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Finite-size scaling in the (2+1)D Ising model

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Abstract. Hamiltonian eigenvalues are calculated for the (2+1)D Ising model on lattices up to 5×5 sites. Finite-size scaling techniques are used to estimate the critical coupling $x_c = 0.329 \pm 0.001$, and index $\nu = 0.635 \pm 0.005$. The prospects are discussed for further applications of these methods in three and four dimensions.

1. Introduction

Finite-lattice techniques have recently been developed (Hamer and Barber 1980, 1981a,b, the last two to be referred to as HBI and HBII respectively, Roomany and Wyld 1980, Nightingale 1976) to explore the spectrum and phase structure of models in lattice field theory and statistical mechanics. The approach involves the calculation of eigenvalues of the Hamiltonian or transfer matrix on a sequence of lattices of increasing size. Sequence extrapolation algorithms (HBII, Barber and Hamer 1982) may then be used to estimate the bulk limit for an infinite lattice, in accord with the hypotheses of finite-size scaling (Fisher 1971, Fisher and Barber 1972, HBI). Critical parameters may be calculated using similar methods.

These procedures have by now been demonstrated to equal or surpass in accuracy any other general numerical technique, for models in two dimensions (HBII, Blöte *et al* 1981), but in three or four dimensions, their efficacy is much less obvious. One needs a sequence of at least four or five different lattice sizes for the extrapolation methods to work, but the sheer numerical size of the problem forbids one from calculating exact eigenvalues for the larger lattices.

The aim of the present work is to 'calibrate' the problem by applying these techniques to the 3D Ising model and pushing them as far as possible. Roomany and Wyle (1980) have already studied the (2+1)D Hamiltonian field theory version of the Ising model on lattices up to 4×4 sites in (spatial) extent. We have continued on to the 5×5 lattice. This calculation employed a basis of 86 056 spin states, which is an order of magnitude larger than previous works in this area (though calculations of similar size have been performed in nuclear physics, cf Whitehead *et al* (1977)).

Applying sequence extrapolation methods (HBII, Barber and Hamer 1982) to these data, estimates of the critical coupling x_c and index ν were obtained:

$$x_c = 0.329 \pm 0.001$$
$$\nu = 0.635 \pm 0.005. \tag{1.1}$$

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These results are consistent with those obtained by series analysis (Marland 1981, Moore *et al* 1969, Baker and Hunter 1973) and renormalisation-group methods (Baker *et al* 1978, Le Guillou and Zinn-Justin 1980). Their accuracy is comparable to that of series analysis, but rather less than that of the renormalisation group. They provide evidence of universality with the 3D Ising model, as expected.

In § 3, it is pointed out that similar success cannot be expected for other models in three or four dimensions. For almost any other model, one will be unable to calculate exact eigenvalues for the 4×4 lattice, let alone the 5×5. Our sequence extrapolation methods then become virtually useless.

Some possible ways out of this situation exist. The logical next step is to explore the use of approximate rather than exact finite-lattice eigenvalues. By making systematic approximations, one may truncate the number of basis states to be considered, and thus treat larger lattice sizes (this is clearly reminiscent of the Monte-Carlo philosophy). It then remains to be seen whether reliable extrapolations of these approximate finite-lattice sequences can be made.

2. Finite-size scaling analysis

The quantum Hamiltonian field theory version of the Ising model has been discussed by Fradkin and Susskind (1978). On a two-dimensional spatial lattice of $M\times M$ sites, with a continuous time variable, the quantum Hamiltonian may be written† (Hamer *et al* 1979), in a 'high-temperature' representation,

$$H=\frac{g}{2a}\Big(\sum_m(1-\sigma_3(m))-x\sum_{m,\hat{\mu}_i}\sigma_1(m)\sigma_1(m+\hat{\mu}_i)\Big). \tag{2.1}$$

Here the index m labels sites on the spatial lattice, and $\{\hat{\mu}_i\}$ are its two unit base vectors. The σ_i are Pauli matrices acting on a two-state spin variable at each site, g is a dimensionless coupling constant (proportional to temperature), a is the lattice spacing and $x=2/g^2$. It is convenient to work, instead, with the reduced Hamiltonian

$$W=\frac{2a}{g}H=M^2-\sum_m\sigma_3(m)-x\sum_{m,\hat{\mu}}\sigma_1(m)\sigma_1(m+\hat{\mu}). \tag{2.2}$$

Periodic boundary conditions are assumed:

$$\sigma_1(m+M\hat{\mu}_i)=\sigma_1(m).$$

The quantities of interest to us are the two lowest-lying eigenvalues of W, denoted ω_0 and ω_1. They have been computed for a sequence of different lattice sizes $M=1$–5. The calculations for the 5×5 lattice were long and tedious, involving a basis of some 86 000 strong-coupling eigenstates. Technical comments on the methods of computation may be found in the appendix.

The correspondences between Hamiltonian field theory and statistical mechanics are by now standard (see e.g. Kogut 1979, HBI, HBII). The quantities of physical interest here can all be deduced from the two eigenvalues ω_0 and ω_1. They include

† In the language of statistical mechanics, this is the 'transverse Ising model' Hamiltonian. The correspondence between the d-dimensional transverse Ising and $(d+1)$-dimensional ordinary Ising models is well known (Elliott *et al* 1970, Pfeuty 1970, Suzuki 1976).

the mass gap or inverse correlation length

$$F(x) = \omega_1(x) - \omega_0(x), \tag{2.3}$$

the Callan–Symanzik β function

$$\frac{\beta(g)}{g} = \frac{F(x)}{(F(x) - 2xF'(x))} \tag{2.4}$$

and the 'specific heat' (HBI)

$$\tilde{C}(x) = -x^2\omega_0''(x). \tag{2.5}$$

Finite-size scaling methods can be used to estimate the behaviour of these functions in the bulk limit, $M \to \infty$ (for details and a history of these methods, the reader is referred to previous work: HBI, HBII, Roomany and Wyld 1980). Away from the critical point, the eigenvalues are expected to converge linearly to their bulk limit, and so an iterated Aitken's algorithm can be used to estimate this limit from the finite-lattice values (HBII). The ensuing results for the ground-state energy per site, the specific heat per site, the mass gap and beta function are illustrated in figures 1 and 2. For the beta function, the upper set of finite-lattice curves are those for the function (2.4); the lower set depict the Roomany–Wyld estimates,

$$\frac{\beta(g)}{g} = \ln R_M(x)\left(\ln\left(\frac{M}{M-1}\right)\right)^{-1}\left(1 - x\frac{\mathrm{d}}{\mathrm{d}x}\ln(F_M(x)F_{M-1}(x))\right)^{-1}. \tag{2.6}$$

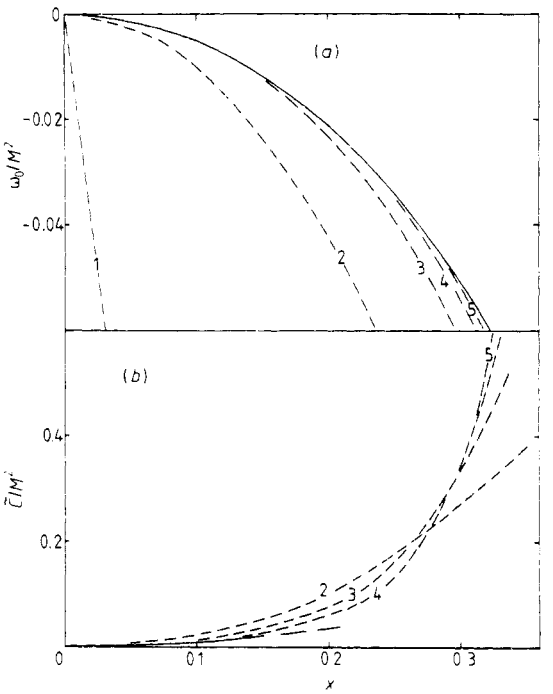

Figure 1. (*a*) Ground-state energy per site, and (*b*) specific heat per site, plotted against the variable x. The broken curves are finite-lattice results, labelled by the lattice size M. The full curve is the estimated bulk limit, and is expected to be accurate to the order of the width of the curve, except where breaks appear.

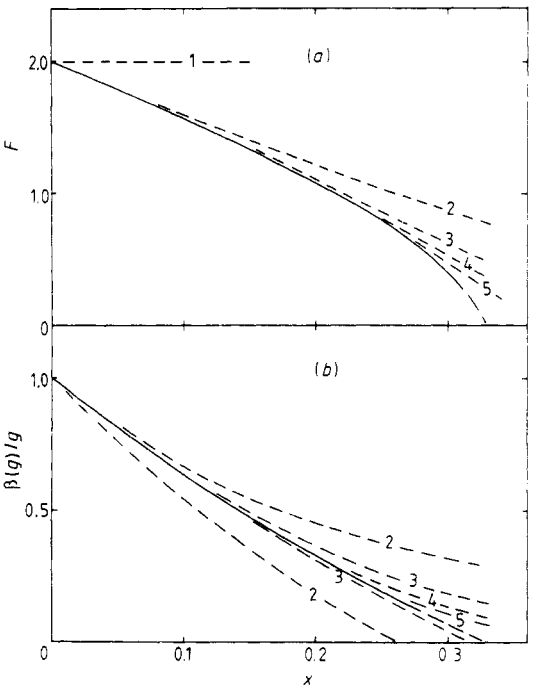

Figure 2. (*a*) The mass gap, and (*b*) the beta function, plotted against the variable x. Conventions are as in figure 1. In (*b*) the upper curves are the direct finite-lattice results, equation (2.4); the lower ones are the Roomany–Wyld estimates, equation (2.6). The Roomany–Wyld estimates for $M = 4$ and 5 are almost indistinguishable from the bulk limit, so for clarity they have been omitted.

Here $F_M(x)$ is the mass gap for lattice size M, and $R_M(x)$ is the 'scaled mass gap ratio' (HBI)

$$R_M(x) = \frac{MF_M(x)}{(M-1)F_{M-1}(x)}. \tag{2.7}$$

As can be seen from figure 1(*b*), the Roomany–Wyld estimates converge remarkably quickly to the bulk limit. A critical point is clearly evident at $x_c \simeq 0.33$: the mass gap and beta function vanish there, and the specific heat shows evidence of a divergence.

Finite-size scaling can now be used to estimate the critical parameters. First of all, a sequence of estimates of the critical point, $\{x_M\}$, may be found (HBI, HBII) as solutions of the equation

$$R_M(x_M) = 1. \tag{2.8}$$

The results are listed in table 1. This sequence is expected to converge logarithmically to the bulk limit. Now in HBII a 'modified VBS algorithm' (Vanden Broeck and Schwartz 1979) was used to extrapolate such sequences. However, this algorithm requires a minimum of five terms in the original sequence, so it is inapplicable here. Instead, we use an algorithm due to Lubkin (1952) which can start on only four terms, and which we have found (Barber and Hamer 1982) to be similar in accuracy and reliability to the VBS one. Let the terms of the original sequence be denoted

Table 1. Finite-size scaling estimates for the critical point x_c, and critical indices $1/\nu$ and α/ν. The finite-lattice estimate for each quantity, respectively, is x_M, $\rho_M(0)$ and $\sigma_M(0)$, as defined by equations (2.8), (2.12) and (2.15), where M is the larger of the two lattice sizes used in each estimate.

M	x_M	$\rho_M(0)$	$\sigma_M(0)$
2	0.260 342	1.278 17	2.000 00
3	0.316 000	1.380 21	0.782 01
4	0.324 249	1.432 43	0.592 47
5	0.326 696	1.463 80	0.512

S_n, $n \geqslant 0$; and define

$$R_n = \frac{S_n - S_{n-1}}{S_{n-1} - S_{n-2}} \qquad (S_{-1} = 0).$$

Then the terms in the transformed sequence are (Lubkin 1952)

$$W_n = S_n + \frac{(S_{n+1} - S_n)(1 - R_n)}{(1 - 2R_{n+1} + R_n R_{n+1})} \qquad n \geqslant 1. \tag{2.9}$$

The new sequence is expected to converge more rapidly than the original one.

The results of this extrapolation are given in table 2. The sequence $\{x_M\}$ is smooth, monotonic and rapidly convergent, so that a fit of the form

$$x_m \underset{M\to\infty}{\sim} x_c - aM^{-\Delta} \tag{2.10}$$

gives the exponent $\Delta \simeq 3.5$. Our final estimate for the critical point is

$$x_c = 0.3289 \pm 0.001. \tag{2.11}$$

The exponent ν can be calculated (HBI, HBII) from the finite-lattice beta function (2.4), evaluated at the 'pseudo-critical points' x_M. Define

$$\rho_M(\varepsilon) = (M + \varepsilon)\left(1 - \frac{\beta_M(x_M)}{\beta_{M-1}(x_M)}\right) \tag{2.12}$$

where ε (the 'end-shift') is a free parameter which is inserted to test the accuracy and reliability of the sequence extrapolation; then we expect

$$\lim_{M\to\infty} \rho_M(\varepsilon) = 1/\nu \qquad \text{for all } \varepsilon. \tag{2.13}$$

Table 2. Typical sequence extrapolation using Lubkin's algorithm for the critical point x_c, and the critical indices $1/\nu$ and α/ν. In each case, the left-hand column lists the finite-lattice estimates, and the right-hand column lists the Lubkin extrapolants.

M	x_M		ρ_M ($\varepsilon = -0.2$)		σ_M ($\varepsilon = 0$)	
2	0.260 342		1.150 35		2.000 00	
3	0.316 000	0.324 821	1.288 20	7.930 31	0.782 01	0.268 61
4	0.324 249	0.328 873	1.360 80	1.574 89	0.592 47	0.277
5	0.326 696		1.405 25		0.512	

Values of $\rho_M(0)$ are listed in table 1. Using the Lubkin algorithm (2.9) to extrapolate this sequence, one obtains the results depicted in figure 3(*a*). The result is stable for $\varepsilon < 0$, and choosing $\varepsilon = -0.2$ we obtain (table 2)

$$1/\nu = 1.575 \pm 0.01$$
$$\nu = 0.635 \pm 0.005. \tag{2.14}$$

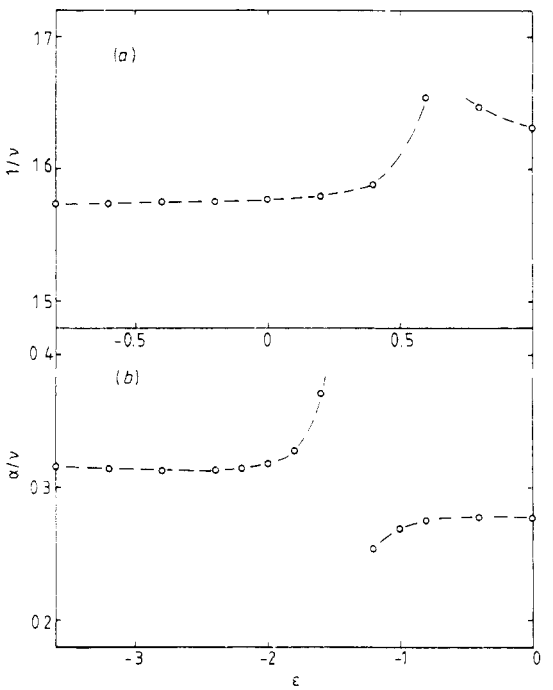

Figure 3. Estimates of (*a*) $1/\nu$, and (*b*) α/ν, as functions of the end-shift ε. The estimates were obtained by Lubkin's method from sequences of finite-lattice results, as discussed in the text.

The exponent Δ governing the convergence of this sequence (cf (2.10)) is $\Delta \simeq 1.0$. Note that our estimate of ν is 'unbiased' in the sense that it does not depend on the critical-point estimate, equation (2.11).

Finally, an attempt was made to estimate the specific heat exponent α. Defining a sequence of values (HBII)

$$\sigma_M(\varepsilon) = (M+\varepsilon)\,|1 - \tilde{C}_M(x_M)/\tilde{C}_{M-1}(x_M)| \tag{2.15}$$

where again ε is a free 'end-shift' parameter, we expect

$$\lim_{M\to\infty} \sigma_M(\varepsilon) = \alpha/\nu \qquad \text{for all } \varepsilon. \tag{2.16}$$

Values of $\sigma_M(0)$ are listed in table 1. The results of a Lubkin extrapolation are shown

in figure 3(*b*). They are fairly stable to changes in ε (except where a switch occurs in the direction of approach to the limit, $\varepsilon \simeq -1.5$), and hence one might assign

$$\begin{aligned} \alpha/\nu &= 0.295 \pm 0.02 \\ \alpha &= 0.19 \pm 0.02. \end{aligned} \tag{2.17}$$

This is a poor result when compared with other approaches which give $\alpha \simeq 0.1$. One might perhaps ascribe this failure to the presence of 'background' terms; however, figure 1(*b*) shows little sign of a strong, constant 'background', and such a term might be expected to decrease the apparent value of α rather than increase it. A more likely explanation is that our sequence is simply too short: the initial entry σ_2, for instance, contains no 'dynamical' information, and a sequence of effectively three members is insufficient even for the Lubkin algorithm.

The accuracy claimed for the critical parameters x_c and ν may seem surprising, in view of the fact that we considered only lattices up to 5×5 sites. The explanation lies in the fact that the Ising model is extremely well behaved, and provides smooth and rapidly convergent estimates in the high-temperature region. This was already seen in previous series analysis work, and it is again evident in the finite-lattice results presented here.

3. Discussion

Our principal results for the critical parameters of the (2+1)D Ising model, in summary, are

$$\begin{aligned} x_c &= 0.3289 \pm 0.001 \\ \nu &= 0.635 \pm 0.005. \end{aligned} \tag{3.1}$$

These were obtained from a sequence of square, $M \times M$ lattices up to $M = 5$. They are therefore expected to be more accurate than the estimates $x_c = 0.320 \pm 0.001$ and $\nu = 0.640 \pm 0.004$ obtained by Roomany and Wyld (1980) using lattices up to $M = 4$.

The most accurate series results for this model are those of Marland (1981), who calculated 'low-temperature' series for the Hamiltonian (2.1) using a linked cluster expansion. He quotes

$$\begin{aligned} x_c &= 0.3285 \pm 0.0005 & \alpha' &= 0.097 \pm 0.001 \\ \beta &= 0.315 \pm 0.005 & \gamma' &= 1.25 \pm 0.002. \end{aligned} \tag{3.2}$$

Our estimate of the critical point is in good agreement with equation (3.2). Unfortunately there is no direct estimate of the exponent ν in this work.

The ordinary 3D Ising model has been studied extensively in statistical mechanics, of course. The various numerical results have been reviewed by Le Guillou and Zinn-Justin (1980). Among the most accurate estimates from high-temperature series analysis are

$$\begin{aligned} \nu &= 0.638^{+0.002}_{-0.001} && \text{(Moore } et\ al \text{ 1969)} \\ \alpha &= 0.13 \pm 0.01 && \text{(Baker and Hunter 1973);} \end{aligned} \tag{3.3}$$

while using field-theoretic renormalisation-group methods, the values obtained are

$$\nu = \begin{cases} 0.630 \pm 0.0015 & \text{(Le Guillou and Zinn-Justin 1980)} \\ 0.630 \pm 0.002 & \text{(Baker } et\ al \text{ 1978)} \end{cases}$$
$$\alpha = \begin{cases} 0.110 \pm 0.0045 & \text{(Le Guillou and Zinn-Justin 1980)} \\ 0.110 \pm 0.008 & \text{(Baker } et\ al \text{ 1978).} \end{cases} \tag{3.4}$$

Allowing for a little hyperbole in the error estimates all round, the estimates (3.1)–(3.4) are in quite good accord for the exponents ν and α, providing evidence of universality between the 3D and (2+1)D formulations.

It thus appears that finite-lattice methods are capable of supplying critical exponents for the 3D Ising model of comparable accuracy to those from series analysis, but they are still not quite competitive with renormalisation-group methods. What then, are the prospects for extending this approach to other models in three and four dimensions?

For the (2+1)D Ising model on a 5×5 lattice, a total of 86 056 strong-coupling basis states were involved in the calculation of each eigenvalue ω_0 and ω_1. This number can be approximately predicted as follows. The total number of states in either the even- or odd-spin sector is $2^{24} \simeq 1.7 \times 10^7$. However, the ground state is symmetric under translations, rotations and reflections: by exploiting this fact, and identifying spin states which are equivalent to each other under these transformations, we may reduce the number of basis states to be considered by a factor of approximately 200, to about 8.5×10^4. For a 6×6 lattice, the corresponding number is $2^{35}/288 \simeq 1.2 \times 10^8$ states. A calculation of this size is quite out of the question at the present time.

For more complicated models, the situation is even worse. For a Z_3 spin model, one might try to solve the 4×4 lattice—but for any more complicated model, even this would be impossible. Now with only 2×2 and 3×3 lattices available, our sequence extrapolation methods are virtually useless: one needs a sequence of reasonable length (four or five entries at least) in order to achieve good quantitative accuracy. Finite-lattice techniques should still give a reliable picture of the phase structure (Roomany and Wyld 1980, Irving and Thomas 1982), but no very accurate estimates of the critical parameters will be possible.

Are there any ways out of this situation? One possibility is to make use of non-square lattices, e.g. the 2×3 lattice, in order to extend the length of the sequence. The scaling behaviour of non-square lattices has been discussed by Ferdinand and Fisher (1969), Roomany and Wyld (1980) and Horn and Karliner (1982). We have made some preliminary investigations of this option: it does not look very hopeful, but needs further exploration. The problems are (i) the 2×3 lattice results seem to merely 'interpolate' half-way between the 2×2 and 3×3 results, and carry no independent information, and (ii) the sequence algorithms of § 2 are postulated upon equally spaced values of M, whereas a 2×3 lattice corresponds to a non-integral effective M. More flexible algorithms could no doubt be found.

A second option is to retreat from the demand that the finite-lattice eigenvalues be exact. One may then employ some systematic method of approximation, truncate the number of basis states used in the calculation and thus obtain results for larger lattices. This option is inevitable, in fact, for models with a continuous symmetry group, because the total number of basis states is infinite, even for a finite lattice. We plan to pursue this idea in future work.

Our conclusion, then, is that the finite-lattice method is unlikely to challenge series analysis and renormalisation-group techniques in the study of conventional second-

order phase transitions in three and four dimensions. However, confining gauge theories have a more complicated singularity structure, so that conventional series analysis methods are inappropriate (Carroll *et al* 1977, Hamer 1979), and renormalisation-group methods have so far proved to be complicated and ineffective. We hope that finite-lattice techniques may have a role to play in these areas.

Acknowledgments

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Appendix. Numerical methods

Previous works (HBII, Roomany *et al* 1980, Irving and Thomas 1982) have discussed the numerical techniques used in finite-lattice calculations. We refer the reader to these papers for a full account, and merely append some comments for *aficionados* relevant to the case of the 5×5 lattice.

(i) The calculations were performed on a VAX 11/780 computer with virtual memory. The total CPU time taken was of order 60 h.

(ii) The basis states were taken as eigenstates of the operator $\Sigma_m (1-\sigma_3(m))$—i.e. ordinary spin states, in a 'strong-coupling' basis. Starting from the strong-coupling ground state, new basis states were generated by application of the pair operators $\sigma_1(m)\sigma_1(m+\hat{\mu}_i)$, until the list of basis states was complete, and the matrix elements of H connecting them had all been calculated and stored on tape. There were a total of 86 056 states and about 2.1×10^6 matrix elements generated in each of the odd- and even-spin sectors.

(iii) Each new binary-coded state vector was transformed by translations, rotations and reflections, and its degeneracy factor under these operations was stored. Thenceforth, the minimum value of the binary state vector obtained during these transformations was used to describe the state. Since this process takes up a major portion of the CPU time, it was carried out by an assembly-language subroutine, and in registers as far as possible, following Roomany *et al* (1980) and Irving and Thomas (1982).

(iv) The different state vectors were held in an address-sorted master file for the purposes of comparing one with another. The hash code used was simply the binary number describing the state vector, suitably scaled down to fit the length of the file (it is advisable to take a square root or logarithm here also). However, the distribution of states is rather 'spiky', and many 'collisions' tended to occur when placing new states in the file. It was therefore found necessary to break the file up into bins, and to reshuffle it from time to time, recalculating the address limits on each bin so as to smooth out the distribution of occupied entries. This operation takes relatively little time, and prevents the number of collisions from escalating unmanageably as the file fills up.

(v) In the second stage of the calculation, tapes containing a list of basis states and the matrix elements connecting them were processed using an iterative algorithm

for large sparse matrices to compute the minimum eigenvalue of H. Following the authors initially quoted, we used a Lanczos routine for this purpose, rather than the conjugate gradient method used previously. The Lanczos method seems somewhat quicker to converge, and for a large calculation like this one, offers the great advantage of requiring less storage space.

(vi) During the Lanczos phase, it was at first found that an excessive number of page faults were occurring as the matrix H was multiplied into the state vectors. This problem was cured by buffering the entries into the new state vector and sorting them in order before emptying the buffer.

(vii) In order to obtain the eigenvalues and their derivatives with sufficient accuracy at the 'pseudo-critical' points x_M, these points were first identified approximately in a 'first pass' calculation, using $M \leqslant 4$ only. In a second pass, eigenvalues were calculated at a cluster of five points, spaced at intervals $\Delta_x = 0.005$, straddling each x_M. The required quantities could then be calculated accurately by finite-difference interpolation algorithms. For the 5×5 case, a single cluster centred at $x = 0.32$ was calculated. The Lanczos routine converged to an accuracy of one part in 10^7 in 18 or 19 iterations; approximately 50 min CPU time was required per iteration for the five-point cluster.

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