PHYSICAL REVIEW B, VOLUME 63, 132205

Elasticity of a one-dimensional tiling model and its implication to the phason elasticity of quasicrystals

Hyeong-Chai Jeong
Department of Physics, Sejong University, Kwangjinku, Seoul 143-747, Korea
(Received 30 November 2000; published 15 March 2001)

A one-dimensional tiling model with matching rule energy (antiferromagnetic Ising Hamiltonian) is studied. We present an analytic study of a transition from the unlocked phase, where free energy is proportional to the square gradient of the perp-space field $[f\sim(\partial w)^2]$, to the locked phase $(f\sim|\partial w|)$ in perp-space elasticity. The phase diagram and the temperature dependence of the elastic constant in the unlocked phase show similarity with the two-dimensional Penrose tiling. The results imply that the unlocking transition of a two-dimensional Penrose tiling model is related to the disordering transition in a one-dimensional Ising model.

DOI: 10.1103/PhysRevB.63.132205 PACS number(s): 61.44.Br

Since the discovery of quasicrystals,[1,2] phason elasticity has been one of the most important issues of quasicrystal structure studies.[3,4] Quasicrystals have two types of low-energy elastic excitations: phonons and phasons. In the long-wavelength limits, phonons become uniform translations while phasons correspond to rearrangements of atoms from one perfect quasicrystalline lattice to another.[5] Phason disorders, either grown in or quenched, have been observed in almost all kinds of quasicrystalline materials.[6–10] Recently, thermal phason fluctuations in quasicrystals have been directly observed in high-resolution transmission electron microscopy images.[11]

There are two different phases in phason elasticity: the locked phase and unlocked phase.[4,12,13] In the locked phase, where the system behaves like a Penrose tiling, the elastic free energy shows a linear dependence on the magnitude of the phason gradient, whereas it varies quadratically with the phason gradient in the unlocked phase as in a random tiling phase.[12,14,15] Phase transitions between these two phases have been studied numerically with tiling models for quasicrystals.[13,16] However, it has been a difficult problem to show the transition analytically and predict the equilibrium thermal fluctuations in the locked phase because the free energy becomes nonanalytic. In this paper, we consider a toy model in which perp-space elasticity (analogous to phason elasticity in quasicrystal model) can be studied analytically and demonstrate the transition in perp-space elasticity from the unlocked phase to the locked phase.

A one-dimensional (1D) commensurate tiling with mismatch energy is considered. A perp-space field $w(x)$ is introduced by assigning $+1$ for one type of tiles and -1 for the other type. This assignment shows that our 1D tiling model is equivalent to a 1D antiferromagnetic Ising model and the perp-space strain is nothing but a magnetization. We derive the perp-space strain (∂w) dependence of the elastic free energy and show that it is quadratic in the strain $[f\sim(\partial w)^2]$ at $T>0$. We also show how the free energy dependence on the strain crosses over to $f\sim|\partial w|$ as $T\to 0$. The connection between this 1D tiling and a two-dimensional (2D) Penrose tiling is also addressed.

Consider a 1D tiling which has two types of tiles A and B shown in Fig. 1(a). The end points of each tile are decorated with arrows. These decorations give rise to four possible states to the vertex, as illustrated in Fig. 1(b).

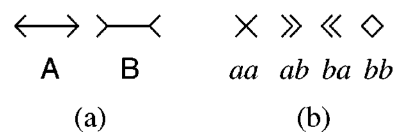

FIG. 1. (a) Two types of tiles A and B in the 1D tiling model. The end points of each tile are decorated with arrows. These decorations give rise to four possible states to the vertex (b).

Our 1D tiling model is introduced by assigning an energy $\varepsilon_v=0$ for the vertices (ab) and (ba), $\varepsilon_v=\epsilon$ for the vertices (aa) and (bb). The ground state has only (ab) or (ba) vertices; hence the A-type tiles and the B-type tiles lie alternately.

The total energy of a tiling χ is defined as a sum of vertex energy:

$$E(\chi)=\sum_{\text{vertex}}\varepsilon_v\,. \tag{1}$$

If we assign spin $S=1$ for an A-type tile and $S=-1$ for an B-type tile, this model is equivalent (except over all energy shift) to a 1D antiferromagnetic Ising model

$$E=\frac{\epsilon}{2}\sum_i S_i\cdot S_{i+1}, \tag{2}$$

with $S_i=+1\ (-1)$ if the ith site is an $A(B)$ type.

Phasons and phonons are elastic Goldstone modes in a quasiperiodic system. Phonons are associated with uniform translations as in a periodic system while phasons are associated with relative translations of incommensurate periodicities, hence found only in a quasiperiodic system. On the microscopic level, phason excitations of finite wavelength correspond to rearrangements of atoms, and in the tiling picture, rearrangements of tiles.

The phason degree of freedom or, more generally, the perp-space (defined below) degree of freedom is easily understood by introducing the concept of the hyperspace. Figure 2 illustrates a way to get the 1D tiling by the projection method from a square lattice in a 2D hyperspace. The lattice sites of the 2D square structure can be projected onto a 1D

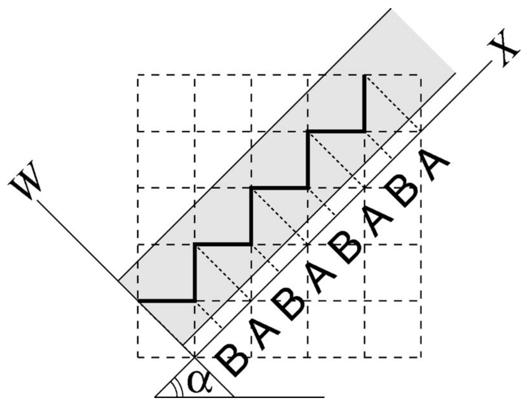

FIG. 2. A 1D tiling on the ''parallel space'' X obtained by the projection method from the square lattice in a 2D ''hyperspace.'' Points in a strip parallel to X and having width $\cos\alpha+\sin\alpha$ (shadowed regions) are projected onto X. The movement of the strip along the ''perp space'' W gives rise to rearrangements of tiles from one perfect sequence $ABABAB\ldots$ to the other perfect sequence $BABABA\ldots$. If the slope of X, $\tan\alpha$, is irrational, the perp space is called a ''phason space'' and the projection gives a quasiperiodic sequence. The figure is for the case of a rational slope with $\tan\alpha=1$.

subspace, which is a straight line X (parallel space) at an angle α with respect to the horizontal rows of the square lattices. The complementary space W is called a ''perp space.'' If the slope of the line is irrational, the projection of all 2D lattice points to X forms a dense set of points. If we restrict projections on X to points confined within a strip which is parallel to X and has a cross section in W equal to the perp-space projection of a square unit cell, then the projection to X gives two types of finite-size tiles and obeys a quasiperiodic sequence. The movement of the strip along the perp space W gives rise to rearrangements of tiles from one perfect quasiperiodic sequence to another. This corresponds to the long-wavelength limit of the phason, and perp space with an irrational slope is called phason space.

For the case of a rational slope, the projection on X is periodic as shown in Fig. 2. The movement (longer than certain amount) of the strip along perp space still causes the rearrangement of tiles from one perfect sequence to another.

In any case, if $w(x)$ is the perp-space field, a smoothed function constructed as an average of the perp-space positions at the vertices near x, uniform perp-space strain $m=\partial w$ produces a number of mismatches (a configuration which is not in a perfect sequence) proportional to $|m|$. Hence the elastic energy is nonanalytic ($F\sim|\partial w|$), and this phase has been called a ''locked phase.''[4,13]

Our 1D tiling model with the Hamiltonian of Eq. (2) corresponds to the case of a rational slope with $\tan\alpha=1$ and 2D lattice constant $=\sqrt{2}$. Both A- and B-type tiles have unit length in physical space. The spin variable $(+1)$ $[(-1)]$ of a type $A[B]$ tile is the perp-space projection values of a type $A[B]$ tile. Hence the perp-space position w at a vertex position x, $w(x)=\Sigma_{i=1}^{x}S_i+w(0)$, and the uniform perp-space strain m is nothing but a magnetization of the Ising model $(m=[w(N)-w(0)]/N=\Sigma_{i=1}^{N}S_i/N)$, and the m dependence of the free energy is easily derived by introducing a magnetization field h to the Hamiltonian of Eq. (2):

$$H=\frac{\epsilon}{2}\sum_{i}^{N} S_i\cdot S_{i+1}-h\sum_{i=1}^{N} S_i . \tag{3}$$

The partition function $Z_N=\Sigma e^{-\beta H}$ of the system of Eq. (3) can be easily calculated using the transfer matrix method:

$$Z_N=\lambda_1^N+\lambda_2^N, \tag{4}$$

where $\lambda_{1,2}=e^{-\beta\epsilon/2}\cosh\beta h\pm e^{-\beta\epsilon/2}[\sinh^2\beta h+e^{2\beta\epsilon}]^{1/2}$ are eigenvalues of the transfer matrix and $\lambda_1\geqslant\lambda_2$.

In the thermodynamic limit, the free energy $g=\ln_{N\to\infty}(Z_N/N)$ depends on the largest eigenvalue (λ_1) of the transfer matrix only and is given by $g=\ln\lambda_1$. Note that g is a function of the intensive variables T and h $[g=g(T,h)]$, since Z_N is so. To get the m dependence of the free energy, we need to do a Legendre transformation

$$\beta f(\beta,m)=\beta g(\beta,h(\beta,m))+mh(\beta,m). \tag{5}$$

The magnetic field h in the above equation is easily expressed in terms of m when we use the fact that $m=-\partial_{(\beta h)}\beta g$:

$$\beta h=\frac{1}{2}\ln[(1-m^2)+2m^2e^{2\beta\epsilon}+2me^{\beta\epsilon}(1-m^2+m^2e^{2\beta\epsilon})^{1/2}]-\frac{1}{2}\ln[1-m^2]. \tag{6}$$

Hence the free energy $f(T,m)$ as a function of the variables T and m is given by

$$\begin{aligned}\beta f(\beta,m)=&-\beta\epsilon/2+\frac{1}{2}\ln[1-m^2]\\&-\ln[1+e^{-\beta\epsilon}(1-m^2+m^2e^{2\beta\epsilon})^{1/2}]\\&+\frac{m}{2}\ln[(1-m^2)+2m^2e^{2\beta\epsilon}+2me^{\beta\epsilon}(1-m^2\\&+m^2e^{2\beta\epsilon})^{1/2}]-\frac{m}{2}\ln[1-m^2].\end{aligned} \tag{7}$$

The $m\to0$ limit of Eq. (6) governs the thermal behaviors of the perp-space elastic excitations of sufficiently long wavelength. In this limit,

$$\beta f(m)=-\beta\epsilon/2-\ln[1+e^{-\beta\epsilon}]+\frac{1}{2}e^{\beta\epsilon}m^2+\mathcal{O}(m^3). \tag{8}$$

We see that the perp-space elastic free energy shows a quadratic dependence on the strain m for sufficiently small strain $[F\sim(\partial w)^2]$. This phase, where the free energy is analytic, has been called an ''unlocked phase.''[4,13]

The elastic constant K in this phase, defined by

$$\beta f=(\text{const})+\frac{1}{2}K(T)m^2-\mathcal{O}(m^4),$$

is given by

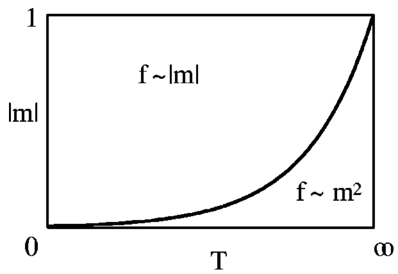

FIG. 3. The phase diagram of the 1D tiling model with Hamiltonian, Eq. (1). The curve $m=e^{-\epsilon/T}$ separates the two regions — the locked phase and the unlocked phase. Here, $m=\partial w$ is a perp-space strain, ϵ is the mismatch energy, and T is the temperature.

$$K(T)=e^{\epsilon/T}. \tag{9}$$

Now let us see how the free energy, which shows a quadratic dependence on the strain at $T>0$, changes to a linear behavior ($F\sim|m|$) at $T=0$. From Eq. (6), at $T=0$,

$$\begin{aligned}\beta f(m)=&-\ln\left[\left(\frac{2e^{\beta\epsilon/2}}{1-m^2}\right)^{1/2}\right]\\&+\frac{m}{2}\ln\left\{2me^{2\beta\epsilon}\left[m\left(1+\frac{1-m^2}{2m^2}e^{-2\beta\epsilon}\right)\right.\right.\\&\left.\left.+|m|\left(1+\frac{1-m^2}{m^2}e^{-2\beta\epsilon}\right)^{1/2}\right]\right\}\\=&-\beta\epsilon/2+\frac{m}{2}\ln[A],\end{aligned}$$

where

$$\begin{aligned}A=&2m^2(1\pm1)e^{2\beta\epsilon}+[(1-m^2)/m](1\pm1)\\&\mp[(1-m^2)/2m]^2e^{-2\beta\epsilon}\end{aligned}$$

($\pm$ represents the sign of m).

For the case of $m>0$, the first term in $[A]$ of the above equation is dominant when we calculate $\ln[A]$ in the limit where T goes to zero, while for the case of $m<0$, the first two terms are zero and the third term is dominant. In both cases, $\ln[A]$ can be expressed as $2\beta\epsilon|m|/m$ and the free energy at $T=0$ is given by

$$f(m)=-\epsilon/2+\epsilon|m|. \tag{10}$$

This equation [Eq. (9)] is valid as long as $|m|e^{\beta\epsilon}\gg1-m^2$; hence the system is in the locked phase if $|m|\gg e^{-\epsilon/T}$.

Figure 3 shows the phase diagram of our model. The thick curve, which separates the two regions — the locked phase and the unlocked phase—is given by $m=e^{-\epsilon/T}$.

Note that the elastic constant $\tilde{K}(T)$ in the locked phase, defined by

$$\beta f(m)=(\mathrm{const})+\tilde{K}(T)|m|-\mathcal{O}(m^2), \tag{11}$$

is linearly proportional to the inverse temperature $[K(T)=\epsilon/T]$.

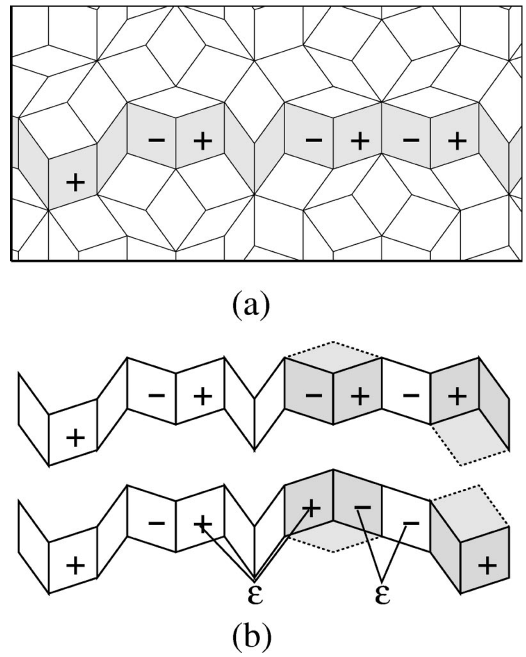

FIG. 4. (a) A piece of Penrose tiling composed from two rhombus shapes, fat and skinny. Along any rail of a perfect Penrose tiling, each shape of tile appears *alternately* in each of its two possible orientations. (+) denotes one orientation of fat tiles and (−) denotes the other orientation of fat tiles. (b) A trail in a perfect Penrose tiling (above) and the trail after flipping some hexagons (shadowed hexagons) (below). Flipping a hexagon which crosses the rail exchanges their positions between tiles of different type in the rail while flipping a hexagon parallel to the rail exchanges tiles of the same type in the rail. Flipping a hexagon of the PPT violates the alternation condition at two places in the rail parallel to the hexagon and costs mismatch energy 2ϵ.

The phase diagram (Fig. 3) and the elastic constant in the unlocked phase [Eq. (8)] shows the same qualitative behaviors as those of 2D Penrose tiling model.[17,12] For the 2D Penrose tiling model, it has been argued that the elastic constant in the unlocked phase should have $K_{\mathrm{Penrose}}=e^{C\epsilon/T}$, where C is a number of the order of 1.[12,17] Using the renormalization methods, Tang and Jaric argued that the boundary between the locked phase and the unlocked phase is given by the curve $m=e^{-2\epsilon/T}$.[12] According to Refs. 12 and 17, the phason fluctuation of wavelength L or longer in a Penrose tiling should occur when the temperature $T>C\epsilon/\ln L$. The disordering transition in our 1D model occurs when the entropy term $T\ln L^{mL}$, due to mL mismatches in a system of size L, is greater than the energy cost $mL\epsilon$:

$$T\ln L^{mL}>mL\epsilon\ (\text{where } m\ll1),\quad T>\epsilon/\ln L. \tag{12}$$

Hence the condition for disordering in the 1D Ising model is the same as that for phason fluctuations in the 2D Penrose tiling (with $C=1$).

The exact connection between our 1D tiling model and the Penrose tiling model is not clear yet. A piece of Penrose tiling composed from two rhombus shapes, fat and skinny, is illustrated in Fig. 4. The shaded tiles in Fig. 4(a) represent a rail,[18] a contiguous strip of tiles which share a common edge direction. In the perfect Penrose tiling (PPT), the fat tiles and the skinny tiles lie quasiperiodically along any rail. Each shape of tile in a rail has two possible orientations, and these two orientations of each shape tiles appear *alternately* in a rail of the PPT.[18] In Fig. 4, $(+)$ denotes one orientation of fat tiles and $(-)$ denotes the other orientation of fat tiles. Two neighboring fat tiles in a rail of the PPT must be either $(+)(-)$ or $(-)(+)$ out of four possible arrangements like the ground state of our 1D model. Flipping a hexagon in a rail of the PPT violates the alternation condition at two places [Fig. 4(b)]. In our model, any arrangement of A and B is possible at $T=\infty$, while possible rearrangements of tile orientations in a rail of the Penrose tiling are restricted by the requirement that the tiles fill a plane without overlaps or gaps. Only tiles forming a hexagon are allowed to change their orientations. Flipping a hexagon parallel to the rail exchanges tiles of the same type while flipping a hexagon which crosses the rail (not parallel to the trail) exchanges the positions of the fat and skinny tiles in a rail and may change the number of hexagons in the rail. Despite these differences, we have found that the phase diagram and the temperature dependence of the elastic constant of our 1D tiling model are similar to those of the 2D Penrose tiling. This seems to indicate that domain-wall-like defects might play a dominant role in determining the phason properties of the Penrose tiling.

In summary, we have presented a toy model which shows a transition from the unlocked phase to the locked phase in perp-space elasticity. By connecting the perp-space field and Ising spin variable, we show how the analyticity of the free energy breaks down as T goes to the transition temperature $T_C=0$. Comparison of the elastic behavior of our model with that of the Penrose tiling model indicates that the unlocking transition of 2D Penrose tiling might be analogous to the disordering transition in a 1D Ising model.

This work was supported by Korea Research Foundation Grant No. KRF-99-015-DP0097.

[1] D. Shechtman, I. Blech, D. Gratias, and J. W. Cahn, Phys. Rev. Lett. **53**, 1951 (1984).

[2] D. Levine and P. J. Steinhardt, Phys. Rev. Lett. **53**, 2477 (1984).

[3] D. Levine, T. C. Lubensky, S. Ostlund, S. Ramaswamy, P. J. Steinhardt, and J. Toner, Phys. Rev. Lett. **54**, 1520 (1985).

[4] C. L. Henley, in *Quasicrystals, The State of Art*, edited by D. P. DiVincenzo and P. J. Steinhardt (World Scientific, Singapore, 1991), pp. 429–524.

[5] T. C. Lubensky, J. E. S. Socolar, P. J. Steinhardt, P. A. Bancel, and P. A. Heiney, Phys. Rev. Lett. **57**, 1440 (1986).

[6] H. Chen, S. E. Burkov, Y. He, S. J. Poon, and G. J. Shiflet, Phys. Rev. Lett. **65**, 72 (1990).

[7] K. Hiraga, W. Sun, F. J. Lincoln, M. Kaneko, and Y. Matsuo, Jpn. J. Appl. Phys., Part 1 **30**, 2028 (1991).

[8] H. L. Li, Z. Zhang, and K. H. Kuo, Phys. Rev. B **50**, 3645 (1994).

[9] S. Ritsch, H.-U. Nissen, and C. Beeli, Phys. Rev. Lett. **76**, 2507 (1996).

[10] G. Zeger, D. Plachke, H. D. Carstanjen, and H.-R. Trebin, Phys. Rev. Lett. **82**, 5273 (1999).

[11] K. Edagawa and K. Suzuki, Phys. Rev. Lett. **85**, 1674 (2000).

[12] L.-H. Tang and M. V. Jaric, Phys. Rev. B **41**, 4524 (1990).

[13] H.-C. Jeong and P. J. Steinhardt, Phys. Rev. B **48**, 9394 (1993).

[14] J. E. S. Socolar, T. C. Lubensky, and P. J. Steinhardt, Phys. Rev. B **34**, 3345 (1986).

[15] H.-C. Jeong and P. J. Steinhardt, Phys. Rev. Lett. **73**, 1943 (1994).

[16] T. Dotera and P. J. Steinhardt, Phys. Rev. Lett. **72**, 1670 (1994).

[17] P. A. Kalugin, Pis'ma Zh. Éksp. Teor. Fiz **49**, 406 (1989) [JETP Lett. **49**, 467 (1989)].

[18] J. E. S. Socolar, in *Quasicrystals*, edited by T. Fujiwara and T. Ogawa (Springer-Verlag, Berlin, 1990), p. 101.