

# First-order to second-order phase transition changeover and latent heats of $q$ -state Potts models in $d=2,3$ from a simple Migdal-Kadanoff adaptation


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The changeover from first-order to second-order phase transitions in  $q$ -state Potts models is obtained at  $q_c = 2$  in spatial dimension  $d = 3$  and essentially at  $q_c = 4$  in  $d = 2$ , using a physically intuited simple adaptation of the Migdal-Kadanoff renormalization-group transformation. This simple procedure yields the latent heats at the first-order phase transitions. In both  $d = 2$  and  $3$ , the calculated phase transition temperatures, respectively compared with the exact self-duality and Monte Carlo results, are dramatically improved. The method, when applied to a slab of finite thickness, yields dimensional crossover.

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## I. INTRODUCTION: ORDER OF POTTS TRANSITIONS AND UNDERLYING PHYSICAL INTUITION

The spatial dimensionality  $d$ , the symmetry of the local degrees of freedom, and the presence of quenched randomness strongly affect the occurrence and order of a phase transition. A simple but effective method in studying the occurrence of a phase transition has been the renormalization-group method under the Migdal-Kadanoff approximation [1,2]. Thus, using this method on widely different systems, the lower-critical dimension  $d_c$  below which no ordering occurs has been correctly determined as  $d_c = 1$  for the Ising model [1,2],  $d_c = 2$  for the XY [3,4] and Heisenberg [5] models, and the presence of an algebraically ordered phase has been seen for the XY model [3,4,6]. In systems with frozen microscopic disorder (quenched randomness), using the simple Migdal-Kadanoff renormalization-group approximation,  $d_c = 2$  has been determined for the random-field Ising [7,8] and XY models [9], and yielding a noninteger value,  $d_c = 2.46$ , for Ising spin-glass systems [10]. Also under the Migdal-Kadanoff approximation, the chaotic nature of the spin-glass phases [11–13] has been obtained and quantitatively analyzed, both for quenched randomly mixed ferromagnetic-antiferromagnetic spin glasses [14–16] and right- and left-chiral (helical) spin glasses [17–19].

An important aspect of an occurring phase transition is the order of the phase transition. The simple Migdal-Kadanoff approximation has not been successful in predicting this for an order-disorder phase transition in a model system. The best example are the  $q$ -state Potts models which, in terms of model system variety and experimental application, offer rich behaviors. The Potts models are defined by the Hamiltonian

$$-\beta\mathcal{H} = J \sum_{\langle ij \rangle} \delta(s_i, s_j), \quad (1)$$

where  $\beta = 1/k_B T$ , at lattice site  $i$  the Potts spin  $s_i = 1, 2, \dots, q$  can be in  $q$  different states, the delta function  $\delta(s_i, s_j) = 1(0)$  for  $s_i = s_j$  ( $s_i \neq s_j$ ), and the sum is over all interacting pairs of spins. The Ising model is obtained for  $q = 2$ . The lower-critical dimension of the Potts models is  $d_c = 1$ , as also seen by the simple Migdal-Kadanoff renormalization-group approximation [20]. However, for  $d > 1$ , the phase transitions of the Potts models are first order for  $q > q_c$  and second order for  $q < q_c$  [21–27]. This has not been obtained by the simple Migdal-Kadanoff approximation, which yields second order for all  $q$ . The actual changeover number of states  $q_c(d)$  depends on dimensionality  $d$ . For  $d = 2$  and  $3$ ,  $q_c = 4$  and  $2$ , respectively. For  $d = 1$ ,  $q_c = \infty$  [24]. This work considers integer values of  $q$ .

As noted above, the  $q$ -state Potts models have a second-order phase transition for  $q \leq q_c$  and a first-order phase transition for  $q > q_c$  [28–30]. In renormalization-group theory [21,27], the latter has been understood, and reproduced, as a condensation of effective vacancies formed by regions of disorder. Disorder is entropically favored for high number of states  $q$ . However, these renormalization-group calculations have required flows in large Hamiltonian parameter spaces, with many different types of interactions, and not connectable to the phase transition temperatures or thermodynamic properties of the original Potts models [Eq. (1)]. The effective vacancy mechanism has not been incorporated into the simple, pliable, otherwise effective, and therefore much used Migdal-Kadanoff transformation.

In this study, we find an also simple, physically motivated adjustment to the usual Migdal-Kadanoff approximation that cures the problem of the order of the phase transition, dramatically improves the calculated transition temperatures both in  $d = 2$  and  $3$ , and appears to be widely applicable to other systems.

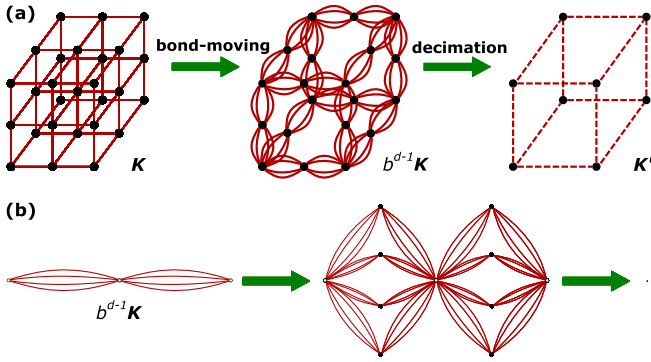


FIG. 1. From Ref. [33]: (a) Migdal-Kadanoff approximate renormalization-group transformation for the  $d = 3$  cubic lattice with the length-rescaling factor of  $b = 2$ . (b) Construction of the  $d = 3$ ,  $b = 2$  hierarchical lattice for which the Migdal-Kadanoff recursion relation is exact.

## II. MIGDAL-KADANOFF AS A SIMPLE EFFECTIVE RENORMALIZATION GROUP

The Migdal-Kadanoff approximation renders a non-doable renormalization-group transformation doable by a physically motivated approximate step, is very easily calculated, applicable to a large number of systems, including, for example, such complexities as the quenched-random helical spin glass [17–19], and effective across physical dimensions  $d$ .

Starting with the example given in Fig. 1(a), an exact renormalization-group transformation cannot be applied to the cubic lattice. Thus, as an approximation, some of the bonds are removed. However, this weakens the connectivity of the system and, to compensate, for every bond removed, a bond is added to the remaining bonds. This whole step is called the bond-moving step and constitutes the approximate step

of the renormalization-group transformation. At this point, the intermediate sites can be eliminated by an exact summation over their spin values in the partition function, which yields the renormalized interaction between the remaining sites. This is called the (exact) decimation step and completes the renormalization-group transformation. As shown in Fig. 1, the renormalization-group recursion relations of the Migdal-Kadanoff approximation are identical to those of an exactly solved hierarchical lattice [20,31,32].

The above can be rendered algebraically in the most straightforward way by writing the transfer matrix between two neighboring spins; for example, for  $q = 3$ ,

$$\mathbf{T}_{ij} \equiv e^{-\beta\mathcal{H}_{ij}} = \begin{pmatrix} e^J & 1 & 1 \\ 1 & e^J & 1 \\ 1 & 1 & e^J \end{pmatrix}, \quad (2)$$

where  $-\beta\mathcal{H}_{ij}$  is the part of the Hamiltonian between the two spins at the neighboring sites  $i$  and  $j$ . In this Eq. (2), the  $q \times q$  transfer matrix is exemplified with  $q = 3$ . Our calculations are done for many values of  $q$ , all the way to  $q = 100$ , as seen in Fig. 2.

The bond-moving step of the Migdal-Kadanoff approximate renormalization-group transformation consists in taking the power of  $b^{d-1}$  of each element in this matrix, where  $b$  is the length-rescaling factor of the renormalization-group transformation, namely, the renormalized nearest-neighbor separation in units of unrenormalized nearest-neighbor separation. The decimation step consists in matrix-multiplying  $b$  bond-moved transfer matrices. The flows, under this transformation, of the transfer matrices determine the phase transition and all of the thermodynamic densities of the system, as illustrated below.

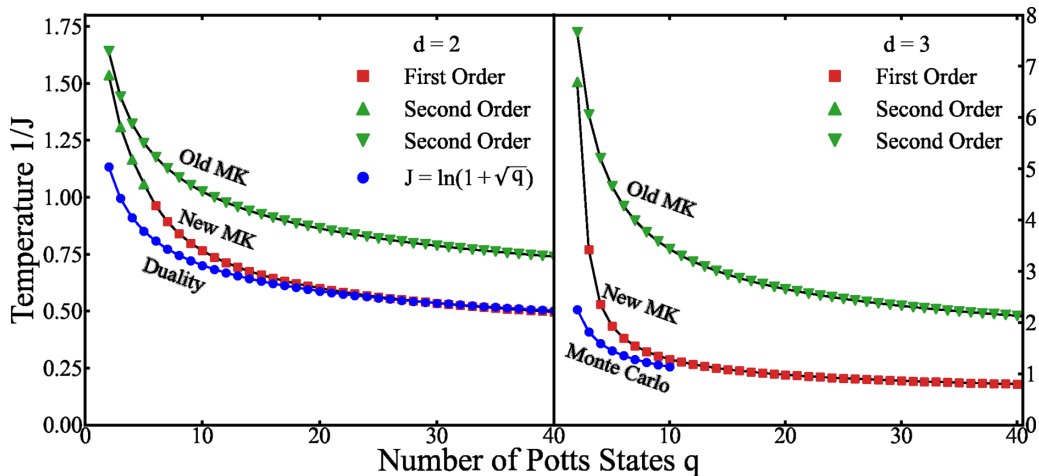


FIG. 2. Calculated transition temperatures  $1/J$  of  $q$ -state Potts models. The top curve is obtained with the conventional Migdal-Kadanoff approximation. In  $d = 2$ , the bottom curve is the exact transition temperatures obtained from self-duality. In  $d = 3$ , the bottom curve is Monte Carlo results [30]. The intermediate curve is obtained with our simply improved Migdal-Kadanoff approximation. First- and second-order phase transitions are given with triangles and squares, respectively. The improved calculation gives the changeover from second to first order exactly (after  $q = 2$ ) in  $d = 3$  and very nearly (after  $q = 5$  instead of  $q = 4$ ) in  $d = 2$ . In the latter case, the changeover can be brought down to  $q = 4$  by a simple physical argument and calculation, as seen in Fig. 4. Both in  $d = 2$  and 3, the values of the phase transition temperatures are dramatically improved with the improved calculation and join the exact results for  $q \gtrsim 10$  and  $q \gtrsim 5$ , respectively.

### III. SIMPLY IMPROVED MIGDAL-KADANOFF RENORMALIZATION-GROUP METHOD

The above is cured simply by including a local disorder state into the two-spin transfer matrix of Eq. (2). Inside an ordered region of a given spin value, a disordered site does not contribute to the energy in Eq. (1), but has a multiplicity

$$\mathbf{T}_{ij} \equiv e^{-\beta\mathcal{H}_{ij}} = \begin{pmatrix} e^J & 1 & 1 & (q-1)^{1/2d} \\ 1 & e^J & 1 & (q-1)^{1/2d} \\ 1 & 1 & e^J & (q-1)^{1/2d} \\ (q-1)^{1/2d} & (q-1)^{1/2d} & (q-1)^{1/2d} & (q-1)^{1/d} \end{pmatrix}. \quad (3)$$

In this Eq. (3), the  $(q+1) \times (q+1)$  transfer matrix is exemplified with  $q=3$ . Our calculations are done for the many values of  $q$ , all the way to  $q=100$ , as seen in Fig. 2. The Hamiltonian, to be studied by renormalization group yielding the exact solution of the hierarchical lattice, thus is

$$-\beta\mathcal{H} = \sum_{(ij)} \{J\delta(s_i, s_j)(1-v_i)(1-v_j) + [\ln(q-1)/2d](v_i+v_j)\}, \quad (4)$$

where  $v_i = 1$  or  $0$  indicates the presence or absence of local disorder at site  $i$ . When  $v_i = 0$ , the Potts spin can have  $q$  different values  $s_i = a, b, c, \dots$ . Thus, the  $q+1$  states of each site are  $(1, a, b, c, \dots)$  [21]. The delta function in the original Potts Hamiltonian [Eq. (1)] indicates that there is no temperature ( $1/J$ ) dependence in local disorder and that there is an entropic effect due to the multiplicity of states, taken into account in Eq. (4). Thus, connecting with the Potts-lattice-gas variables [21], the unrenormalized vacancy chemical potential  $-\Delta$  depends on the multiplicity and the unrenormalized vacancy-vacancy interaction  $K$  is zero.

Using this transfer matrix of Eq. (3), the renormalization-group calculation yields  $q_c$ . The first-order phase transition is recognized by the disordered side at the phase transition having, under repeated rescalings, the effective-vacancy position of  $(q+1) \times (q+1)$  dominant in the transfer matrix, rather than the elements of the  $q \times q$  upper-left submatrix being simultaneously dominant. The first-order phase transition is explicitly seen from the calculation, using this Migdal-Kadanoff transformation, of the latent heat and from the eigenvalue exponents of the discontinuity fixed point to which the first-order phase transition points flow under repeated renormalization-group transformations (Sec. IV).

The phase transition temperatures  $1/J$  of  $q$ -state Potts models, calculated with the simply improved Migdal-Kadanoff transformation, are shown in Fig. 1. The top curve in this figure is obtained with the conventional Migdal-Kadanoff approximation. In  $d=2$ , the bottom curve is the exact transition temperatures obtained from self-duality [29]. In  $d=3$ , the bottom curve is Monte Carlo results [30]. The intermediate curve is obtained with our simply improved Migdal-Kadanoff approximation. First- and second-order phase transitions are distinguished in the figure. The improved calculation gives the changeover from second to first order exactly (after  $q=2$ ) in  $d=3$  and very nearly (after  $q=5$  instead of  $q=4$ ) in  $d=2$ .

of  $q-1$ . The subtraction is because the disordered site cannot be in the spin state of its surrounding ordered region. This is equivalent to the exponential of an on-site energy and, with no approximation, is shared on the transfer matrices of the  $2d$  incoming bonds. The transfer matrix does become, for example for  $q=3$ ,

In the latter case, the changeover can be brought down to  $q=4$  by a simple physical argument and calculation, as seen below. Both in  $d=2$  and  $3$ , the values of the phase transition temperatures are dramatically improved with the improved calculation and join the exact results for  $q \gtrsim 10$  and  $q \gtrsim 5$ , respectively.

### IV. LATENT HEATS OF THE $Q$ -STATE POTTS MODELS IN $D=2, 3$ AND $(Q+1)$ -STATE COEXISTENCE AT THE DISCONTINUITY FIXED POINT

The position-space renormalization-group solution of a system yields the entire statistical mechanics of the system, at and away from the phase transitions, including the thermodynamic densities [33]. The calculation of the latter requires following the entire range of renormalization-group trajectories. In the ordered phases, the trajectories lead to strong coupling behavior. To avoid numerical overflow problems, with no approximation, at the beginning of a trajectory and after each decimation, the transfer matrix is divided by its largest element, so that its largest element then becomes 1. This division is equivalent to subtracting the constant from the Hamiltonian. This division is not necessary after bond moving, since the largest element, taken to the power  $b^{d-1}$ , remains 1. The logarithm of the dividing element, namely, the subtractive constant  $G(n) = \ln(T_{ij})_{\max}$ , where  $n$  indicates the  $n$ th renormalization-group transformation, summed over the trajectory, yields the free energy, and therefore the thermodynamic densities.

The dimensionless free energy per bond  $f = F/kN$  is thus obtained by summing the constants generated at each renormalization-group step,

$$f = \frac{1}{N} \ln \sum_{\{s_i\}} e^{-\beta\mathcal{H}} = \sum_{n=0}^{\infty} \frac{G(n)}{b^{dn}}, \quad (5)$$

where  $N$  is the number of bonds in the initial unrenormalized system, the first sum is over all states of the system, the second sum is over all renormalization-group steps  $n$ , and  $G^{(0)}$  is the constant from the first division at the beginning of the trajectory. This sum quickly converges numerically.

A derivative of the free energy  $f$  with respect to  $J$  gives the energy density  $\langle \delta(s_i, s_j)(1-v_i)(1-v_j) \rangle$ . The calculated  $q$ -state Potts energy densities in  $d=2$  and  $3$  are shown in Fig. 3. The latent heat discontinuities are shown with the dashed

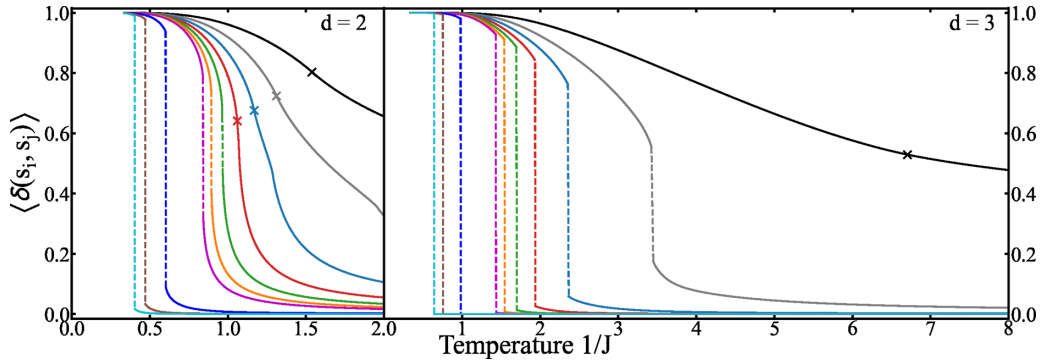


FIG. 3. Calculated  $q$ -state Potts energy densities in  $d = 2$  and  $3$ . In each panel, the curves are, from right to left, for  $q = 2, 3, 4, 5, 6, 7, 8, 20, 50, 100$ . The latent-heat discontinuities of the first-order phase transitions are shown with the dashed lines. The second-order phase transitions are marked with  $\times$ .

lines and are consistent with order of the phase transition yielded by the renormalization-group flows. The latent heats are also given in Table I and compared with the exactly known values in  $d = 2$  [28,29]. The correct  $q_c = 2$  is obtained for  $d = 3$ . In  $d = 2$ , we need a first-order transition for  $q = 5$  to obtain  $q_c = 4$ . However, this is a near miss in the calculation, physically explained: In the middle of a disordered island, all spin states contribute to the local multiplicity introduced above. Thus, the subtraction  $q - 1$  is an oversubtraction. In fact, when  $q - 0.25$  is used, the first-order transition with the latent heat is obtained, as seen in Fig. 4. This would also improve the latent heat values at low  $q$  in Table I.

The first-order phase transition points, under repeated renormalization-group transformations, flow to an unstable strong-coupling fixed point with eigenvalue  $b^d$  [34,35]. In our case, at this fixed point of the first-order phase transitions, the many-times renormalized  $(q + 1) \times (q + 1)$  transfer matrix reduces to

$$\mathbf{T}_{ij} = \begin{pmatrix} e^{E_q} & 0 & 0 & 0 \\ 0 & e^{E_q} & 0 & 0 \\ 0 & 0 & e^{E_q} & 0 \\ 0 & 0 & 0 & e^{E_0} \end{pmatrix}, \quad (6)$$

From this matrix, under renormalization group,  $(q + 1)$  independent recursion relations of the form  $E'_u = b^d E_u$  are obtained, yielding  $(q + 1)$  separate eigenvalues  $b^d$ . The number of  $b^d$  eigenvalues is the number of coexisting phases [36,37] at the fixed point and at all points renormalizing onto the fixed point, which is the generalization of the Nienhuis-Nauenberg condition [34].

TABLE I. Exact [28,29] and our calculated latent heats  $L$  in  $d = 2$ .

$q$	Exact $L$	Calculated $L$
6	0.474	0.176
7	0.586	0.333
8	0.659	0.457
20	0.889	0.847
50	0.958	0.945
100	0.980	0.973

### V. DIMENSIONAL CROSSOVER AND CORRELATION LENGTH FROM FINITE-THICKNESS SLAB CALCULATIONS

Our simple approach can easily be used in a variety of systems. For example, we consider the Potts models on a two-dimensional slab of finite thickness in the third dimension. As described by the work of Shnidman and Domany [38], this system is solved by doing  $d = 3$  renormalization-group transformations until the many-renormalized system is reduced to  $d = 2$ , followed by  $d = 2$  renormalization-group transformations. As explained by these authors [38], if the correlation length of the original (unrenormalized) system is less than the thickness of the slab, specifically at a first-order phase transition since the correlation length diverges at a second-order phase transition, the first-order phase transition of  $d = 3$  should be observed in the  $d = 2$  slab. Conversely, if the correlation length is greater than the slab thickness, the two-dimensionality of the system is sensed and the  $d = 2$  phase transition occurs. We have verified this dimensional crossover with the  $(q = 3)$ -state Potts model, which has a

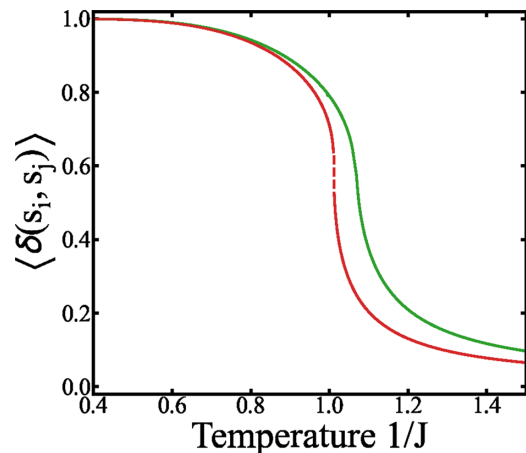


FIG. 4. Calculated energy density in  $q = 5$  and  $d = 2$ . The left curve uses the  $q - 0.25$  for the local disorder multiplicity. The correct first-order phase transition is obtained (left curve) by simple, physically motivated adjustment.



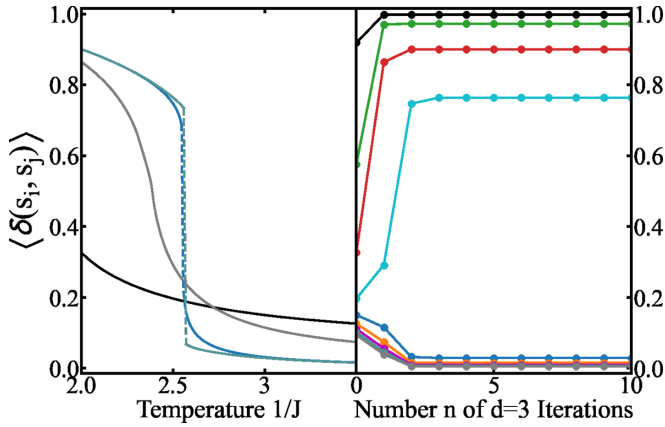


FIG. 5. Calculated energy densities for a two-dimensional slab of finite thickness  $b^n$ , for  $q = 3$ . The system is solved by performing  $n$  renormalization-group transformations for  $d = 3$ , reducing the system to  $d = 2$ , followed by infinitely many renormalization-group transformations for  $d = 2$ . Left panel: The temperature variation of the energy density. The curves are, from bottom to top on the left,  $n = 0, 1, 2, 3$ . The curves for  $n \geq 3$  coincide to the accuracy of the figure. For the narrow slabs,  $n = 0, 1$ , the correlation length at the would-be  $d = 3$  first-order transition is larger than the slab thickness and the second-order phase transition of  $d = 2$  occurs. For thicker slabs,  $n \geq 2$ , the correlation length at the first-order phase transition of  $d = 3$  is less than the slab thickness and thus this first-order phase transition actually occurs. Right panel: Slab thickness dependence of the energy density. The curves are, from top to bottom, for temperatures  $T = J^{-1} = 0.5, 1.0, 1.5, \dots, 5.5$ . The first-order transition of  $n \geq 2$  is seen by the gap opening. From both panels, it is seen that the latent heat does not depend on the slab thickness for  $n \geq 3$ , since the correlation length at the first-order phase transition is less than  $b^n$ .

first-order phase transition in  $d = 3$  and a second-order phase transition in  $d = 2$  (Fig. 3).

Our calculated results are shown in Fig. 5, for a two-dimensional slab of finite thickness  $b^n$ , for  $q = 3$ . The system is solved by performing  $n$  renormalization-group transformations for  $d = 3$ , reducing the system to  $d = 2$ , followed by infinitely many renormalization-group transformations for

$d = 2$ . The left panel gives the temperature variation of the energy density. The curves are, from bottom to top on the left,  $n = 0, 1, 2, 3$ . The curves for  $n \geq 3$  coincide to the accuracy of the figure. For the narrow slabs,  $n = 0, 1$ , the correlation length at the would-be  $d = 3$  first-order transition is larger than the slab thickness and the second-order phase transition of  $d = 2$  occurs. For thicker slabs,  $n \geq 2$ , the correlation length at the first-order phase transition of  $d = 3$  is less than the slab thickness and thus this first-order phase transition actually occurs. The right panel gives the slab thickness dependence of the energy density. The curves are, from top to bottom, for temperatures  $T = J^{-1} = 0.5, 1.0, 1.5, \dots, 5.5$ . The first-order transition of  $n \geq 2$  is seen by the gap opening. From both panels, it is seen that the latent heat does not depend on the slab thickness for  $n \geq 3$ , since the correlation length at the first-order phase transition is less than  $b^n$ .

Thus, our estimated correlation length of  $b^n \simeq 4$  at the  $d = 3$  Potts model transition is consistent with the Monte Carlo measured values of 7 (11) lattice spacings for approaching the transition from low (high) temperatures [39] and with the general arguments presented in Ref. [38].

## VI. CONCLUSION

The changeover from first-order to second-order phase transitions in  $q$ -state Potts models is obtained in spatial dimensions  $d = 2$  and 3 by a physically inspired simple adaptation of the simple Migdal-Kadanoff renormalization-group transformation. The phase transition temperatures are dramatically improved by this physical adaptation. The latent heats at the first-order phase transitions are calculated using the renormalization-group transformation. The inclusion of the local disorder state, which is the essence of our adaptation, can be used for numerical improvement and to take into account the possibility of a first-order phase transition.

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