is very different and powerful. I believe that $IMCRG$ provides a complete framework to analyze the critical behavior of spin systems. With the increased availability of supercomputer time we shall have very accurate and reliable results.

3: Truncation Errors In The LTM

Consider the matrix equation for T in block form

$$\begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix} \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} \tag{3.1}$$

where D_{11} and U_{11} are the 2 derivative matrices calculated in some truncated space of operators that are considered dominant. The elements of the sub-matrix T_{11} will have no truncation errors provided we can calculate

$$T_{11} = D_{11}^{-1} \{U_{11} - D_{12}T_{21}\} . \tag{3.2}$$

In the $IMCRG$ method the matrix D is diagonal and known, so D_{12} is 0. Thus elements of T_{11} determined from U_{11} have no truncation errors. The errors in the eigenvalues and eigenvectors arise solely from diagonalizing T_{11} rather than the full matrix T. Calculations in the $d = 2$ Ising model have shown that these errors are large, *i.e.* of order 10%, if all operators of a given range are not included. An open problem right now is a robust criterion for classifying operators into sets such that including successive sets decreases the truncation error geometrically by a large factor.

The errors arising from using a sub-matrix T_{11} can be reduced significantly by diagonalizing

$$T_{11} + T_{11}^{-1}T_{12}T_{21} = D_{11}^{-1}U_{11} + \{-D_{11}^{-1}D_{12} + T_{11}^{-1}T_{12}\}T_{21} \qquad (3.3)$$

as shown by Shankar, Gupta and Murthy[29]. The correction term $T_{11}^{-1}T_{12}T_{21}$ is the 2^{nd} order perturbation result valid for all eigenvalues that are large compared to those of T_{22}. The matrix $T_{12}T_{21} \approx (T^2)_{11} - (T_{11})^2$ can be calculated approximately in $IMCRG$. There are errors (which I have ignored) due to the RG flow, because of which T^2 is evaluated at a different point than T. The errors depend on how close to H^* the calculation is done. For the $d = 2$ Ising model we[28,29] find that the perturbative correction significantly decreases truncation errors in the relevant eigenvalues. However, straight $MCRG$ works just as well with far less work as explained below. The other thing we have learnt from this study is that the difference between the calculated eigenvalue at $n = 1$ $(1.97 \pm .01)$ and the exact result, 2, is not due to truncation errors or statistics. It is due to irrelevant operators causing corrections to scaling.

In standard $MCRG$, the calculations with $T_{11} = D_{11}^{-1}U_{11}$ have shown good convergence once few operators, $O(5 - 10)$, are included in T_{11}. The reason for this is an approximate cancellation between the two types of truncation errors. If in Eq. (3.1) we ignore terms with T_{22} and approximate $T_{11} = D_{11}^{-1}U_{11}$ then

$$-D_{11}^{-1}D_{12} + T_{11}^{-1}T_{12} \sim -D_{11}^{-1}D_{12} + U_{11}^{-1}U_{12} \ .$$

Further, usually these derivative matrices are roughly proportional, *i.e.* $U \sim \lambda_t D$ and the corrections fall off as the ratio of non-leading eigenvalues to the leading one λ_t. The derivation follows from the arguments of section 1.1 and can be checked by expanding operators in term of eigenoperators. Thus Swendsen[7] by calculating just $D_{11}^{-1}U_{11}$ and ignoring all truncation problems was effectively cancelling a large part of the truncation error (2^{nd} term in Eq. (3.3)) against the error arising from diagonalizing a truncated matrix (perturbative correction, 3^{rd} term in Eq. (3.3)). This explains his success. Shankar[30] has found a correction term to further decrease the truncation effects in $MCRG$. Given the assumptions, the flow under a RG and the success of the procedure as it exists, an improvement will be hard to evaluate. However, the check needs to be made.

Thus, at present the best way to get accurate results is to use $IMCRG$ to calculate the Renormalized couplings and Swendsen's $MCRG$ method to calculate the eigenvalues.

4: DETERMINATION OF THE RENORMALIZED HAMILTONIAN.

The advantage of using a hamiltonian close to H^* in MC simulations is to reduce the effect of operators that lead to scaling violations. There are, to the best of my knowledge, 11 methods in existence to calculate the renormalized couplings. These have been reviewed in ref.[8]. I shall here briefly describe only those methods most relevant to spin systems.

The generic problem of systematic errors in the estimate of the couplings due to a truncation in the number of couplings kept in the analysis will be referred to as "truncation errors". This is a serious drawback because the errors can be very large and there is no way of estimating them without a second long simulation. Unlike $IMCRG$, all the following methods have uncontrolled truncation errors.

4.1) Swendsen's method[31] using the Callen representation: The block expectations values of interactions are calculated in two ways. First as simple averages over block configurations, and second using the Callen representation[32] with a guess for the block couplings. From these two estimates, the block couplings at n levels are determined simultaneously. The estimate is improved iteratively. The method is fast and easy to implement but it does have undetermined truncation errors.

4.2) Callaway-Petronzio-Wilson[33,34] method of fixed block spins: This method is useful for discrete spin systems like the Ising model and models in the same universality class. A $MCRG$ calculation is modified by fixing all the block spins except one such that only a controllable few block interactions are non-zero. The system is simulated with the RGT used as an additional weight in the Metropolis algorithm. The ratio of probability of this unfixed spin being up to it being down is equal to a determined function of a certain number (depending on how many block interactions are non-zero) of block couplings. By using different configurations of fixed block spins a system of linear equations is set up from which the block couplings are determined. The drawback of this method, even for the Ising model, is that it is hard to set up the block spins so that only a few (≈ 10) block interactions are nonzero. Wilson showed that this can be done if one uses the lattice gas representation *i.e.* 0 or 1 for spin values. The couplings in the ± 1 representation are then given by an expansion in the lattice gas couplings. The second improvement due to Wilson is that instead of a MC determination of the ratio of probabilities, the exact result can be obtained in the transfer matrix formalism. In the $d = 2$ Ising model, the convergence of the ± 1 couplings in terms of the lattice gas couplings is slow[34]. About a 1000 lattice gas couplings were necessary for an accuracy of $\approx 10^{-4}$. However, the calculation is non-statistical and very fast.

4.3) Microcanonical (Creutz's Demon) Method[35]: This method is very efficient if from a previous $MCRG$ calculation expectation values of m block interactions at each of the n block levels are determined. To determine the corresponding couplings at the n^{th} level, a microcanonical simulation is then done (on a same size lattice as on which the block expectation values were calculated) with the corresponding m energies fixed and with one demon per interaction. The desired m couplings are then determined from the distribution of demon energies. The accuracy has a fundamental limitation for discrete spin systems because the demon energy and the total energy is discrete. The truncation errors are the same as in Swendsen's method with which it also shares an advantage; A single original calculation is necessary to determine the block interactions on many levels. Thus if the simulated H is critical, then at each blocking level H^n is also on the critical surface.

The renormalized couplings and H^* are no. universal but depend on the specific RGT. Therefore this improvement program is tied heavi' 'th $MCRG$.

Umrigar and I[24] have performed the following test in the $d = 2$ Ising model: We used $IMCRG$ to determine H^1 in the subspace of all 2-spin and 4-spin interactions that exist in a 3×3 square. This was then used to perform a standard MCRG calculation for the eigenvalues. The result was remarkable; the thermal eigenvalue is 2.001 ± 0.001 and the magnetic 3.669 ± 0.001 at the first level. The exact answers are 2 and 3.668. We are extending the calculation to include more blocking levels and use H^2 before proceeding to the $d = 3$ Ising model. If these stability tests work then we shall feel confident that a good way to calculate the exponents is to first calculate the renormalized couplings using $IMCRG$ and then c lculate the exponents by $MCRG$.

5: OPEN PROBLEMS

I shall just list the problems that have already been discussed before and elaborate on the rest.

[1] The accuracy of $MCRG$ in models with known violations of hyperscaling.

[2] Optimization of the RGT to improve convergence to H^*. The key here is to understand why the value of the magnetic exponent becomes worse as the kernel becomes longer ranged.

[3] A result obtained from the study of the $d = 2$ Ising model is that the LTM has elements that grow along rows and fall along columns[29]. The leading left eigenvector is normal to the critical surface. Its elements give an estimate of the growth in the elements along the rows of the LTM. For two spin interactions these grow like $x^{\frac{1}{\nu}}$. Therefore apriori the matrix T is badly behaved. The reason one gets sensible results is because the elements along the columns are observed to fall off faster (presumababiy exponentially). An open problem is to develop a theory for how elements along the columns fall-off. In problems examined so far we can arrange T to look like

$$\begin{pmatrix} A & B \\ \epsilon & D \end{pmatrix} \tag{5.1}$$

with A the minimal truncated $n \times n$ block matrix that should be calculated. The case $\epsilon = 0$ is simple; there are no truncation errors in either method and diagonalizing A gives the n largest eigenvalues. Otherwise for $IMCRG$ the truncation error depends on the dot product of terms in ϵ and B. The requirement of absolute convergence in the dot product only guarantees that this product is finite but it may be arbitrarily large i.e. $O(1)$. Therefore for each model, a careful study of the signs and magnitude of the elements in ϵ as a function of the RGT becomes necessary.

[4] So far I have only talked about the leading thermal eigenvalue. The irrelevant eigenvalues are known to be $\frac{1}{2^m}$. These are not well reproduced. For example we consistently find a value close to 0.4 rather than 0.5 for the leading irrelevant eigenvalue. The second unknown in this case is the statistical accuracy. While for the relevant eigenvalue determined by Swendsen's method there seems to be an amazing cancellation of sweep to sweep correlations between the matrices U and D, this is not true for the rest.

[5] A classification scheme for operators according to the range of the interactions. The criterion of success to use here is that on including a complete set, there should be a geometric decrease in truncation errors.

REFERENCES

[1] K. G. Wilson, in *Recent Developments in Gauge Theories*, Cargese (1979), eds. G. t' Hooft, *et al.* (Plenum, New York, 1980).

[2] R. H. Swendsen, Phys. Rev. Lett. **42**, (1979) 859.

[3] S. H. Shenker and J. Tobochnik, Phys. Rev. **B22** (1980) 4462.

[4] S. K. Ma, Phys. Rev. Lett. **37**, (1976) 461.

[5] L. P. Kadanoff, Rev. Mod. Phys. **49**, (1977) 267.

[6] K. G. Wilson, in *Progress in Gauge Field Theories*, edited by G. 't Hooft *et al.*, (Plenum, New York 1984).

[7] R. H. Swendsen, in *Real Space Renormalization, Topics in Current Physics*, Vol 30, edited by Th. W. Burkhardt and J. M. J. van Leeuwen (Springer, Berlin, 1982) pg. 57.

[8] R. Gupta, in *Proceedings of the Wuppertal Conference on Lattice Gauge Theories: A challange in large scale computing*, Plenum Press 1986.

[9] K. Binder, in *Monte Carlo Methods in Statistical Physics*, edited by K. Binder (Springer, Berlin,1979) Vol 7 , and in *Applications of Monte Carlo Methods in Statistical Physics*, (Springer Verlag, Heidelberg, 1983).

[10] M. Fischer in *'Advanced Course in Critical Phenomenon'*; Lecture Notes in Physics, Vol 186, Springer Verlag 1983.

[11] K. G. Wilson and J. Kogut, Phys. Rep. **12C**, (1974) 76.

[12] P. Pfeuty and G. Toulouse, *Introduction to the Renormalization Group and Critical Phenomenon*, (John Wiley & Sons, New York 1978).

[13] D. Amit, *Field Theory, the Renormalization Group and Critical Phenomenon*, (World Scientific, 1984).

[14] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller and E. Teller, J. Chem. Phys. **21** (1953) 1087.

[15] M. Creutz, Phys. Rev. D **21** (1980) 2308.

[16] D. Callaway and A. Rehman, Phys. Rev. Lett. **49** (1982) 613.
M. Creutz, Phy. Rev. Lett. **50** (1983) 1411.
J. Polonyi and H. W. Wyld, Phys. Rev. Lett. **51** (1983) 2257.

[17] G. Parisi and Wu Yongshi, Sci. Sin. **24** (1981) 483.

[18] G. G. Batrouni, G. R. Katz, A. S. Kronfeld, G. P. Lepage, B. Svetitsky, and K. G. Wilson, Cornell Preprint CLNS-85(65), May 1985.

[19] A. Brandt, in *Multigrid Methods*, Lecture Notes in Math 960, (Springer Verlag 1982) and references therein.

[20] The idea was first discussed by G. Parisi in *Progress in Gauge Field Theories*, edited by G. 't Hooft, *et al.*, (Plenum, New York, 1984).

[21] A more careful statement is made by M. E. Fischer and M. Randeria, Cornell Note (1985).

[22] R. Shankar and R. Gupta, Phys. Rev. B32 (1985) 6084.

[23] R. H. Swendsen, Phys. Rev. Lett. **52** (1984) 2321.

[24] R. Gupta and C. Umrigar, In progress

[25] H. Gausterer and C.B. Lang, Graz preprint UNIGRAZ-UTP 4/86.

[26] R. Gupta and R. Cordery, Phys. Lett. **A105** (1984) 415.

[27] R. Gupta in *Proceedings of the Tallahassee Conference on Advances in Lattice Gauge Theory,* World Scientific (1985).
[28] R. Gupta, in progress
[29] R. Shankar, R. Gupta and G. Murthy, Phys. Rev. Lett. **55** (1985) 1812.
[30] R. Shankar, Phys. Rev. B33 (1986) 6515.
[31] R. H. Swendsen, Phys. Rev. Lett. **52** (1984) 1165.
[32] H. B. Callen, Phys. Lett. **4B** (1961) 161.
[33] D. Callaway and R. Petronzio, Phys. Lett. **139B** (1984) 189.
[34] K. G. Wilson and C. Umrigar, unpublished.
[35] M. Creutz, A. Gocksch, M. Ogilvie and M. Okawa, Phys. Rev. Lett. **53** (1984) 875.