Crumpling transition of the discrete planar folding in the negative-bending-rigidity regime

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The folding of the triangular lattice embedded in two dimensions (discrete planar folding) is investigated numerically. As the bending rigidity K varies, the planar folding exhibits a series of crumpling transitions at $K \approx -0.3$ and $K \approx 0.1$. By means of the transfer-matrix method for the system sizes $L \leq 14$, we analyze the singularity of the transition at $K \approx -0.3$. As a result, we estimate the transition point and the latent heat as $K = -0.270(2)$ and $Q = 0.043(10)$, respectively. This result suggests that the singularity belongs to a weak-first-order transition.

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At sufficiently low temperatures, a polymerized membrane becomes flattened macroscopically [1]; see Refs. [2–5] for a review. It still remains unclear [6–8] whether the crumpling transition (separating the flat and crumpled phases) is critical [9–21] or belongs to a discontinuous one with an appreciable latent heat [22–24].

In this Brief Report, we investigate a discretized version of the polymerized membrane embedded in two dimensions [25–28]; details are overviewed afterward. This model, the so-called discrete planar folding, exhibits a series of crumpling transitions at $K \approx -0.3$ and 0.1 [27,28], as the bending rigidity K changes. The latter transition exhibits a pronounced discontinuous character, whereas the nature of the former transition remains unclear. In this Brief Report, we utilized the transfer-matrix method [27] for the system sizes $L \leq 14$. We implemented a modified folding rule [29] [Eq. (5)], which enables us to impose the periodic-boundary condition. Technically, the restoration of the translational symmetry admits a substantial reduction in the transfer-matrix size.

To begin with, we explain a basic feature of the discrete planar folding [27,28]; see Fig. 1(a). We consider a sheet of the triangular lattice. Along the edges, the sheet folds up. The fold angle θ is either $\theta=0$ (complete fold) or π (no fold). The elastic energy at each edge is given by $K \cos \theta$ with the bending rigidity K. The thermodynamic property of the planar folding has been studied extensively [27,28]. The transfer-matrix simulation for the system sizes $L \leq 9$ [27] revealed a series of crumpling transitions at $K \approx -0.3$ and $K = 0.11(1)$. The behavior of the specific heat around $K \approx -0.3$ indicates that this transition would be a continuous one. The cluster variation method (CVM) of a single-hexagon-cluster approximation [28] indicates that there occur crumpling transitions at $K = -0.284$ and $K = 0.1013$ of the continuous and discontinuous characters, respectively.

The crumpling transition $K \approx -0.3$ is closely related [32] to that of an extended folding [30–32] at $K_3 \approx -0.8$. (The extended folding, the so-called three-dimensional folding, has four possibilities, $\cos \theta = \pm 1, \pm 1/3$, as to the joint angle θ.) That is, according to an argument based on a truncation of the configuration space [32], the following (approximate) relations should hold:

$$K = K_3/3, \tag{1}$$

$$Q = Q_3. \tag{2}$$

Here, the variables Q and Q_3 denote the latent heat for the planar- and three-dimensional-folding models, respectively. A number of results, $(K_3, Q_3) = (-0.852, 0)$ [32], $(-0.76(1), 0.03(2))$ [33], and $(-0.76(10), 0.05(5))$ [29], have been obtained via the CVM, density-matrix renormalization-group, and exact-diagonalization analyses, respectively. The nature of its transition at $K_3 \approx -0.8$ is not fully clarified, because the three-dimensional folding is computationally demanding. It is a purpose of this Brief Report to shed light on

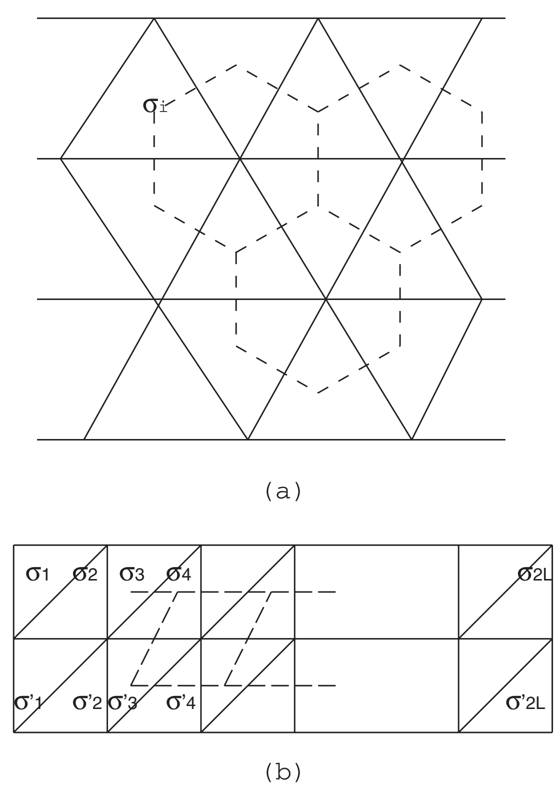

FIG. 1. (a) We consider a discrete folding of the triangular lattice. The fold angle (with respect to the adjacent triangular plaquettes) is discretized into either $\theta=0$ or π. (b) A drawing of a transfer-matrix strip is shown.

this longstanding issue from the viewpoint of the planar folding. (It has to be mentioned that the planar folding has relevance to a wide class of systems [26,34–37].)

For the sake of self-consistency, we present the transfer-matrix formalism for the discrete planar folding explicitly. We place the Ising variables $\{\sigma_i\}$ at each triangle i (rather than each joint); see Fig. 1(a). Hereafter, we consider the spin model on the dual (hexagonal) lattice. The Ising-spin configuration specifies each joint angle between the adjacent triangles. That is, provided that the spins are (anti)parallel, $\sigma_i\sigma_j=1$ (-1), for a pair of adjacent neighbors, i and j, the joint angle is $\theta=\pi$ (0). The spin configuration is subjected to a constraint (folding rule); the prefactor of the transfer-matrix element [Eq. (3)] enforces the constraint. As a consequence, the discrete folding reduces to an Ising model on the hexagonal lattice. In Fig. 1(b), a drawing of the transfer-matrix strip is presented. The row-to-row statistical weight $T_{\{\sigma_i\},\{\sigma'_i\}}$ yields the transfer-matrix element. The transfer-matrix element for the strip length L is given by [27]

$$T_{\{\sigma'_i\},\{\sigma_i\}}=\left(\prod_{i=1}^{L}\delta(\sigma_{2i}+\sigma_{2i+1}+\sigma_{2i+2}+\sigma'_{2i-1}+\sigma'_{2i} + \sigma'_{2i+1} \bmod 3,0)\right)\exp\left(-\sum_{i=1}^{L}H_i(K)/T\right), \quad (3)$$

with the local Hamiltonian

$$H_i(k)=-\frac{K}{2}(\sigma_{2i}\sigma_{2i+1}+\sigma_{2i+1}\sigma_{2i+2}+\sigma_{2i+2}\sigma'_{2i+1} + \sigma'_{2i+1}\sigma'_{2i}+\sigma'_{2i}\sigma'_{2i-1}+\sigma'_{2i-1}\sigma_{2i}), \quad (4)$$

due to the bending-energy cost for spins surrounding each hexagon i. Here, the parameter K denotes the bending rigidity, and the expression $\delta(n,m)$ is Kronecker's symbol. The periodic-boundary condition $\sigma_{L+i}=\sigma_i$ is imposed. We set $T=1$, considering it as a unit of energy.

In practice, the above scheme does not work. The folding rule is too restrictive to impose the periodic-boundary condition. So far, the open-boundary condition has been implemented; more specifically, the range of the running index i in Eq. (3) was set to $1\leq i\leq L-1$ [27]. In this Brief Report, following Ref. [29], we make a modification as to the constraint [prefactor of Eq. (3)] to surmount the difficulty. We replace the above expression with

$$T_{\{\sigma'_i\},\{\sigma_i\}}=\frac{1}{L}\sum_{l=1}^{L}\left(\prod_{i\neq l}\delta(\sigma_{2i}+\sigma_{2i+1}+\sigma_{2i+2}+\sigma'_{2i-1}+\sigma'_{2i} + \sigma'_{2i+1} \bmod 3,0)\right)\exp\left(-\sum_{i\neq l}H_i(K)-H_l(K')\right). \quad (5)$$

That is, the constraint is released at a defect hexagon $i=l$. Additionally, the local bending rigidity at the defect is set to K'. In order to improve the finite-size behavior, we adjust K' to

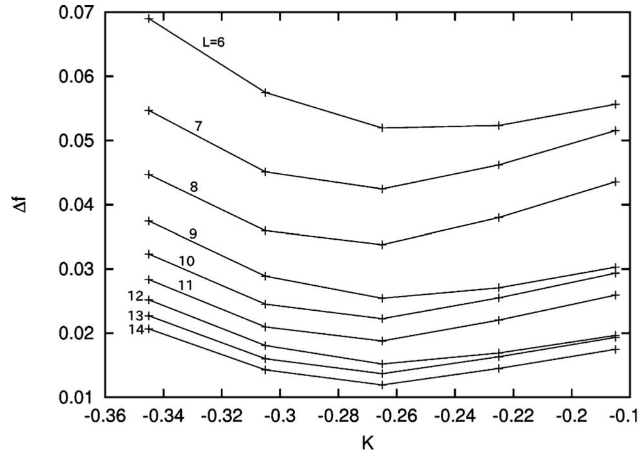

FIG. 2. The free-energy gap (7) is plotted for the bending rigidity K and the system sizes $6\leq L\leq 14$.

$$K'=2K. \quad (6)$$

A justification is shown afterward.

Based on the transfer-matrix formalism with a modified folding rule (5), we simulated the planar folding numerically. The numerical diagonalization was performed within a subspace specified by the wave number $k=0$ and the parity even; here, we made use of the spin-inversion symmetry $\sigma_i\to-\sigma_i$.

In Fig. 2, we plot the free-energy gap

$$\Delta f=f_2-f_1, \quad (7)$$

for the bending rigidity K and various system sizes $L=6,7,\ldots,14$. Here, the free energy per unit cell is given by $f_i=-\ln\Lambda_i/(2L)$ with the (sub)dominant eigenvalue $\Lambda_{1(2)}$ of the transfer matrix. (Here, the unit cell stands for a triangle of the original lattice rather than a hexagon of the dual lattice; see Fig. 1.) From Fig. 2, we see a signature of a crumpling transition (closure of Δf) at $K\approx-0.27$. The location of the transition point appears to be consistent with the preceding estimates [27,28].

In Fig. 3, the approximate transition point $K(L)$ is plotted for $1/L^2$ and $6\leq L\leq 14$. The approximate transition point minimizes Δf; namely, the relation

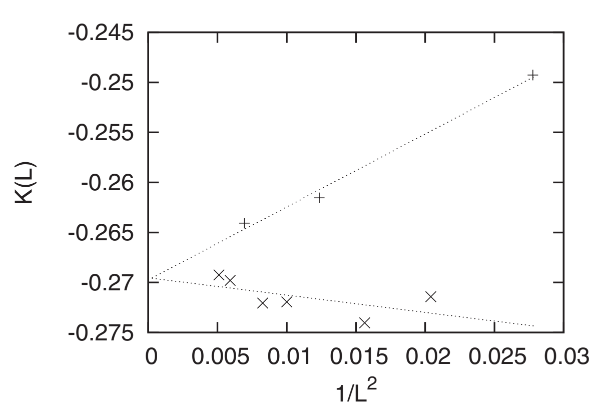

FIG. 3. The transition point $K(L)$ (8) is plotted for $1/L^2$. The linear least-squares fit for $L=0$ (+) and $1,2 \bmod 3$ (×) $(6\leq L\leq 14)$ yields $K=-0.2697(12)$ and $-0.2695(14)$, respectively.

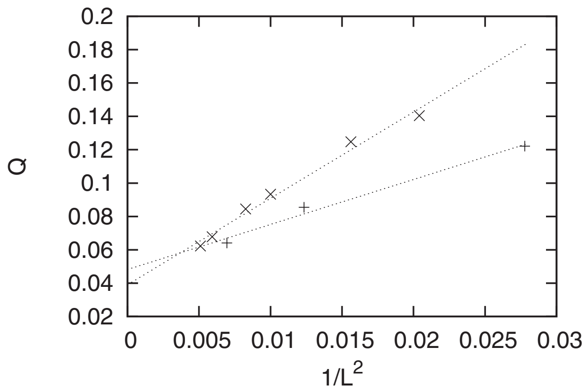

FIG. 4. The latent heat $Q(L)$ (11) is plotted for $1/L^2$. The linear least-squares fit for $L=0$ (+) and 1,2 mod 3 ($\times$) ($6 \leq L \leq 14$) yields $Q=0.0482(59)$ and 0.0391(38), respectively.

$$\partial_K \Delta f|_{K=K(L)} = 0 \tag{8}$$

holds. The least-squares fit to a series of results for $L=6,9,12$ yields an estimate $K=-0.2697(12)$ in the thermodynamic limit $L\to\infty$. Similarly, for $L=1,2$ mod 3, we obtain $K=-0.2695(14)$. (An observation that the data $L=0$ and 1,2 mod 3 behave differently was noted in Ref. [27].) The above independent results appear to be consistent with each other, validating the $1/L^2$-extrapolation scheme. As a result, we estimate the transition point as

$$K=-0.270(2). \tag{9}$$

We then proceed to estimate the amount of the latent heat with Hamer's method [38]. A basis of this method is as follows. At the first-order transition point, the low-lying spectrum of the transfer matrix exhibits a level crossing, and the discontinuity (sudden drop) of the slope reflects a release of the latent heat. However, the finite-size artifact (level repulsion) smears out the singularity. According to Hamer [38], regarding the low-lying levels as nearly degenerate, one can resort to the perturbation theory of the degenerated case and calculate the level-splitting (discontinuity of slope) explicitly. To be specific, we consider the matrix

$$V=\begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix}, \tag{10}$$

with $V_{ij}=\langle i|\partial_K T|j\rangle$ and the transfer matrix T. The bases $|1\rangle$ and $|2\rangle$ are the (nearly degenerate) eigenvectors of T with the eigenvalues $\Lambda_{1,2}$, respectively. The states $\{|i\rangle\}$ are normalized so as to satisfy $\langle i|T|i\rangle=1$. According to the perturbation theory, the eigenvalues of Eq. (10) yield the level-splitting slopes due to K. Hence, the latent heat (per unit cell) is given by a product of this discontinuity and the coupling constant $K(L)$,

$$Q(L)=|K(L)|\sqrt{(V_{11}-V_{22})^2+4V_{12}V_{21}}\frac{1}{2L}, \tag{11}$$

for the system size L.

In Fig. 4, we plot the latent heat Q (11) for $1/L^2$ and $6 \leq L \leq 14$. The least-squares fit for $L=6,9,12$ yields an estimate $Q=0.0482(59)$ in the thermodynamic limit $L\to\infty$.

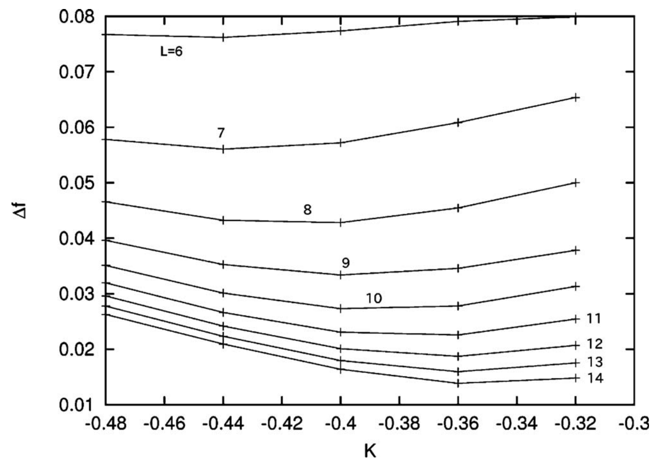

FIG. 5. The free-energy gap (7) is plotted for the bending rigidity K and the system sizes $6 \leq L \leq 14$. Tentatively, the defect parameter (5) is set to $K'=0$.

Similarly, for $L=1,2$ mod 3, we obtain $Q=0.0391(38)$. Considering the deviation of these results as a possible systematic error, we obtain

$$Q=0.043(10). \tag{12}$$

The error margin covers both the statistical and systematic errors.

We consider the $1/L^2$-extrapolation scheme. The finite-size data are expected to converge rapidly (exponentially) to the thermodynamic limit around the first-order transition point for periodic boundary conditions, because the correlation length (typical length scale) ξ remains finite. Hence, the dominant finite-size corrections in our case should be described by $1/L^2$ (rather than $1/L$). On one hand, the curve in Fig. 4 appears to be concave down, indicating an existence of a correction of $O(1/L)$. However, this possibility (second-order phase transition) should be excluded: in a preliminary stage, we made a finite-size-scaling analysis and arrived at a conclusion that the scaling theory does not apply; the critical index ν estimated from the excitation gap tends to diverge as $L\to\infty$. Therefore, we set the abscissa scale in Fig. 4 to $1/L^2$; actually, the result in Fig. 3 demonstrates that the abscissa scale $1/L^2$ is sensible.

As a comparison, we provide a simulation result, setting the defect parameter to $K'=0$ tentatively. In Fig. 5, we present the free-energy gap Δf for the bending rigidity K; the scale of K is the same as that of Fig. 2, Clearly, the data in Fig. 5 are less conclusive. As a matter of fact, the signatures of the crumpling transition strongly depend on the system size L. This result indicates that the choice of the defect parameter K' affects the finite-size behavior. In the preliminary stage, we survey a parameter space of K' and arrive at a conclusion that the above choice [Eq. (6)] is an optimal one.

In summary, the crumpling transition of the discrete planar folding in the $K<0$ regime was investigated with the transfer-matrix method for $L \leq 14$. We adopted a modified folding rule (5), which enables us to implement the periodic-boundary condition. As a result, we estimate the transition point and the latent heat as $K=-0.270(2)$ and $Q=0.043(10)$, respectively. The planar- and three-dimensional-folding models are closely related; see Eqs. (1) and (2). Making use of $K_3=-0.76(1)$ [33] and the present result $K=0.270(2)$, we arrive at $K_3/K=2.815(43)$ (~ 3). Relation (1) appears to hold satisfactorily; a slight deviation indicates that the truncation of the configuration space is not exactly validated. Encouraged by this result, we estimate $Q_3=0.043(10)$ via Eq. (2). This result is consistent with $Q_3=0.03(2)$ [33] and $Q_3=0.05(5)$ [29], indicating that the singularity belongs to a weak-first-order transition rather definitely. Because a direct approach to the three-dimensional folding is computationally demanding, an indirect information from the planar folding would be valuable. A further justification of the configuration-space truncation would be desirable to confirm this claim. This problem will be addressed in the future study.

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