The Dobrushin–Shlosman Phase Uniqueness Criterion and Applications to Hard Squares

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The rigorous Dobrushin–Shlosman phase uniqueness criterion is reviewed, then applied to the hard square model to prove that only a single phase exists at activity $z = 1.185$. The criterion is violated (for a five-site by five-site lattice cell) at $z = 1.35557$, but this does not imply phase nonuniqueness. This work complements that of Dobrushin, Kolafa, and Shlosman, who proved phase uniqueness for all $z \leqslant 1$. Certain "experimentally" discovered regularities are presented as conjectures: one for a more general problem and two for the application to hard squares. Even with these regularities, however, substantial further improvements in the algorithmic implementation of the criterion will be required before it can become a practical tool for locating phase transitions.

1. INTRODUCTION

The problem of locating phase transitions is both important and difficult. The critical temperature of even the simple three-dimensional Ising model, for example, has not been located rigorously, although useful upper and lower bounds have been established. One method of establishing such bounds is through a "phase uniqueness criterion," i.e., a criterion which, when satisfied, guarantees that the system in question has only a single equilibrium phase. Since at temperatures below the critical temperature the Ising model exhibits two-phase coexistence, any temperature at which the system satisfies the uniqueness criterion is an upper bound on the critical temperature. In this paper we discuss a new phase uniqueness criterion, due to Dobrushin and Shlosman,[1] and apply it to the hard square model.

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Currently, the most important and successful phase uniqueness criteria are applicable only to ferromagnetic spins with pair interactions. Most of the phase uniqueness criteria applicable to general systems (such as the earlier criterion of Dobrushin[2]) have a serious limitation: If, at a given temperature, the system satisfies the criterion, then it is known to be in the single-phase regime. If, on the other hand, it fails to satisfy the criterion, then the test gives no information and, even worse, nothing can be done to improve matters. The new Dobrushin–Shlosman result escapes this limitation because the criterion is applied to an arbitrary subset of the lattice (the so-called "lattice cell"). If the criterion is satisfied, the system has only a single phase. But if it is not, the criterion can be applied again to a different (presumably larger) lattice cell. It has been conjectured that extending this process to ever larger cells will locate the transition exactly.[1,3] (Dobrushin's earlier criterion[2] is precisely the Dobrushin–Shlosman criterion applied to a cell of a single lattice site.)

The Dobrushin–Shlosman criterion can thus in principle locate transition points, but the question remains of whether it can do so efficiently enough to become a useful tool. An answer can be supplied only by testing the criterion on a non-trivial statistical mechanical system: we follow the lead of Dobrushin et al.[4] and investigate the system of hard squares.[5] We find that despite the fact that this system is ideally suited for analysis by the phase uniqueness criterion, the transition location bounds obtained are in fact quite far from the true location, which is known to high precision from nonrigorous series analysis techniques.[6]

An outline of the paper follows: Section 2 states (without proof) the Dobrushin–Shlosman criterion. In Section 3 we show how to apply the criterion using linear programming techniques with the assistance of a computer. Our tests have shown that such algorithmic implementations are far easier and faster than one might at first suppose, and we formalize this discovery as a conjecture. Section 4 applies the criterion to the hard square model. Once again unexpected regularities appear, and these are formalized into two conjectures. A summary of the hard square results and a general discussion of the prospective utility of the Dobrushin–Shlosman criterion are given in Section 5.

2. THE CRITERION

The Dobrushin–Shlosman criterion is a precise refinement of the observation that the macroscopic state of a system with only one phase is insensitive to changes in the boundary conditions, while the state of a system in which two or more phases coexist can be very sensitive to such changes. [Consider, for example, an Ising model in zero field. At high

temperatures (and for large enough systems), the magnetization per spin vanishes whether the boundary consists of all up spins or of all down spins. But below the critical temperature, in the two-phase regime, flipping all the boundary spins from up to down will dramatically alter the system's character, as reflected by a change in the sign of the magnetization.] To turn this motivation into a mathematical tool, Dobrushin and Shlosman provide the following precise definitions. (The theorem applies to lattice systems with continuous or discrete variables at each lattice site. For simplicity, this paper treats only discrete variables.)

A *lattice cell* V is a finite set of (usually contiguous) lattice sites. Their number is denoted $|V|$.

The *boundary* of V, denoted ∂V, consists of all those sites that interact with sites in V but are not themselves in V. Thus, the boundary of V for a system with nearest-neighbor and next-nearest-neighbor interactions is larger than the boundary of V for a system with nearest-neighbor interactions alone.

The *configuration* of V will be represented by either i or j. The *boundary condition*, i.e., the configuration of the boundary ∂V, will be represented by either x or y.

If the boundary ∂V is in configuration x, then the *probability* that V is in configuration i is denoted $p(i \mid x)$. Generally this probability will be a normalized Boltzmann factor,

$$p(i \mid x) = \exp[-H(i \mid x)/k_B T]/Z(x; T)$$

where $H(i \mid x)$ is the energy of configuration i with boundary x and

$$Z(x; T) = \sum \exp[-H(i \mid x)/k_B T]$$

is a normalization factor. Hence $p(i \mid x)$ will vary with the temperature T.

The *state* (or, more precisely, the *Gibbs state*) of V is the function $p(\cdot \mid x)$. Note the distinction between microscopic configurations i, j and macroscopic states $p(\cdot \mid x)$. *The states are probability distributions over the configurations.* In general they vary with the boundary condition and with the temperature.

In order to say whether a system is "sensitive" or "insensitive" to boundary conditions, we must be able to say whether the state changes a little or a lot as the boundary condition changes. In short, we need some sort of distance between states or, more generally, between probability distributions. The Dobrushin–Shlosman criterion uses the so-called *Vasserstein distance.*[7] (Also called the Kantorovich–Rubinstein–Ornstein–Vasserstein metric: see Ref. 8 for a historical review.)

The Vasserstein distance between states is defined in terms of a simpler distance between configurations. This *configuration distance* d_{ij} is simply the number of sites in V where the configurations i and j differ. The Vasserstein distance $\mathscr{R}[p(\cdot | x), p(\cdot | y)]$ between two states $p(\cdot | x)$ and $p(\cdot | y)$ is a linear combination of distances between configurations, weighted to increase the importance of the more probable configurations. The distance is

$$\mathscr{R}[p(\cdot | x), p(\cdot | y)] \equiv \min \left\{ \sum_{ij} w_{ij} \, d_{ij} \right\} \tag{1}$$

where the minimization is performed over all joint probability distributions w_{ij} such that

$$\sum_{j} w_{ij} = p(i | x); \qquad \sum_{i} w_{ij} = p(j | y); \qquad w_{ij} \geqslant 0 \tag{2}$$

It is easy to verify that $\mathscr{R}$ satisfies the requirements for a distance: it is nonnegative (vanishing only if the two states are identical), commutative, and obeys the triangle inequality.[9]

The maximum change in state that can be produced by altering a single boundary site t is

$$k_t \equiv \max \{ \mathscr{R}[p(\cdot | x), p(\cdot | y)] \} \tag{3}$$

where the maximization is over pairs of boundary conditions x, y that differ only at site t. Phase uniqueness holds when such changes are small enough:

Theorem (Dobrushin–Shlosman phase uniqueness criterion). If for some V

$$\sum_{t \in \partial V} k_t < |V| \tag{4}$$

then the infinite system has only a single equilibrium phase.

The theorem is proved in Ref. 1.

3. ALGORITHMIC IMPLEMENTATION OF THE CRITERION

Application of the Dobrushin–Shlosman criterion involves nothing more than arithmetic, but it involves so much arithmetic that recourse must be made to the computer. It is easy to produce algorithms that implement all aspects of checking the criterion except for one: the con-

strained minimization that defines the Vasserstein distance. The task of minimizing linear functions subject to linear constraints is called linear programming.[10,11] In conformity with linear programming conventions, we now write a_i for $p(i|x)$ and b_j for $p(j|y)$, so the Vasserstein problem is to minimize

$$\sum_{ij} d_{ij} w_{ij} \tag{5}$$

by varying the values w_{ij} subject to

$$\sum_j w_{ij} = a_i; \qquad \sum_i w_{ij} = b_j; \qquad w_{ij} \geqslant 0 \tag{6}$$

In this notation the problem will immediately be recognized (by a linear programmer) as an example of the "transportation problem." This problem usually arises in a context somewhat different from that of finding distances between probability distributions. Suppose a company owns a number of mattress factories, labeled by i, and a number of stores, labeled by j. The factory labeled i produces a_i mattresses a day, and the store labeled j sells b_j mattresses a day. Total mattress production equals total mattress sales. The number of mattresses shipped daily from factory i to store j is w_{ij}, and the unit cost of shipping on this route is d_{ij}. Constraints (6) simply require that each factory ships its entire production and that each store receives the amount it sells. The sum (5) represents the total cost for shipping mattresses, which the company clearly wishes to minimize. The origin of the term "transportation problem" should now be clear.

The transportation problem is readily and efficiently solved by Dantzig's simplex algorithm.[12] The general scheme of this algorithm is as follows (details are given by, for example, Murty:[10] It starts by producing a set of variables $\{w_{ij}\}$ that satisfies the constraints (6). It then applies a test to determine whether this set minimizes the sum (5). If so, the algorithm stops. Otherwise it alters the original variables w_{ij} in such a way that the constraints are still satisfied and the value of the sum is either decreased or remains constant: this alteration is called a "pivot." The new variables are then tested for minimization of the sum. The algorithm continues pivoting and testing, pivoting and testing, until the test is passed, signaling that the minimum is found.

A number of different starting techniques exist for producing the initial set of constraint-satisfying variables. Each technique has its own advantages and disadvantages, which depend upon the problem studied. When we tested several starting technique to find out which best suits our problem, we discovered that in each of thousands of trials one of them, the so-called "greedy method," produced variables w_{ij} that not only satisfy the

constraints (6), but also minimize the sum (5). It seems that if the greedy method is used, no pivoting is required! This is significant theoretically, because it reveals a hitherto unsuspected structure in the Vasserstein distance, and also practically, because pivoting and testing are time-consuming, complicated processes, whereas application of the greedy method is fast and easy.

The greedy method[10,13] selects values for the w_{ij} that surely satisfy the constraints but are also chosen with an eye toward minimizing the total cost (5). It does so by assigning as much "traffic" w_{ij} as the constraints permit to the route with the smallest unit cost d_{ij}. After this assignment is made the problem can be formally reduced to a smaller transportation problem. The process is continued until all routes have been assigned. Specifically:

G1. Select the smallest coefficient d_{ij} in the transportation problem. If several such coefficients are equal, select one of them at random. Denote the corresponding values of i and j by I and J.

G2. Assign $w_{IJ} = \min\{a_I, b_J\}$.

G3a. *If $a_I \leqslant b_J$, then*: The constraint $\sum_j w_{Ij} = a_I$ demands that we assign $w_{Ij} = 0$ for all $j \neq J$. Form the smaller transportation problem by elminating all of the just-assigned routes (I, j) and by replacing b_J with $b_J - a_I$.

G3b. *If $b_J < a_I$ then*: The constraint $\sum_i w_{iJ} = b_J$ demands that we assign $w_{iJ} = 0$ for all $i \neq I$. Form the smaller transportation problem by eliminating all of the just-assigned routes (i, J) and by replacing a_I with $a_I - b_J$.

The method is called "greedy" (or sometimes "myopic") because it never looks ahead to see what might be gained by assigning traffic to routes not at the current minimum cost. In general, it will not minimize the total transportation cost (5). However, we believe:

Conjecture A (Greed succeeds). The greedy method produces the minimum transportation cost (5) in the Vasserstein problem, for pairs of boundaries that differ at only one site.

Our evidence for this conjecture rests upon thousands of tests on several different models: hard squares, zero-field square and triangular lattice Ising ferromagnets, triangular lattice Ising antiferromagnet (with and without field), random bond square lattice Ising model. Tests were applied to cells of various sizes and shapes and at various temperatures (or, in the case of hard squares, at various activities). Never did the greedy method fail to minimize the transportation cost.

There are a small number of transportation problems for which the greedy method has been proven to succeed.[13] For example, if the pairs (i, j) can be arranged in a sequence such that

$$d_{pq} + d_{rs} \leqslant d_{ps} + d_{rq} \tag{7}$$

whenever (p, s) and (r, q) fall after (p, q) in the sequence (the "Monge condition"), then the greedy method will succeed regardless of the values of the constraint coefficients a_i, b_j. Similarly, there is a condition on the constraint coefficients that will assure the method's success regardless of the cost coefficients d_{ij}. We have found that our problem satisfies neither condition, because changes made to either the cost or constraint coefficients will generally cause the greedy method to fail.

4. APPLICATION TO HARD SQUARES

The Dobrushin–Shlosman criterion is undeniably correct, but its truth does not imply its utility. To see how well the criterion works in practice, we have applied it to the model of hard squares.[5] This model is easily specified: The sites of a square lattice are either occupied or unoccupied, but two nearest-neighbor sites cannot both be occupied. Because all configurations have zero energy, the concept of temperature is inapplicable and the macroscopic (thermodynamic) state of a hard square system is completely specified by a single variable, the activity z. This model is believed to exhibit a single critical transition at activity z_c, showing phase uniqueness when $z < z_c$ and two-phase coexistance when $z > z_c$. A careful series analysis study[6] suggested that

$$z_c = 3.7962 \pm 0.0001 \tag{8}$$

but, before the advent of the Dobrushin–Shlosman criterion, the only rigorous bound[14] on the transition activity was $z_c > 1/2$.

In many ways the hard square model is ideally suited to the Dobrushin–Shlosman criterion. The limiting factor in applying the criterion is the sheer arithmetic required to check every boundary of every configuration, and in the hard square model many configurations are flatly prohibited: for example, a five by five lattice cell can support $2^{25} = 33,554,432$ spin-$\frac{1}{2}$ Ising model configurations, but only 55,447 hard square configurations. All but 0.16% of the Ising configurations are prohibited! Thus, it is not surprising that the first application of the Dobrushin–Shlosman criterion was to hard squares, when Dobrushin et al.[4] (hereafter called DKS) used a three by four lattice cell to prove that $z_c > 1$. (This bound is particularly interesting because it has implications

for the phase diagram geometry of the square-lattice Ising antiferromagnet.[4])

Let us pause to mention two important differences between the work of DKS and our own. First, DKS use an algorithmic implementation of the Dobrushin–Shlosman criterion that proves phase uniqueness over a range of activities rather than at a single value of z. They apply this technique to a number of abutting intervals in order to rigorously prove phase uniqueness throughout the interval $0 \leqslant z \leqslant 1$. Although our implementation is also capable of proving uniqueness over intervals in the same way, we have in fact checked the criterion only at isolated activity points. (A proof of Conjecture C below would allow intervals of uniqueness to be determined accurately and easily without recourse to supplementary computations.) The second difference is that we find Vasserstein distances using the classic simplex algorithm as described in Section 3, while DKS employ a specialized technique, which generates not the Vasserstein distance itself, but an upper bound only.

Now that our attention is restricted to a single model, we can describe the Dobrushin–Shlosman criterion more precisely. First, recall that a "boundary condition" (or "boundary configuration") is a configuration of the sites immediately adjacent to the lattice cell V. A configuration i of V is called "compatible" with a boundary configuaration x when none of the sites occupied in i are adjacent to sites occupied in x. If $n(i)$ is the number of sites occupied in configuration i, then the probability of finding the lattice cell in configuration i given that the boundary configuration is x and the activity is z is

$$p(i \mid x) = \begin{cases} z^{n(i)}/Z(x; z) & \text{if } i \text{ is compatible with } x \\ 0 & \text{otherwise.} \end{cases} \tag{9}$$

Here the normalizing factor $Z(x; z)$ is the sum of $z^{n(j)}$ over all hard square configurations j compatible with boundary configuration x.

Given these preliminaries, we can write down the following algorithm for applying the Dobrushin–Shlosman criterion to hard squares.

H1. Pick an activity z and a lattice cell V.

H2. For all sites t in the boundary of V, perform steps H3 and H5.

H3. For all boundary configurations with t vacant, perform step H4.

H4. Calculate the Vasserstein distance between two states: one with the current boundary configuration and the other with a boundary condition identical except that site t is occupied.

H5. Select the maximum such Vasserstein distance and call it k_t.

H6. Sum all the values k_t. Apply the Dobrushin–Shlosman test (4).

For the sake of example, we can apply this algorithm to a three by four lattice cell. At $z = 1$ we find

$$\sum_{t \in \partial V} k_t = \frac{119{,}026}{10{,}605} = 11.22357... \tag{10}$$

whereas DKS produce only the upper bound

$$\sum_{t \in \partial V} k_t < 11.99998 \tag{11}$$

Again, applying the algorithm at $z = 1.074$, we find

$$\sum_{t \in \partial V} k_t = 11.996924 \tag{12}$$

This result was obtained via algorithm H using 30 sec of CPU time on the DEC-2060, a computer with a cycle time of 100 nsec.

The time-consuming step in the hard square algorithm is H4, so it is important to optimize the preformance of this step. We noted in Section 3 that the greedy algorithm, which assigns values to the variables w_{ij} starting with those of minimum distance d_{ij}, appears to produce in every case the proper Vasserstein distance. This conjecture remains unproven, but DKS were able to show that the first stage of the greedy algorithm, namely the assigning of values to those w_{ij} with $d_{ij} = 0$, is rigorously correct. (It is easy to see that this is true for the general case as well.) We have further proven the correctness of the second and third stages of the process, in which values are assigned to those w_{ij} with $d_{ij} = 1$ or 2. The simplification afforded by these improvements is considerable. For example, in a three by four lattice cell the Vasserstein distance between the boundary with no sites occupied and the boundary with one corner-adjacent site occupied is found naively by solving a transportation problem with 35,295 variables and 382 equality constraints. After the variables with $d_{ij} = 0$ are eliminated the problem has 11,160 variables and 227 constraints, while after the variables with $d_{ij} = 1$ and 2 are eliminated it has 1624 variables and 114 constraints.

Even with these improvements step H4 is still time-consuming and, even worse, it must be executed once for every other boundary configuration, a number that grows exponentially with the number of sites in the boundary. Some of these boundaries can be eliminated from consideration through symmetry or other elementary arguments (see DKS, Section 4.2), but even so the remaining computational problem is large. It also seems pointless, as all but one of the computed Vasserstein distances are thrown away at step H5! If we could tell beforehand which boundary configuration would lead to the maximum Vasserstein distance, then we

would only need to execute step H4 once. With this in mind we have searched for patterns obeyed by the "maximizing" boundary condition. Throughout our extensive tests, the following rule has never failed.

Conjecture B (Maximizing boundary configuration). For a rectangular lattice cell in the hard square model, the maximum Vasserstein distance between two states at the same activity and with boundary configurations differing only at site t is achieved when the boundary configuration $\hat{x}$ in which t is vacant has either all sites vacant or else only one site occupied. If the activity is small enough, then $\hat{x}$ is given precisely by:

   a. If t is adjacent to a lattice cell site which is itself adjacent to a corner site, then $\hat{x}$ is the configuration with only the site next to that corner occupied (see Fig. 1).

   b. Otherwise, $\hat{x}$ is the configuration with all sites vacant.

The precise meaning of "small enough" in this conjecture is as yet uncertain. In our tests the conjecture held for all values of z less than or equal to 10 (by comparison, z_c is about 3.8). We suspect that it applies for all values of z at which the Dobrushin–Shlosman criterion is satisfied.

When conjecture B is adopted, the CPU time required to produce result (12) falls from 30 sec to 4 sec.

4.1. Conjectured Formula for the Hard–Square Vasserstein Distance

In this subsection we conjecture a simple formula for the Vasserstein distance between two given boundary configurations as a function of activity. If the conjecture is correct, then the entire domain of uniqueness ensured by a given lattice cell can be obtained by solving a few linear programming problems and by finding the zero of a simple polynomial.
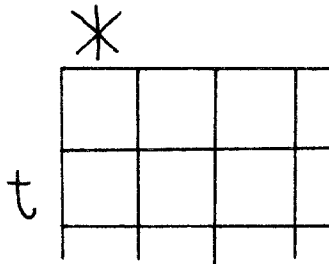

Fig. 1.   Conjecture B, part a. The site labeled by the star is the only site occupied in boundary configuration $\hat{x}$.

Consider the problem of finding the Vasserstein distance between two hard-square lattice-cell states with different boundary configurations. (Usually we will be interested in this problem when the two boundary configurations differ at only a single site, but in this subsection we discuss the more general problem.) Equation (9) shows that the constraint coefficients (represented by a_i and b_j in Section 3) of this transportation problem are rational functions of z with integer coefficients. Now imagine implementing the greedy method to find a value for the sum (5), which, provided Conjectured A is correct, is the Vasserstein distance. Recall that each stage of the greedy method eliminates a row or column of variables w_{ij} to produce a smaller transportation problem. It is clear from step G3 that the constraint coefficients of this smaller problem are still rational functions, so step G2 always assigns to w_{ij} a rational function of z. One is tempted to conclude that the Vasserstein distance produced by the greedy method is a rational function of z, but this is not necessarily correct. The rows and columns will generally be eliminated in a different order at each different value of z, so we may deduce only that the value for the sum (5) produced by the greedy method is a piecewise rational function of z. Indeed, one can easily find boundary conditions for which the Vasserstein distance is not a rational function of z. However, our tests indicate that:

Conjecture C (Vasserstein distance is rational). For a rectangular lattice cell in the hard suqare model, the Vasserstein distance between two states at the same activity z but with boundary configurations which differ at a single site is a rational function of z with positive integer coefficients.

Further discussion of this result is presented in Ref. 15.

For small lattice cells it is easy enough simply to work out the Vasserstein distance and confirm the conjecture (DKS, Section 4.3). For larger cells it is not hard to keep track of the polynomial coefficients by computer. For example, we conjecture that for a three by four lattice cell the Vasserstein distance between a state with all boundary sites vacant and a state with only a site next to the corner occupied is

$$\frac{z + 10z^2 + 33z^3 + 46z^4 + 28z^5 + 6z^6}{1 + 11z + 40z^2 + 59z^3 + 35z^4 + 8z^5 + z^6} \tag{13}$$

If Conjecture C were proven, then one could obtain the sum $\sum_{t \in \partial V} k_t$ as a rational function $N_V(z)/D_V(z)$ [$N_V(z)$ and $D_V(z)$ polynomials], and the Dobrushin–Shlosman criterion (4) could be expressed as the simple polynomial inequality

$$N_V(z) - |V| \, D_V(z) < 0 \tag{14}$$

where $|V|$ is the number of sites in the lattice cell V. Executing this program for the three by four lattice cell, for example, gives the criterion

$$210z^{16} + 4001z^{15} + 31941z^{14} + 140719z^{13} + 374807z^{12} + 606528z^{11}$$
$$+ 518795z^{10} - 6113z^9 - 591942z^8 - 780398z^7 - 566829z^6$$
$$- 266119z^5 - 83705z^4 - 17511z^3 - 2334z^2 - 179z - 6 < 0 \quad (15)$$

for phase uniqueness. [The polynomial vanishes for some z between 1.074 and 1.075; compare Eq. (10).] One can easily show (using induction on the order of the polynomial) that a polynomial with a string of positive coefficients followed by a string of negative coefficients has exactly one positive zero. If Conjecture C is correct, then this zero is z_V^*, the smallest activity at which the Dobrushin–Shlosman criterion fails. Furthermore, the criterion is satisfied for all $z < z_V^*$ and violated for all $z \geqslant z_V^*$.

5. RESULTS AND CONCLUSIONS

We have programmed a computer to apply the Dobrushin–Shlosman criterion to several rectangular hard square lattice cells. For each cell V the criterion was satisfied for all the tested activities below some value z_V^* and violated for all the tested activities at or above z_V^*. The results are summarized below:

$$
\begin{array}{lcccc}
\text{Lattice cell} & 3 \times 3 & 3 \times 4 & 3 \times 5 & 4 \times 4 \\
z_V^* & 0.982+ & 1.074+ & 1.139+ & 1.185+
\end{array}
\qquad (16)
$$

(The plus signs indicate that, for example, when V is a three by four cell, the criterion is satisfied at $z = 1.074$ and violated at $z = 1.075$.) These results were obtained without recourse to the conjectures mentioned in Sections 3 and 4.

We would like to continue checking the criterion for even larger lattice cells, but checking even the four by four cell is already a large computational task. Realistically, the criterion can be applied to larger cells only by accepting a conjecture and hence sacrificing rigor. We have promulgated three conjectures: Conjecture A simplifies the computation of the Vasserstein distance, Conjecture B decides which boundary configuration gives rise to the value k_t used in the Dobrushin–Shlosman test (4), and Conjecture C provides an easily evaluated analytic expression for k_t. Which of these can be put to the most effective use? Virtually all of the computer time is devoted to solving the transportation problem. Our experience indicates that it takes as long to test a candidate solution for optimality as it does to produce the canditate using the greedy method, so

adoption of Conjecture A would halve the required computer time. Furthermore, since the greedy method produces a rigorous upper bound on k_t, the criterion generates a rigorous proof of phase uniqueness even when the optimality test is omitted. Only the comfort of knowing that the algorithm has produced the best possible bound from the given lattice cell has been lost.

In contrast, an algorithm that assumes Conjecture B produces lower bounds for k_t, and hence can be used to show rigorously that the criterion is violated. An activity that violates the criterion is an upper bound for z_V^*, and since z_V^* is a lower bound on z_c such a result can say nothing about the transition. But if we can accept this limitation, then the payoff from Conjecture B is enormous. Only one transportation problem must be solved for each boundary site, whereas previously in, say, a five by five cell, about 10 million transportation problems were required for each boundary site!

Conjecture C is most useful in conjunction with Conjecture B. If Conjecture C is ignored, one must run the full program at several different activities in order to close in on z_V^*. If Conjecture C is adopted, the transportation problems are solved but once, and then the value of z_V^* is obtained in seconds by finding the zero of a polynomial.

We extended the calculation to larger cells using this strategy: Conjecture A was not used at all. Conjecture C was used to find candidate values for z_V^*, and these values were rounded upward to produce activities at which the criterion was expected to fail. This expectation was confirmed using Conjecture B. The resulting activities are shown below: since the criterion rigorously fails at these activities, they are upper bounds on z_V^*.

$$
\begin{array}{lcc}
\text{Lattice cell} & 4\times 5 & 5\times 5 \\
\text{Upper bound on } z_V^* & 1.268 & 1.35557
\end{array}
\tag{17}
$$

The bound on z_V^* for the five by five cell is our must computationally intensive result. It was obtained using 16 hr of CPU time on the Cyber 205, a supercomputer with a cycle time of 20 nsec. (We did not use extensively the vector arithmetic features of the Cyber 205, so it is possible that further improvements in CPU time can still be achieved.) Of these 16 hr, 4 hr was employed to find the Vasserstein function using Conjecture C, 4 hr was used to produce initial solutions of the transportation problems at $z = 1.35557$ using the greedy algorithm, and 8 hr was used to verify that these initial solutions were indeed correct. The bounds in (16) and (17) should be compared with the estimated[6] transition activity $z_c = 3.796$.

One might object that none of the numerical statements in this paper [with the exception of Eq. (10)] are rigorous, because all of them were obtained using nonexact floating-point computer arithmetic. This objection

is in fact valid, but a technique exists that can overcome the objection. The technique involves replacing the computer's floating-point arithmetic with "interval arithmetic." In interval arithmetic the result of, say, a multiplication is reported not as a single number that approximates the true product, but as a pair of numbers that rigorously bound the true product. One can (usually) produce rigorous bounds on Vasserstein distances by solving the relevant transportation problem subject to two precautions: first, by always keeping the exact integer polynomial form of the constraint coefficients (the a_i and b_j of Section 3) and second, by evaluating these polynomials using interval arithmetic. We have not carried out this ambitious program. However, we have applied interval arithmetic to the criterion (14), which applies to the five by five lattice cell, and we find that at $z = 1.35557$ the polynomial expression is rigorously positive.

The Dobrushin–Shlosman theorem is the most powerful general phase uniqueness cirterion yet proven. It has opened up a fertile field of interesting new questions in both linear programming and statistical mechanics, as the conjectures set forth in this paper amply demonstrate. The hard square transition bounds obtainable through the criterion are without doubt the best rigorous bounds now available. Even so, however, these bounds remain far from the estimated transition activity, and were obtained only at enormous cost in computer time. This work has shown the Dobrushin–Shlosman criterion to be an important tool in rigorous statistical mechanics, but further improvements in the algorithmic implementation of the criterion will be required before it can compete with established nonrigorous methods in the practical location of phase transition points.

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REFERENCES

1. R. L. Dobrushin and S. B. Shlosman, in *Statistical Physics and Dynamical Systems*, J. Fritz, A. Jaffe, and D. Szász, eds. (Birkhäuser, New York, 1985), pp. 347–370.
2. R. L. Dobrushin, *Theory of Probability and its Applications* **15**:469–497 (1070).
3. R. L. Dobrushin and S. B. Shlosman, in *Statistical Physics and Dynamical Systems*, J. Fritz, A. Jaffe, and D. Szász, eds. (Birkhäuser, New York, 1985), pp. 371–403.
4. R. L. Dobrushin, J. Kolafa, and S. B. Shlosman, *Commun. Math. Phys.* **102**:89–103 (1985).
5. D. S. Gaunt and M. E. Fisher, *J. Chem. Phys.* **43**:2840–2863 (1965).
6. R. J. Baxter, I. G. Enting, and S. K. Tsang, *J. Stat. Phys.* **22**:465–489 (1980).
7. L. N. Vasserstein, *Problemy Peredachi Informatsii* **5**:64–73 (1969).
8. S. T. Rachev, *Theory Prob. Appl.* **29**:647–676 (1985).
9. R. L. Dobrushin, *Theory Prob. Appl.* **15**:458–486 (1970).
10. K. G. Murty, *Linear Programming* (Wiley, New York, 1983).
11. J. Franklin, *Methods of Mathematical Economics* (Springer-Verlag, New York, 1980).
12. G. B. Dantzig, in *Activity Analysis of Production and Allocation*, T. C. Koopmans, ed. (Wiley, New York, 1951), Chapter 23.
13. A. J. Hoffman, in *Surveys in Combinatorics 1985*, I. Anderson, ed. (Cambridge University Press, Cambridge, 1985), pp. 97–112.
14. L. K. Runnels and J. B. Hubbard, *J. Stat. Phys.* **6**:1–20 (1972).
15. D. C. Radulescu and D. F. Styer, to be published.