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A New MCRG Calculation of the Critical Behavior of the 3d Ising Model – Preliminary Results*

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Abstract

We have undertaken a large-scale computer simulation of the 3d Ising model using the Monte Carlo Renormalization Group (MCRG) method. Our calculation improves on past calculations in three ways. Firstly, larger lattices are used – we have run on 128^3 as well as 64^3. Secondly, many more spin operators – 53 even and 46 odd – are measured. Lastly, we have incorporated more efficient ways of spin update – Wolff's single-cluster variant of the Swendsen and Wang algorithm. In addition to calculating the critical temperature, the thermal and magnetic exponents, and improving the estimate of the correction-to-scaling exponent, we are aiming to verify the presence of redundant operators. We do not yet have sufficient statistics to give final results so here we describe our calculation and present preliminary results which demonstrate that we have control over both finite size effects and systematic errors arising from truncation.

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1. Introduction

The Ising model is the simplest model for ferromagnetism that predicts phase transitions and critical phenomena. This model, introduced by Lenz in 1920 [1] , was solved in one dimension by Ising in 1925 [2] , and in two dimensions by Onsager in 1944 [3] . However, it has not been solved analytically in three dimensions, so Monte Carlo computer simulation methods have been one of the methods used to obtain numerical solutions. One of the best available techniques for this is the Monte Carlo Renormalization Group (MCRG) method [4] . The Ising model exhibits a second-order phase transition in $d = 3$ dimensions at a critical temperature T_c. As T approaches T_c, the correlation length ξ diverges as a power law with critical exponent ν:

$$\xi = \xi_0 (T/T_c - 1)^{-\nu} \tag{1}$$

and the pair correlation function $G(r)$ at $T = T_c$ falls off to zero with distance r as a power law defining the critical exponent η:

$$G(r) = G_0 r^{-(d-2+\eta)}. \tag{2}$$

T_c, ν and η determine the critical behavior of the 3d Ising model and it is their values we wish to determine using MCRG.

Five years ago, this was done by Pawley, Swendsen, Wallace and Wilson [5] in Edinburgh on the ICL DAP computer with high statistics. They ran on four lattice sizes – $8^3, 16^3, 32^3$ and 64^3 – measuring seven even and six odd spin operators. With at least one million sweeps, measuring every fourth sweep, they were able to determine the critical coupling (inverse temperature) K_c to six decimal digits and the critical exponents ν and η to three, within their statistical errors. We are essentially repeating their calculation, which from now on we shall refer to as the "Edinburgh" calculation, on the new AMT DAP. Why should we do this? There are five main reasons. Firstly, to investigate finite size effects – we have run on the biggest lattice used by Edinburgh, 64^3, and on a bigger one, 128^3 (we can also go to 256^3). Secondly, to investigate truncation effects – qualitatively the more operators we measure for MCRG, the better, so we have included 53 even and 46 odd operators. Thirdly, we are making use of the new cluster-updating algorithm due to Swendsen and Wang [6] , implemented according to Wolff [7] . Fourthly, we would like to try to more accurately measure another critical exponent, the correction-to-scaling exponent ω. And finally, Edinburgh speculate that they found a redundant operator – we would like to substantiate this.

2. MCRG

The formulation of Monte Carlo Renormalization Group (MCRG) was completed in 1979 by Wilson and by Swendsen [4]; key ingredients were provided earlier by Ma and by

Kadanoff [8] . MCRG combines Monte Carlo (MC) simulations techniques of statistical mechanical models [9] with a renormalization group (RG) analysis of their critical properties [10] . The renormalization group is a set of scale transformations. The basic idea is that, since the critical properties of a system are not strongly affected by details on a short length scale, some fraction of the variables associated with short wavelength fluctuations may be integrated out, transforming the original system into a new one with fewer degrees of freedom. Such transformations are called renormalization group transformations. Typically they involve a local grouping of the variables into "blocks" and assigning a value to each "block variable" on the basis of the variables in each block. Block-variable transformations reduce the linear dimensions of a d-dimensional system by a scale factor s, where s^d is equal to the number of variables in a block. For the 3d Ising model, we divide the simple cubic lattice of spins into 2x2x2 blocks ($s = 2$) and assign the block spin the values +1 or -1 depending on the sign of the sum of the spins in the block. (When the sum is zero, +1 and -1 are assigned with equal probability.) If we write the Hamiltonian of the original system as

$$\mathcal{H} = \sum_{\alpha} K_{\alpha} S_{\alpha}, \tag{3}$$

where the S_{α}'s are combinations of the spins and the K_{α}'s are the corresponding coupling constants, then the RG transformation R_s produces a new system with renormalized Hamiltonian

$$\mathcal{H}' = R_s \mathcal{H} = \sum_{\alpha} K'_{\alpha} S'_{\alpha} \tag{4}$$

parameterized in terms of a new set of coupling constants $\{K'_{\alpha}\}$, with S'_{α} being combinations of the block spins. Thus the RG transformation is a mapping of the space of coupling constants onto itself, with its fixed points determining the critical surface by the standard theory [11] . To determine the critical coupling $K_c \equiv K_{1_c}$, one performs independent MC simulations on a large lattice L of size M^3 and on smaller lattices S of size $(M/2^m)^3, m = 1, 2, ...$, and compares the operators measured on the large lattice blocked m times more than the smaller lattices. $K_1 = K_{1_c}$ when

$$< S_{\alpha}^{(n)} >_L = < S_{\alpha}^{(n-m)} >_S . \tag{5}$$

Since the effective lattice sizes are the same, unknown finite size effects should cancel. The critical exponents y_a are obtained directly from the eigenvalues λ_a of the stability matrix $T_{\alpha\beta}$ according to $\lambda_a = 2^{y_a}$. In particular, the leading eigenvalue of $T_{\alpha\beta}$ for the even S_{α} gives ν from $y_1 = 1/\nu$, and similarly $y_1 = (d + 2 - \eta)/2$ from the odd $T_{\alpha\beta}$. $T_{\alpha\beta}$ is the linearized RG transformation matrix R_s near the fixed point and is defined by

$$T_{\alpha\beta} = \frac{\partial K_{\alpha}^{(n+1)}}{\partial K_{\beta}^{(n)}}. \tag{6}$$

By performing simulations at K_{1_c}, one can obtain estimates for the stability matrix by solving the linear equations

$$\frac{\partial < S_\gamma^{(n+1)} >}{\partial K_\beta^{(n)}} = \sum_\alpha T_{\alpha\beta} \frac{\partial < S_\gamma^{(n+1)} >}{\partial K_\alpha^{(n+1)}}. \tag{7}$$

In both eqs. (5) and (7) the best results are obtained from the largest blocking level n. Thus, in order to calculate all the quantities of interest using MCRG, we must evaluate the operators S_α. Unfortunately there are rather a lot of them. In [5] the calculation was restricted to seven even spin operators and six odd; we are evaluating 53 and 46, respectively. Specifically we have decided to evaluate the most important operators in a 3x3x3 cube. We do this by evaluating all of the operators in each of the three 3x3 planes forming the sides of the cube along the coordinate directions, and all of the operators in the 2x2x2 sub-cube lying in the corner of the 3x3x3 cube. In [12] we show all the spin operators for a 3x3 square and a 2x2x2 cube, and describe a computer code written to generate them.

3. Implementation on the DAP

The Distributed Array Processor (DAP) is a Single Instruction, Multiple Data (SIMD) computer consisting of $D \times D$ bit-serial processing elements (PEs) configured as a cyclic two-dimensional grid with nearest-neighbor connectivity. Originally made by ICL with $D = 64$, the DAP is currently made by AMT with $D = 32$ or 64. The Ising model computer simulation is very well suited to such a machine since the spins can be represented as single bit (logical) variables. In 3d the system of spins is configured as a $M \times M \times M$ simple cubic lattice which is "crinkle mapped" onto the $D \times D$ DAP by storing $N \times N$ pieces of each of M planes in each PE: $M \times M \times M = M \times (N \times D) \times (N \times D)$, with $N = M/D$.

When we began our simulation, we updated the spins using the standard Metropolis algorithm [13] , performing 100 sweeps between measurements. Now we are using a hybrid algorithm consisting of 10 such Metropolis sweeps plus 1 cluster-update using Wolff's single-cluster variant of the Swendsen and Wang algorithm [14] . Empirically, we found that the cluster-update evolves the magnetization more quickly than the energy, whereas Metropolis updates evolve the energy faster. By using this hybrid algorithm, we hope to obtain the best of both worlds. In fact, on a 128^3 lattice, the autocorrelation length of the magnetization reduces from 73 ± 2 sets of 100 sweeps for Metropolis alone to 5.0 ± 0.2 sets of 10 Metropolis plus 1 cluster-update for the hybrid algorithm.

In order to measure the spin operators S_α, the DAP code simply histograms the spin *configurations* so that an analysis program can later pick out each particular spin operator using a look-up table. In fact, four histograms are made: three with $512(= 2^9)$ entries for the 3x3 planes and one with $256(= 2^8)$ for the 2x2x2 sub-cube. The obvious way to

implement this on the DAP, namely by storing one histogram per PE, is inefficient because the PEs lack the hardware functionality to individually index different locations in their respective memories. Instead, we store a 512-entry histogram in D pieces along rows of the DAP. Then each of these histogram parts is decomposed as D columns and H memory locations, with $D \times H = 512$. During the measurement, the D partial histograms are updated in parallel and then summed into the complete histogram. Currently the code requires the same time to do 1 four-histogram measurement, 1 Wolff single-cluster-update or 100 Metropolis updates. Therefore, our hybrid of 10 Metropolis plus 1 cluster-update takes about the same time as a measurement.

4. Preliminary Results

We have run on lattices of size 64^3 and 128^3 at two values of the coupling: 0.221654 (Edinburgh's best estimate of the critical value) and 0.221644. On the smaller lattice we have measured $10K$ histograms, on the larger we have $30K$ for 0.221654 and $20K$ for 0.221644. These statistics are not very impressive compared to Edinburgh who had $250K$ measurements. However, our measurements are separated by either more (100 vs. four) Metropolis sweeps or by cluster-updates so our autocorrelation length is much smaller, and we are still running. Moreover, as will be demonstrated below, we have control over both finite size effects and systematic errors arising from truncation of the number of spin operators.

In order to analyze our results, the first thing we have to decide is the order in which to arrange our 53 even and 46 odd spin operators. Naively, they can be arranged in order of increasing total distance between the spins [12](as was done in [5]). However, the ranking of a spin operator is determined, physically, by how much it contributes to the energy of the system. Thus we initially did our analysis with the operators in the naive order to calculate their energies, then subsequently we used the "physical" order dictated by these energies. This physical order of the first 20 even operators is shown in Fig. 1 with six of Edinburgh's operators indicated; the seventh Edinburgh operator (E-6) is our 21st. This order is important because in order to access the systematic effects of truncation we are going to analyze our data as a function of the number of operators included. Specifically, we successively diagonalize the 1x1, 2x2, ..., 53x53 (for even, 46x46 for odd) stability matrix $T_{\alpha\beta}$ to obtain its eigenvalues and thence the critical exponents. Therefore, it is important both physically and numerically to have the operators arranged in order of decreasing importance. Since here we are reporting preliminary results, we shall present only plots of the eigenvalues, not the values of the critical exponents.

Firstly, we look at the truncation effects in the leading even eigenvalue which determines ν. In Fig. 2 we plot this eigenvalue vs. number of spin operators included in the analysis for the second, third, fourth and fifth RG blocking levels starting from the 128^3 lattice at an inverse temperature of 0.221654. (We ignore the first blocking level because

it suffers from strong transient effects and the sixth because being only 2^3 it is too small to accommodate all of the operators.) We see that there are strong truncation effects – the value of the eigenvalue does not settle down until at least thirty and perhaps forty operators are included. Also shown in Fig. 1, as horizontal lines, are the relevant results from the Edinburgh calculation: the dotted line is their value of the eigenvalue from the corresponding blocking level starting from their 64^3 lattice, and the dashed line is their extrapolation to the infinite lattice also taking into account their significant truncation errors. Firstly, note that our value agrees with Edinburgh's when around seven operators are included – this is a significant verification that the two calculations are consistent. Secondly, Edinburgh's 64^3 result is systematically off from our value with all 53 operators included. In fact, on the fifth blocking level, their value is off the top of the plot which is presumably due to the fact that their lattice is only 2^3 in size forcing them to drop their E-7 operator and therefore incur even worse truncation errors. Lastly, amazingly, Edinburgh's "phenomenological" extrapolation [15] appears to have saved the day on the higher blocking levels so that within statistical errors their result agrees with ours!

Turning to finite size effects, we show our results for the leading even eigenvalue on the first four blocking levels starting from the 64^3 lattice in Fig. 3, and on the first five blocking levels from the 128^3 lattice in Fig. 4, both at 0.221654. The values on the respective lattices agree, and the agreement improves with increasing blocking level. Thus we feel that we have overcome the finite size effects so that a 64^3 lattice is just large enough. However, the advantage in going to 128^3 is obvious in Fig. 4: there we can perform one more blocking, which reveals that the results on both the fourth and fifth blocking levels are consistent. This means that we have eliminated most of the transient effects near the fixed point in the MCRG procedure.

Unfortunately, the results for the leading odd eigenvalue are not quite as good as those for the even. In Figs. 5 and 6 we show the analogous plots to Figs. 3 and 4. The first three blocking levels are consistent but the fourth appears to have too large a value on the 64^3 lattice. This may be a problem with statistics as we only have $10K$ measurements on the 64^3 lattice; we shall find out when we run some more.

The second largest even eigenvalue gives the correction-to-scaling exponent according to $\lambda_2 = 2^{-\omega}$. Our results for this are shown in Fig. 7. The fourth and fifth blocking levels are not consistent and there is a very strong dependence on truncation so again we should reserve judgement until we have more statistics.

Finally, perhaps the most important number, as it can be determined the most accurately, K_c. Our first set of runs at Edinburgh's value for the critical coupling $K = 0.221654$ on the two lattice sizes 64^3 and 128^3 indicated that $K - K_c = 0.000005(2)$. Therefore we are carrying out a second set of runs at $K = 0.221644$ hoping to find the same value for $K - K_c$ but with the opposite sign. So far, we do not have enough data to extract a reliable

estimate for this.

5. Conclusions

We set out to do five things and are making good progress. We believe that we have overcome finite size effects for the leading even eigenvalue and with more data hope to do the same for the leading odd and second largest even eigenvalues. We seem to have control over the truncation effects – all of the eigenvalues settle down to a constant value when at least thirty or forty spin operators are included. We are successfully using Wolff's single-cluster variant of the Swendsen and Wang algorithm, along with some standard Metropolis sweeps, to update our lattices. We have measured the correction-to-scaling exponent, it comes out significantly less than one but we do not yet have a consistent value. In order to look for redundant operators, one has to calculate the eigenvectors as well as the eigenvalues of the stability matrix; we are just beginning to do this now. As for our preliminary results, the leading even and odd eigenvalues disagree with Edinburgh's 64^3 numbers but agree with their extrapolated values; the critical coupling may be a little less than Edinburgh's estimate. We intend to at least double our statistics before publishing final results.

While this work was in progress, we learned of a similar simulation performed on the DISP at Delft [16] . They measured about half the number of operators as we did and only ran on the same lattice sizes as Edinburgh.

Acknowledgements

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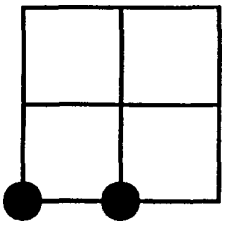
Fig. 1: Our Order for Even Spin Operators



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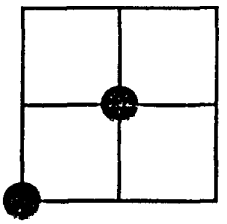

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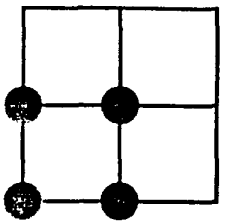

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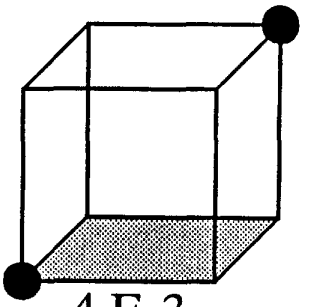

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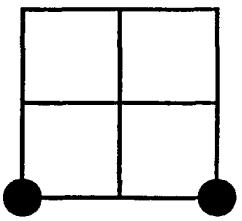

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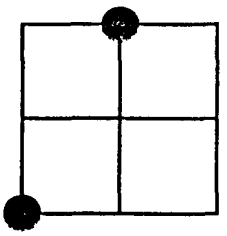

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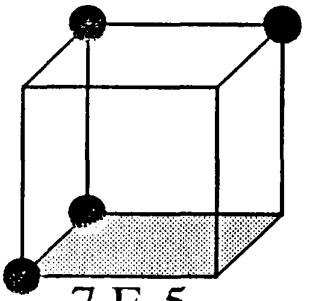

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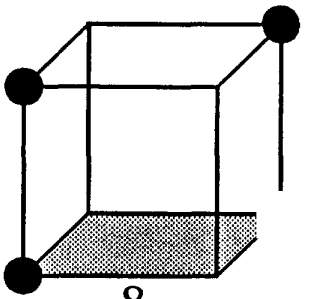

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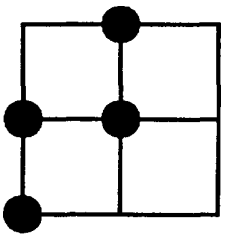

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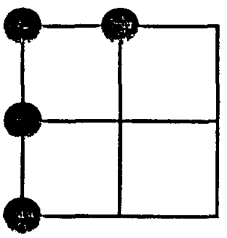

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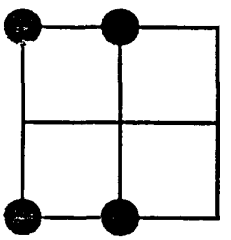

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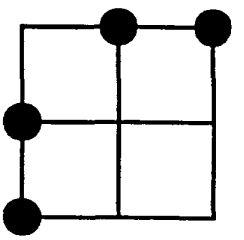

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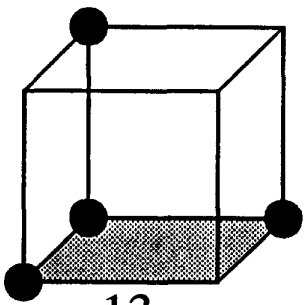

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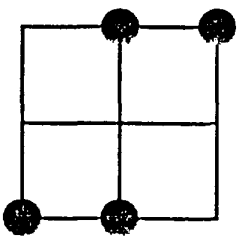

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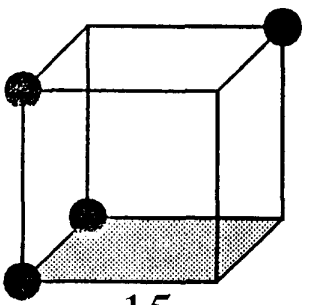

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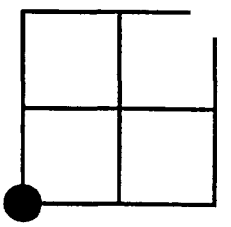

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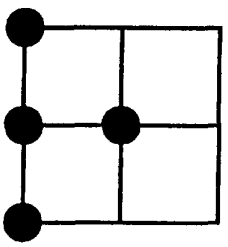

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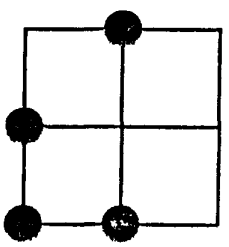

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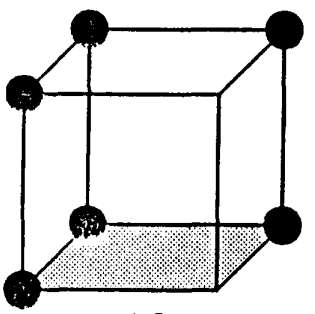

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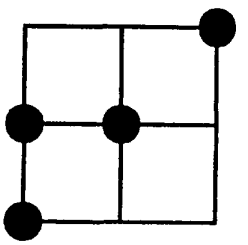

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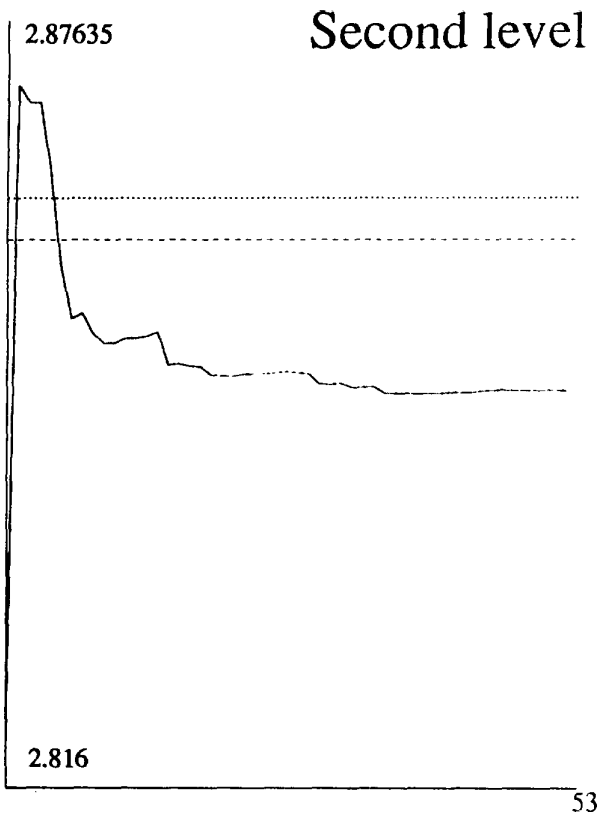
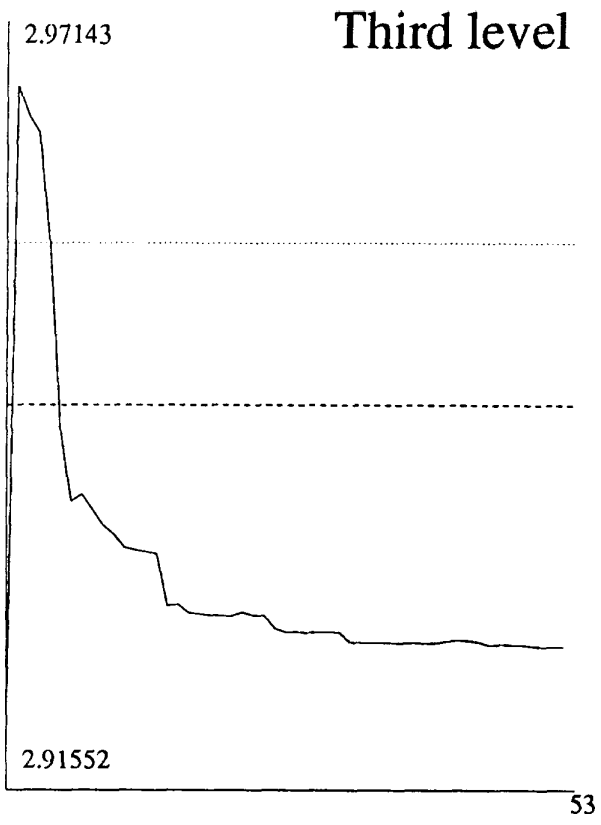
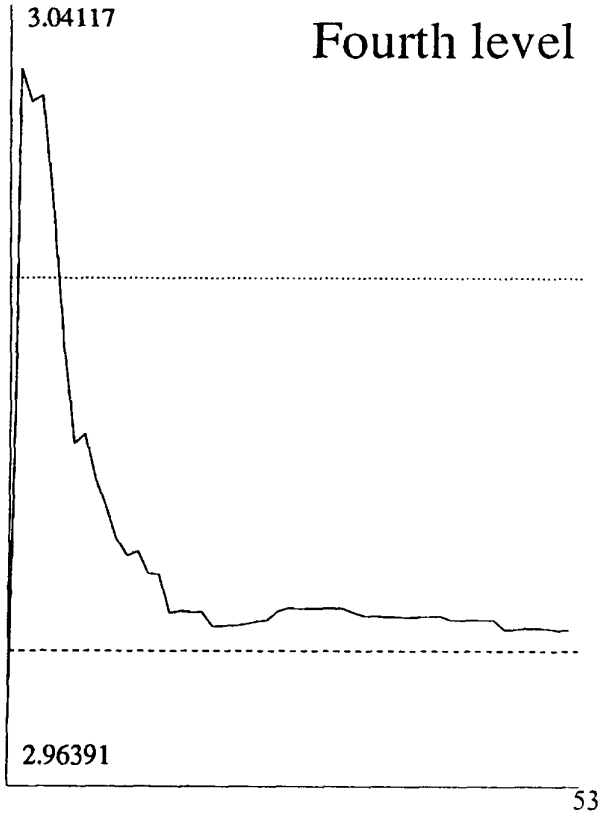
Fig. 2: Leading Even Eigenvalue vs. No. Operators







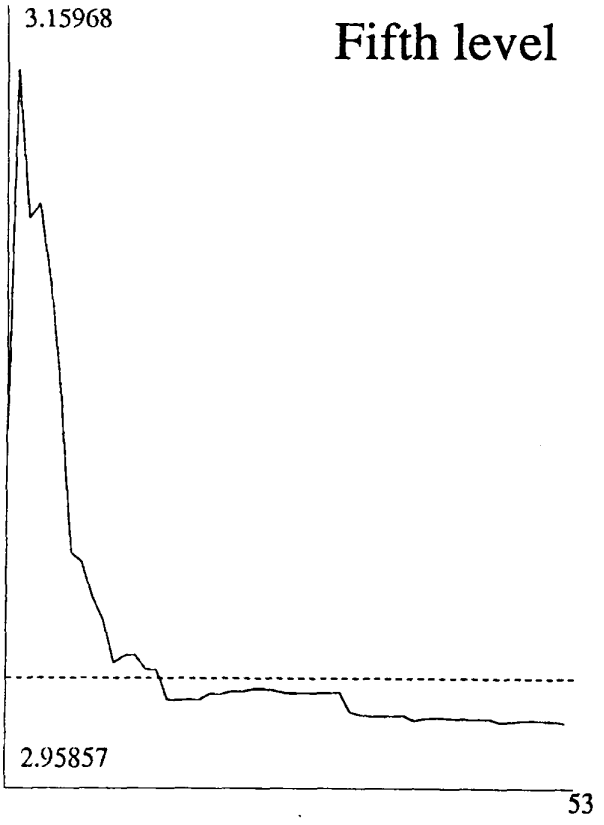


Fig. 3: Leading Even Eigenvalue

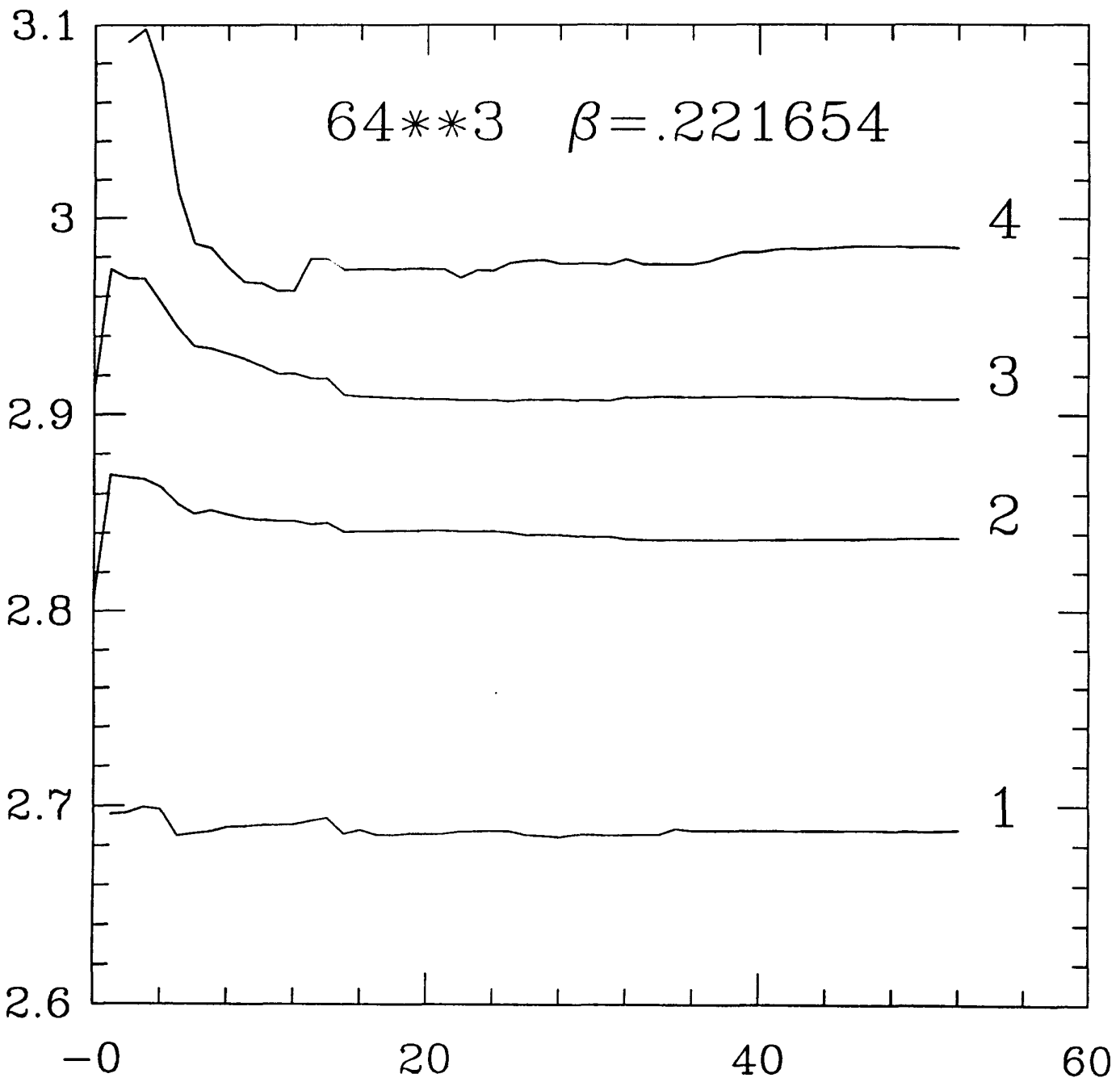


Fig. 4: Leading Even Eigenvalue

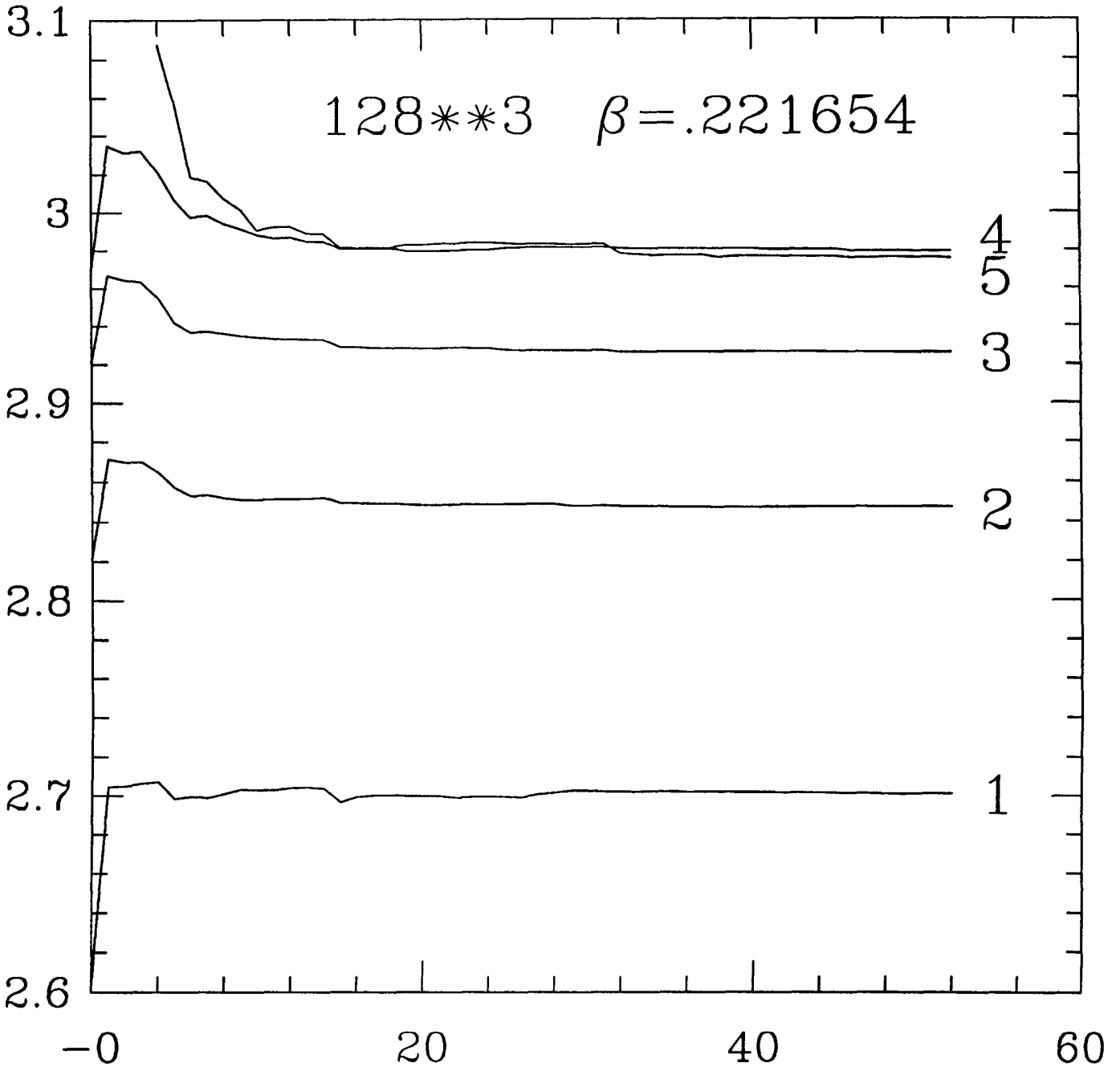


Fig. 5: Leading Odd Eigenvalue

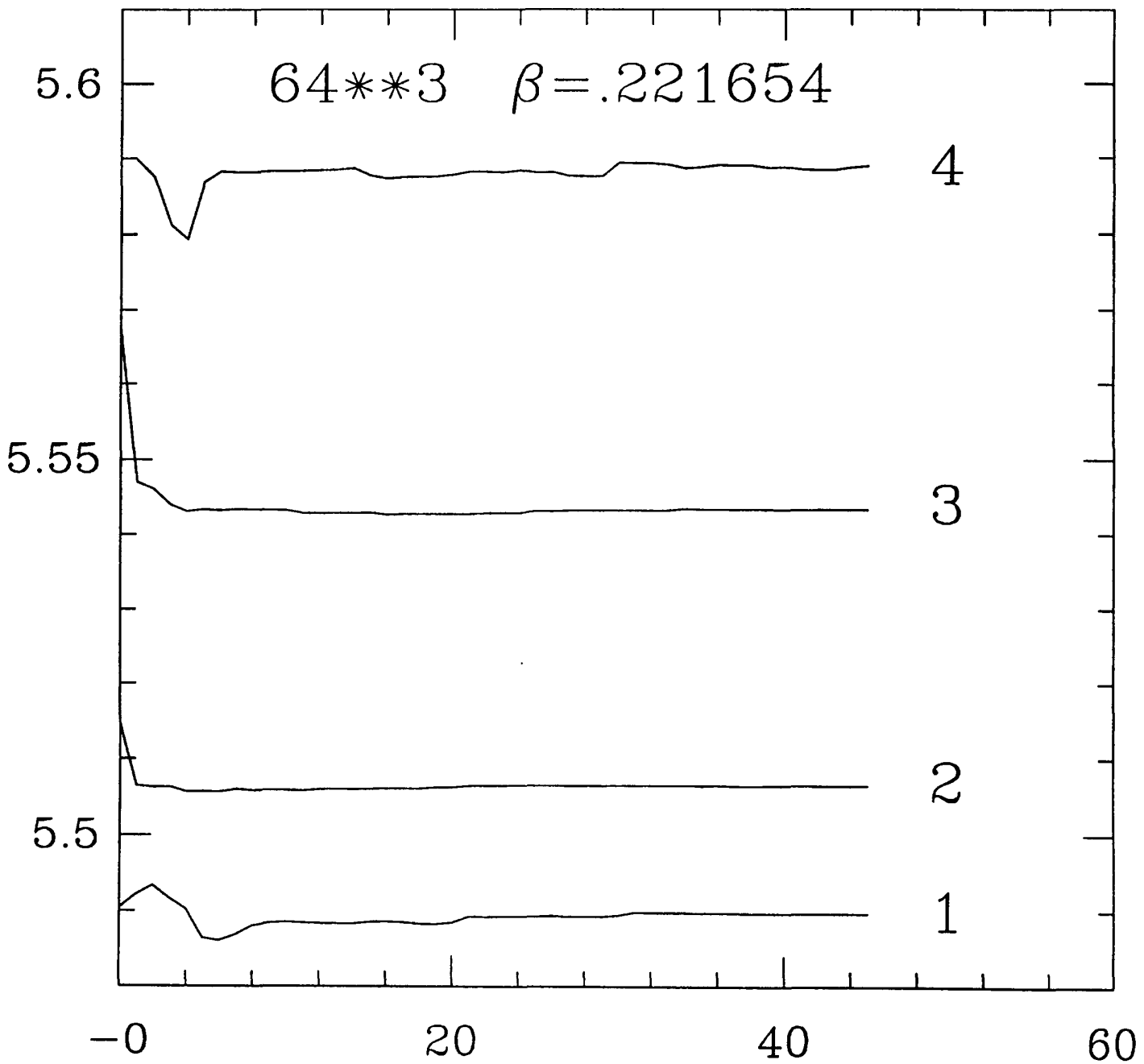


Fig. 6: Leading Odd Eigenvalue

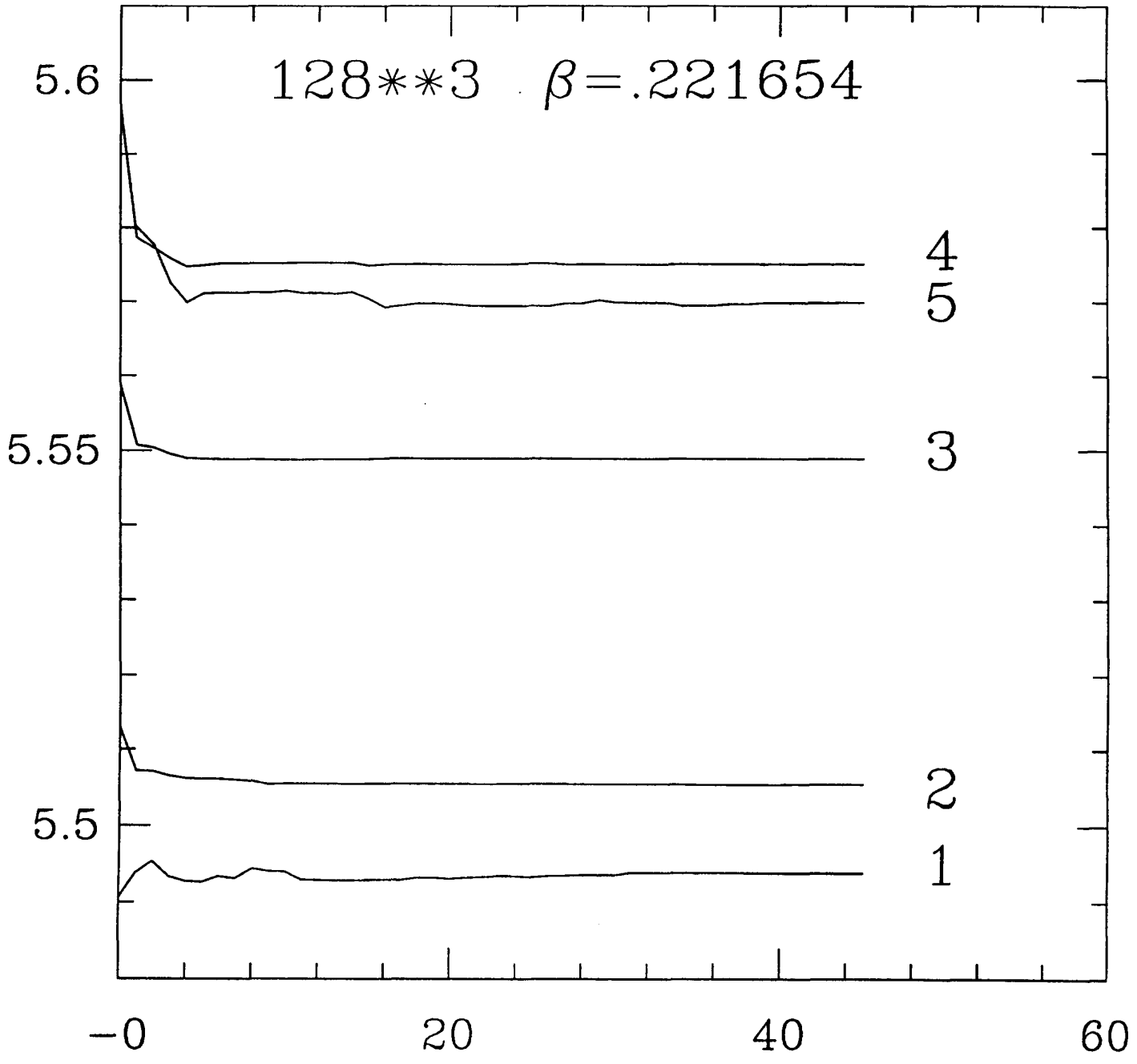


Fig. 7: Second Even Eigenvalue