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Alan Middleton
Syracuse University

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Numerical Results for the Ground-State Interface in a Random Medium

A. Alan Middleton

Department of Physics, Syracuse University, Syracuse, NY 13244

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Abstract

The problem of determining the ground state of a d -dimensional interface embedded in a $(d + 1)$ -dimensional random medium is treated numerically. Using a minimum-cut algorithm, the exact ground states can be found for a number of problems for which other numerical methods are inexact and slow. In particular, results are presented for the roughness exponents and ground-state energy fluctuations in a random bond Ising model. It is found that the roughness exponent $\zeta = 0.41 \pm 0.01, 0.22 \pm 0.01$, with the related energy exponent being $\theta = 0.84 \pm 0.03, 1.45 \pm 0.04$, in $d = 2, 3$, respectively. These results are compared with previous analytical and numerical estimates.

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In many physical systems, the equilibrium and non-equilibrium behavior of interfaces determine the thermodynamic and dynamic properties of the system. Examples of such interfaces include the phase boundary between spin-up and spin-down domains in an Ising magnet and the fluid-vapor interface in porous media. A number of problems in statistical mechanics can be mapped onto questions about surfaces in a higher dimensional system; for example, the Potts models can be cast as “height models” [1]. The study of interfaces has also been applied to the fracture in solids, where the fracture location relative to the original whole body is treated as an interface [2]. Quenched disorder greatly affects the equilibrium and dynamical properties of interfaces and phase boundaries [3]. An interface is distorted by the random forces or potential caused by the disorder, so that its shape is much rougher than in a pure system.

The problem considered here is that of finding the ground state, or zero-temperature configuration, of a d -dimensional interface in a $(d + 1)$ -dimensional medium with quenched disorder, i.e., spatially varying couplings that are fixed in time. Given a method for finding the minimal energy configuration of an interface for a particular realization of the disorder, statistical properties can be found by averaging over many realizations. One can then determine, for example, how the perpendicular width W of the interface and the fluctuations in the ground state energy depend on the linear size L of the interface. These quantities capture many of the features of the low energy state and are relevant to thermodynamic properties of the interface at low temperatures. This information can also be used to place lower bounds on the barriers between low energy configurations [3,4], to study the sensitivity of the location of the interface to perturbations [5], and to help to analyze the motion of an interface subject to an external drive [4].

The approach to finding the ground state used in this paper applies a minimum-cut (or “mincut”) algorithm [6] to find the exact ground state. Algorithms for finding the mincut take a time bounded by a polynomial in the volume of the system; finding the “best” algorithm is still a matter of active research in combinatorial optimization. The polynomial time bound means, however, that this algorithm is extremely fast compared to annealing

techniques, exhaustive search techniques, or transfer-matrix algorithms [7] that take a time exponential in the size of the system. Given such an algorithm, quantities of interest can be measured and averaged over many realizations of the quenched disorder. A type of mincut algorithm has been applied previously to the random field Ising magnet [8]. The mincut algorithm is applicable to many other physical problems, however. In this paper, I describe the general technique and summarize the results for the interface in the random bond Ising model.

The problem of finding the ground state of a random bond Ising model (RBIM) in zero field is that of minimizing the total energy

$$E = - \sum_{\langle ij \rangle} J_{ij} s_i s_j, \quad (1)$$

where the spin variables s_i take on the values ± 1 and the sum is over nearest neighbor pairs $\langle ij \rangle$ on a $(d + 1)$ -dimensional lattice. The $J_{ij} \geq 0$ are independent identically-distributed random variables; in this paper, the J_{ij} are taken to be uniformly distributed in the range $[0, 1)$. I consider here a lattice of dimensions $H \times L^d$, with coordinates $\{y, x_1, \dots, x_d\}$, $0 \leq y < H$, and $0 \leq x_\alpha < L$ for $1 \leq \alpha \leq d$. Boundary conditions must be chosen to induce an interface; this is done by setting the spins s_i to have the value $+1$ on the surface $y = 0$ and to be equal to -1 on the surface $y = H - 1$. Nearest neighbors are defined so that the constant x_0 surfaces represent slices of a “cubic” lattice taken along the $[11 \dots 1]$ direction [9]. The RBIM is used to describe a ferromagnet with random variation in the coupling strength due to spatial disorder of the spins or impurities. This model has also been used to describe fracture in materials, where the J_{ij} represents the local force needed to break the material [2] and it is assumed the fracture occurs along the surface of minimum total rupture force.

The problem of the random bond Ising magnet was treated numerically by Huse and Henley [10] for $d = 1$, in the case of the directed polymer, where the interface is restricted to be described by a single valued function $y(x_1)$. The algorithm used, an iterative transfer-matrix method, will find the lowest energy state subject to this restriction. Though the

algorithm used here need not be subject to this restriction, the single-valued- y approximation is convenient for analytical work and is believed to not affect the long wavelength behavior. Huse and Henley found that the transverse width

$$W = \left\{ \sum_{\{x_\alpha\}} y^2(x_\alpha) - \left[\sum_{\{x_\alpha\}} y(x_\alpha) \right]^2 \right\}^{1/2} \quad (2)$$

scaled with the length L of the interface as W^ζ , with $\zeta \approx 0.66$. It was also found that the sample-to-sample rms fluctuations in the ground state energy varied as $\Delta E \sim L^\theta$, with $\theta \approx 0.33$. Subsequently the $d = 1$ case was solved analytically by Huse, Henley and Fisher [10], who showed that $\zeta = 2/3$ and $\chi = 1/3$ in $d = 1$, consistent with the numerical work of Huse and Henley. Numerical work for interface dimension $d = 2$ was done by Kardar and Zhang [7], using a transfer matrix which operates on the space of paths; this algorithm, though exact, requires a time exponential in one of the dimensions of the system; they were consequently restricted to lattices with linear dimension $L \leq 16$. From their simulations, they found $\zeta = 0.50 \pm 0.08$ and $\theta = 1.10 \pm 0.05$ in $d = 2$. Analytical arguments have been given for the roughness exponents in higher dimensions [2,11,12].

The algorithm used to find the ground state is based upon a maximum network flow algorithm. The network flow problem is defined on a graph with given ‘‘capacities’’ indicating the rate at which fluid can flow from one node of the graph to another along a directed edge that connects the two nodes. The goal is to determine the maximum amount of flow that can be sustained between two given points, the source and the sink, given current conservation at each of the non-terminal nodes. It is straightforward to show that the maximum flow value is equivalent to the value for the minimum ‘‘cut’’, which is defined as the weight of the set of edges with minimum total capacity that, when cut, disconnect the source and the sink. This minimum cut can be imagined as describing a minimal flow surface that separates the source and the sink by intercepting the flows through the removed edges. The equivalence of the network flow and the minimum cut is due to the fact that the minimum cut is the ‘‘bottleneck’’ through which all flow must pass.

To apply this algorithm to the RBIM, a graph is constructed whose minimum cut directly

reflects the minimum energy interface in the spin lattice. This is done by attaching two fictitious spins to the lattice, the source and the sink, which can be seen as setting the boundary conditions for the spin in the Ising magnet. The source is connected by an edge to each $y = 0$ site; each $y = H - 1$ site is connected to the sink. The capacity on each of these auxiliary edges is set to be a very large value ($2d$ times the maximum J_{ij}) so that the minimum cut surface does not pass through these edges and instead lies in the bulk. One then has the choice of whether or not to implement the single-valued- y approximation, according to the choice of the capacities of the edges connecting the bulk nodes. If for each pair of nearest neighbors $\langle ij \rangle$, two edges are created, one from i to j and the other from j to i , each with capacity $2J_{ij}$, the maximum flow algorithm will give the interface and energy of the unrestricted interface problem. The cost of the minimum cut, i.e., the minimum of $2 \sum J_{ij}$ over all surfaces which separate the source and the sink, is then equal to the minimal energy of an interface, above the ground state (which has all spins equal). See Fig. (1) for a diagram of this construction.

For $d = 2, 3$, I simulated the restricted, single-valued, problem by choosing the capacity of the edge connecting i to j to be J_{ij} if $y(i) < y(j)$ and to be $2d \max(J_{ij})$ if $y(i) > y(j)$. (Because of the choice of lattice alignment, $y(i) \neq y(j)$ for nearest neighbors $\langle ij \rangle$.) The high cost of the “backwards” edges, those connecting higher y -coordinate sites to those with smaller y -coordinates, excludes them from the minimal cut [13]. In order to minimize the effects of the boundary surfaces on the energy associated with the minimum cut, the edge costs were increased to $2d \max(J_{ij})$ on a single line of bonds from one boundary to the other, except on the center edge. The minimal cut surface will not intersect this line except at the midpoint, where the energy is not raised. This modification therefore “pins” the interface at one point, which is halfway between the boundaries.

Once the corresponding graph is constructed, the max-flow/min-cut algorithm can be directly applied. Specifically, the algorithm and code developed by Cherkassky and Goldberg [14] was adapted to the class of graphs studied here; this code was approximately 2-3 times faster than other code applied to this problem. The computer time for the solution of a

particular realization on an IBM RS/6000-390 workstation was found to average 230s for $d = 2, L = 120, H = 50$ and 146s for $d = 3, L = 30, H = 20$, with the time for smaller systems being nearly proportional to the volume of the sample. The program gives both the minimum-cut cost, i.e., the ground state energy, and the location of the minimum-cut. The width of the interface was computed by finding the rms fluctuation of the y -coordinate of the cut bonds; the cut can be visualized by drawing the plaquettes that are dual to the cut bonds.

The results for the sample-averaged interface widths and energy fluctuations are shown in Fig. (2) and Fig. (3), for $d = 2$ and $d = 3$, respectively. The scaling plots assume a scaling form for the average width

$$\overline{W(L, H)} = L^\zeta w(H/L^\zeta), \quad (3)$$

with $w(x) \sim x$ for $x \rightarrow 0$ and $w(x) \sim \text{const}$ for $x \rightarrow \infty$, and a scaling form for the rms energy fluctuations of

$$\overline{\Delta E(L, H)} = L^\theta u(H/L^\zeta), \quad (4)$$

with $u(x) \sim x^{\theta/\zeta}$ for $x \rightarrow 0$ and $w(x) \sim c$ for $x \rightarrow \infty$. The best scaling fits for the largest L are obtained for the values $\zeta = 0.41 \pm 0.01, 0.22 \pm 0.01$ and $\theta = 0.84 \pm 0.03, 1.45 \pm 0.04$, in $d = 2, 3$, respectively. The statistical errors due to sample-to-sample fluctuations in the width W are relatively small (for almost all sizes, 10^4 samples were generated; at least 10^3 samples were generated in all cases). The statistical errors in the energy fluctuations ΔE are somewhat larger, as can be seen from the scatter in the plots. The dominant source of errors in these fits are from the unknown corrections to scaling; the uncertainty in the exponents indicates the range of values over which the curves for the three largest L values agree to within statistical error when scaled. The larger relative errors in θ are also due to a long crossover in the scaling plots; the widths W appear to converge more quickly, yet also have a slow convergence after a sharp crossover. The exponent values satisfy the scaling relation $2\zeta = \theta + d - 2$ to within numerical error [10]. Applying this scaling relation using

the numerical values of ζ gives $\theta = 0.82 \pm 0.02, 1.44 \pm 0.02$ for $d = 2, 3$, respectively. The exponents found here are in disagreement with the results of Ref. [7]; this is likely due to finite size effects in the smaller systems examined there. Given the current numerical accuracy, it is difficult to differentiate between the analytical results of Fisher and those of Halpin-Healy, which are very close in value ($\zeta = 0.208(4 - d)$ and $\zeta = 2(4 - d)/9$, respectively). The numerical results are in agreement with both. The constraint preventing computations for larger systems on workstations is memory (> 256 MB will be required) rather than total CPU time.

The max-flow algorithm for determining min-cuts has been applied to several problems in the past, most notably the random field Ising magnet [8], but this is the first time that it has been applied directly to the random bond Ising model. As has been noted, this technique is also applicable to other systems of current interest. This technique is not restricted to single-valued height interfaces. For example, from simulations without the single-valuedness restriction, I find the roughness exponent $\zeta = 0.67 \pm 0.02$ for $d = 1$, in agreement with theory and numerical results for the case where overhangs are forbidden (the directed polymer problem) [3].

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FIGURES

FIG. 1. Example of the construction of the graph whose minimum-cut corresponds to the ground state of a random-bond Ising model with twisted boundary conditions. (a) The sites and bonds for an Ising problem, with dimensions $L = 2$ and $H = 4$ (in $(d = 1) + 1$ dimensions). The stronger bonds (larger J_{ij}) are indicated by thicker widths. The sites are labeled according to their values in the ground state configuration, with sites fixed to take on the values $-$ and $+$ on the left and right sides, respectively. (b) The corresponding graph for the minimum-cut problem. The “source” and “sink” nodes are auxiliary nodes added to the bulk lattice to define the boundary conditions. Nodes are connected by directed edges, with the capacity of the edges indicated by the width of the lines. The bulk forward edges have capacities J_{ij} . “Forbidden” backwards edges with large weights (greatest thicknesses) both enforce boundary conditions and prevent overhangs in this example; see text for the case with overhangs. The minimum-cut surface separating the sink from the source is indicated by the broken line.

FIG. 2. Scaling plots for average ground state quantities in $2 + 1$ dimensions. All lengths are measured in units of the lattice constant. (a) Scaling of the average sample width $W(L, H) = \overline{\langle y^2(x) \rangle - \langle y(x) \rangle^2}$. The scaled width W/L^ζ is plotted vs. the scaled transverse sample size H/L^ζ for different L , using the value $\zeta = 0.41 \pm 0.01$. (b) Scaling plot for the sample-to-sample fluctuations in the ground-state energy. The scale energy fluctuations $\Delta E/L^\theta$ are plotted as a function of scaled transverse sample size H/L^ζ for varying L , using $\theta = 0.84 \pm 0.03$.

FIG. 3. Scaling plots for average ground state quantities in $3 + 1$ dimensions. The plotted quantities are the same as in Fig. (2), with $\zeta = 0.22 \pm 0.01$ and $\theta = 1.45 \pm 0.04$.

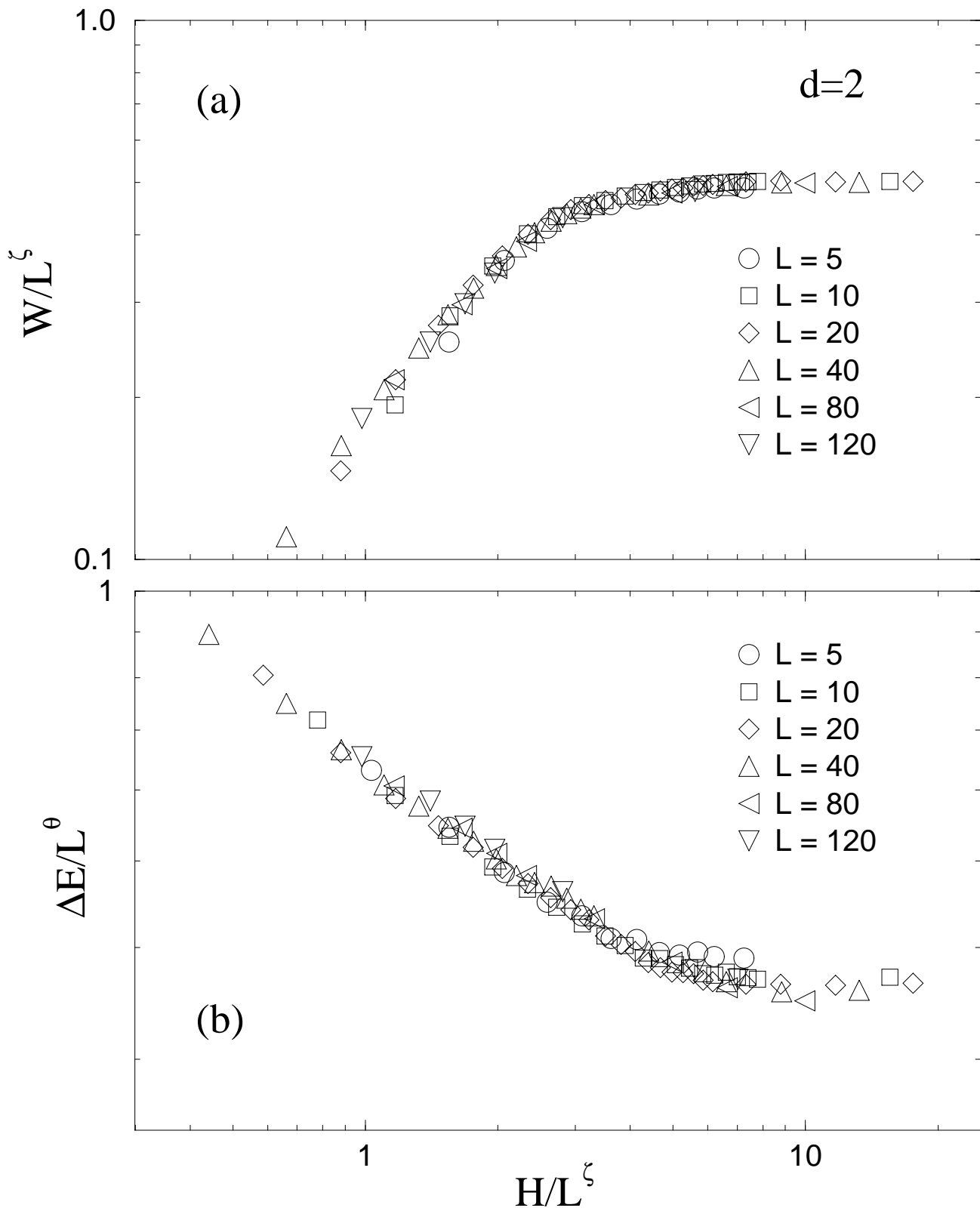


Fig. 2 - Middleton, Numerical Results for the Ground-State...

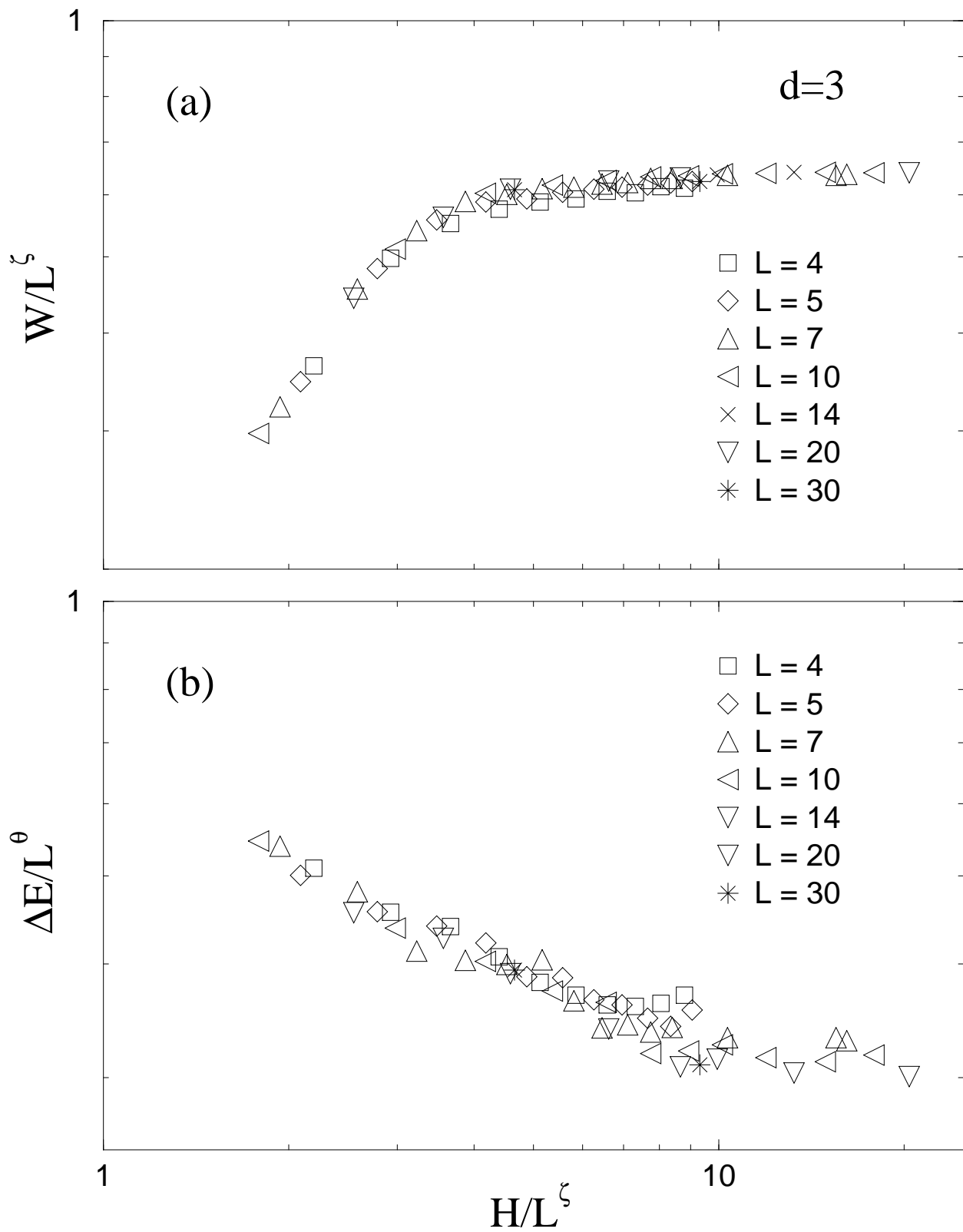


Fig. 3 - Middleton, Numerical Results for the Ground-State...