Interface Roughening in Two-Dimensional Quasicrystals

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The equilibrium fluctuations of interfaces in two-dimensional quasiperiodic lattices, such as Penrose tilings, are considered. By a transfer-matrix formulation, this problem is mapped to the one-dimensional Schrödinger equation with a quasiperiodic potential; from the scaling properties of the eigenstates near the band edge, one can extract the exponent ζ characterizing the interface roughness. For a cosine potential, we find a true roughening transition in $d=2$ dimensions. For a Fibonacci tiling, which approximates the Penrose tiling, we find that ζ is nonuniversal, $\zeta<\frac{1}{2}$, and $\zeta\to 0$ continuously as $T\to 0$.

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This Letter explores the thermal roughening of quasicrystal interfaces and surfaces. This is motivated by observations of dodecahedral grains of icosahedral Al-Mn, Al-Mn-Si, and U-Pd-Si alloys,[1] and smooth-faceted triacontahedral "crystals" of the equilibrium icosahedral phase of Al-Cu-Li.[2] We will consider ideal quasicrystals[3]: Like ideal crystals, they contain high-density planes of infinite extent—i.e., they possess translational long-range order—but these planes are arranged quasiperiodically rather than periodically.

In simple lattice-gas models defined on Penrose tilings,[4] it is easy to verify that (as with crystals) there are well-defined facets at temperature $T=0$. The aim of this paper is to investigate the effects of $T>0$ on an interface in thermal equilibrium, for the case $d=2$. Surprisingly, we find that an interface in a quasiperiodic lattice is *less* rough than in the periodic case. In contrast to the periodic case,[5] it may even exhibit a roughening transition at a finite roughening temperature $T_R>0$.

In the first part of this paper, we will consider a solid-on-solid (SOS) model on a rectangular lattice, where the interaction strength is modulated quasiperiodically in the direction normal to the interface. For one case, where the modulation is described by a one-dimensional Fibonacci tiling, the interface is rough at any nonzero temperature, but the roughness exponent ζ is smaller than in a uniform system and goes continuously to zero as $T\to 0$; for a second case, where the modulation is described by an analytic function, there is a genuine roughening transition ($T_R>0$). In the second part of the paper, we consider a model defined on a Penrose tiling, which has quasiperiodic modulations in *five* directions, and show how this problem can be mapped (approximately) to one of the class solved in the first part.

We will take fixed quasiperiodic lattices, and consider simple lattice-gas models which are equivalent to purely ferromagnetic Ising spin models with no external field. We parametrize the interface (running in the x direction) by $z(x)$, with a pinned boundary condition at one end, $z(0)=z_0$. Then we can define a *roughness* (also known as *wall wandering* or *spatial anisotropy*) exponent ζ by[5-7]

$$\langle (z(x)-z_0)^2\rangle^{1/2}\simeq x^{\zeta}. \tag{1}$$

An interface is *localized* (corresponding to a facet) when the left-hand size of (1) is bounded as $x\to\infty$ (which implies $\zeta=0$); otherwise it is called *rough*. In ordinary systems in $d=2$ dimensions we always have $\zeta=\frac{1}{2}$.

Let us now consider a toy model consisting of a rectangular lattice with all ferromagnetic bonds. The bonds in the x direction are all taken equal to a constant $J/2$; however, those in the z direction have the value $V(z)/2$, where $V(z)$ is a quasiperiodic function of z. The energy of an interface is given by

$$H=\sum_x \{V(z(x))+J\,|z(x+1)-z(x)|\}. \tag{2}$$

Let $W(x;z)$ be the total Boltzmann weight of all interfaces ending at (x,z). We use a transfer-operator approach[7] to calculate $W(x;z)$, building out the lattice in the x direction. The state space for each x is labeled by just $z(x)$. We have

$$W(x+1;z)=\sum_{z'=-\infty}^{\infty} e^{-J|z'-z|/T} e^{-[V(z')+V(z)]/2T} W(x;z'). \tag{3}$$

Now, in the limit $T\to 0$, we can work to $O(e^{-J/T})$:

$$W(x+1;z)-W(x;z)=\mathcal{L}W(x;z)\equiv -\tilde{V}(z)W(x;z)+e^{-J/T}[t(z,z+1)W(x;z+1)+t(z,z-1)W(x;z-1)], \tag{4}$$

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where

$$\tilde{V}(z) \equiv 1 - \exp[-V(z)/T],$$

and

$$t(z,z+1) \equiv t(z+1,z) = \exp\{-[V(z)+V(z+1)]/2T\}.$$

Note that, for large x, the same x dependence follows from the continuum form $dW/dt = \mathcal{L}_{\text{cont}} W(z)$, where $\mathcal{L}_{\text{cont}} \equiv \ln(1+\mathcal{L})$ has the same form as (4) but with $\tilde{V}(z) = V(z)/T$, and $t(z,z+1) = f([V(z)-V(z+1)]/2T)$ for $f(y) \equiv (\sinh y)/y$. We will consider, in general, any quasiperiodic $\tilde{V}(z)$ and $t(z,z+1)$, not just the cases arising from (2). In particular, the Penrose tiling model (see below) has *temperature-independent* $\tilde{V}(z)$ and $t(z,z+1)$ as $T \to 0$.

The operator $-\mathcal{L}$ is that of the Schrödinger equation defined on a discrete chain, with $\tilde{V}(z)$ the potential and $t(z,z+1)$ the hopping. The equilibrium state of the interface is specified by the eigenvector of $\mathcal{L}$ with maximum eigenvalue, which corresponds to the ground-state eigenfunction of the Schrödinger equation. When the ground state (and the states near it) are localized, we have a *localized* interface. When the ground state is extended, we have a *rough* interface. From the scaling of the eigenfunctions near the ground state, one can understand the correlations of the interface, in particular its roughness exponent ζ.

What follows is the argument for how the exponent ζ can be extracted from the (known) exponents for the scaling of the energies of eigenstates near the ground state. We can decompose $W(x;z)$ into eigenstates $\psi_E(z)$:

$$W(x;z) = e^{-E_0 x} \int d\mu(E) e^{-(E-E_0)x} c_E \psi_E(z), \quad (5)$$

where $\mu(E)$ is the integrated density of states and E_0 is the ground-state energy. (For simplicity, we consider the continuous formulation of the x evolution.) With the pinned boundary condition, $W(0;z) = \delta(z - z_0)$, it is obvious that the initial "wave packet" contains a broad energy spectrum. After x steps, most of the amplitudes will have decayed to zero apart from those with $E - E_0 < 1/x$. Now, an eigenfunction with energy E close to E_0 looks indistinguishable from the ground state up to a coherence length ξ_c which (see below) scales as

$$\xi_c \sim (E - E_0)^{-\alpha} \quad (6)$$

for some exponent α. The surviving eigenstates in $W(x;z)$, then, are coherent up to $|z| \simeq \xi_c$, beyond which they interfere destructively. Hence $\langle z^2 \rangle^{1/2} \simeq \xi_c$, and

$$\zeta = \alpha. \quad (7)$$

For the case $t(z,z+1) \equiv \text{const}$, equations of form (4) have been intensively studied for two special cases of $\tilde{V}(z)$, both described by $\tilde{V}(z) \equiv v(\tau^{-1} z)$, where τ is the golden ratio, $\tau \equiv (1+\sqrt{5})/2$, and $v(y)$ is periodic, $v(y+1) \equiv v(y)$. Case 1 is the piecewise constant "Fibonacci" potential:

$$v(y) = \begin{cases} 0, & 0 < y < \tau^{-1}, \\ U, & \tau^{-1} < y < 1. \end{cases} \quad (8)$$

In this case, $\tilde{V}(z)$ is always either 0 or U, so that at $T = 0$ there are many degenerate locations for a ground-state interface, as in the uniform case. Equation (8) produces a Fibonacci sequence of values, $00U0U00\cdots$. Our Eq. (4) is a generalization of this case to two values of the hopping coefficient, $t(z,z+1) = t_{00}$ or t_{0U}. Case 2 is Harper's potential,

$$v(y) = U \cos(2\pi y). \quad (9)$$

An essential method for previous studies of the one-dimensional quasiperiodic chain is the 2×2 transfer matrices $A_E(z)$ which, for a given energy E, propagate the corresponding eigenfunction $\psi_E(z)$ down the chain $(\psi_E(z+1), \psi_E(z)) = A_E(z)(\psi_E(z), \psi_E(z-1))$. For the Fibonacci case (8), the matrix $A_E(z)$ just takes on one of two values A_1, A_0 depending on whether $V(z) = U$ or 0. One can construct a renormalization group for the matrices by taking advantage of the self-similarity of the Fibonacci lattice under a kind of decimation called "deflation." One blocks together the pair $U0 \to U$ and $U \to 0$, which reduces the number of sites by a rescale factor τ. This induces an iteration of the transfer matrices which propagate the wave function on the decimated lattice[8]: $A_{n+1} = A_n A_{n-1}$. The nature of an eigenstate is just determined by its A_1 and A_0.

It remains to derive (6) for the Fibonacci case (8). Under the renormalization group, we produce a sequence of eigenstates with coherence lengths $\xi_{c,n}$ and growing differences $\Delta A_n = A_n - A_n^{(0)}$, where the $A_n^{(0)}$ are the iterates of the ground-state transfer matrices. An eigenstate is coherent with the ground state up to ξ_c if its next iterate is coherent up to ξ_c/τ: Hence, $\xi_{c,n} \simeq \tau^{-n} \xi_{c,0}$. Also, $\Delta A_n \simeq \delta^n \Delta A_0$, where δ is the more relevant eigenvalue of the matrix iteration.[8,9] Finally, $\Delta A_0 \sim (E - E_0)$, from the definition[8,9] of (A_1, A_0). Now, $\xi_{c,n} \simeq 1$ at the same step where $\Delta A_n \simeq 1$; solving for $\xi_{c,0}$ in terms of $E - E_0$, we see that (6) holds with $\alpha = \ln\tau/\ln\delta$.

It turns out that δ is just the eigenvalue corresponding to the simple one-dimensional map obeyed by the traces of the transfer matrices.[6,7] For the ground state (corresponding to the two-cycle of the trace map), Kohmoto, Sutherland, and Tang[9] found

$$\delta = [K_I + (K_I^2+4)^{1/2}]/2, \quad K_I \equiv (25+16I)^{1/4}, \quad (10a)$$

where I is the invariant of the trace map, given by

$$I = (e^{J/T}/2)^2 [U t_{00}/t_{0U}^2 + E_0(1/t_{00} - t_{00}/t_{0U}^2)]^2. \quad (10b)$$

Recalling Eq. (7), we have finally

$$\zeta = \ln\tau/\ln\delta, \tag{11}$$

where δ is given by Eqs. (10). As a check, note that for the uniform case, $V(z)\equiv 0$, $t_{00}\equiv t_{0U}$, then $I=0$, and so $\delta=\tau^2$, which indeed gives the usual $\zeta=\frac{1}{2}$.

The roughness exponent ζ is nonzero, and so the interface has unbounded fluctuations, but these are anomalously weak: $\zeta<\frac{1}{2}$, and the exponent ζ depends continuously on the temperature through I. When U, t_{00}, and t_{0U} are temperature independent, then as $T\to 0$, $E_0 \to$ const and (10b) implies $I\simeq e^{2J/T}$; as $I\to\infty$, $\delta\sim I^{1/4}$, so that

$$\zeta \approx 2\ln\tau(T/J). \tag{12}$$

The behavior (12) follows whether or not $t_{00}=t_{0U}$.

Numerical iteration of (4) using the Fibonacci potential (8) with $U=1-\exp(-0.4)$, fitted to (1) over the range $10^3<x<10^5$, gave $\zeta=0.35\pm 0.01$ and 0.27 ± 0.02 for $T/J=0.4$ and 0.3, respectively, in full agreement with the values 0.347 and 0.280 predicted from (10b).

Next we consider the other case, that of Harper's potential (9). Take the case of constant $t(z,z+1)\equiv t$: If $Ue^{J/T}/t<2$ ($Ue^{J/T}/t>2$), then *almost all* states,[10] in particular those near the ground state,[11] are extended (localized). This implies a roughening temperature T_R such that the interface is localized for $T<T_R$ and rough, with $\zeta=\frac{1}{2}$, for $T>T_R$. In the actual model derived from (2) and (9), $t(z,z+1)$ has an (analytic) quasiperiodic modulation. We still expect a second-order roughening transition in this case, although the value of T_R (and possibly of ζ) will be changed.

Exactly at $T=T_R$, we expect critical scaling near the ground state with a nontrivial ζ. Indeed, using (7) we extract $\zeta\cong 0.421$ from Ref. 11. Furthermore, fluctuations of the interface will diverge at T_R characterized by correlation lengths $\xi_\parallel\sim|T-T_R|^{-\nu_\parallel}$ and $\xi_\perp\sim|T-T_R|^{-\nu_\perp}$ in the x and z directions, respectively, with

$$\nu_\perp=1, \quad \nu_\parallel=1/\zeta\cong 2.38. \tag{13}$$

Here $\nu_\perp=1$ is well known for the localization length of the one-dimensional Schrödinger equation[10] and $\nu_\perp=\zeta\nu_\parallel$ follows from scaling.[6] The interfacial free energy satisfies hyperscaling: It scales as $1/\xi_\parallel$ and so the exponent α_s of the interface specific heat at T_R is given by $\alpha_s=2-1/\zeta<0$.

We now study the interface roughening in the "cell" model, defined on the version of the Penrose tiling with two kinds of rhombi.[12] The center of each rhombic cell has one spin, with four ferromagnetic bonds (strength $J/2$) to the spins in the neighboring rhombi. An interface between ferromagnetic ground states is just a path along the edges of the tiling, and its cost is J times its length.

The $T=0$ interface paths can be found[4,13] with the grid, or dual, construction of the Penrose tiling[12]: The optimal interface runs normal to an edge direction (which we will call the z direction). It consists of *any* path of steps which have a positive projection on the x direction. (See Fig. 1.) For a fixed starting point, z_0, the path is *not* unique, but is confined within a "lane," bounded by rows of tiles with $\pm z$ edges. (These rows are called "tracks" in Ref. 4. Consequently, the interface is smooth at $T=0$.

There are two general classes of lanes (Fig. 1): narrow ones, which have a width zero in places, and wide ones, which have a minimum of two sites in parallel. The wide and narrow lanes are stacked vertically so as to form a Fibonacci sequence, which we will number by $z=1,2,3,\ldots$.

We now let $W_0(x;z)$ be the the number of paths (up to x) in lane z: obviously it is larger for the wide lanes. With use of the projection construction of the tiling,[12] it can be shown that the same sequence of environments repeats quasiperiodically along each lane. Thus each lane has a well-defined entropy, $W_0(x;z)\simeq\exp[S_{\rm lane}(z)x]$, which is quasiperiodic in z: $S_{\rm lane}(z)=s_{\rm lane}(\tau^{-1}z)$, where $s_{\rm lane}(y)\equiv s_{\rm lane}(y+1)$.

We next approach the interface fluctuations in the same spirit as with the lattice model. At $T>0$, the interface may jump from one lane to the next (along a z edge) with a Boltzmann cost $e^{-J/T}$. At low temperatures we may take a continuum approximation in the x direction, exactly as with the lattice model. In place of $V(z)/T$, the potential term in the Schrödinger operator in (4) is now $\tilde V(z)=-S_{\rm lane}(z)$. The form of $s_{\rm lane}(y)$ is similar to Eq. (8). We find that $s_{\rm lane}(y)$ ranges, depending on y, from 0.451 58 to 0.454 44 for narrow lanes (an analytic result) and for wide lanes from 0.540 363 3 to 0.540 364 7 (numerical result). The hopping rate between lanes is also quasiperiodic as a function of z, and is similar in form to the model with two hopping coefficients, $t_{00}\cong 0.47$ and $t_{0U}\cong 0.44$. Here $t(z,z+1)<1$

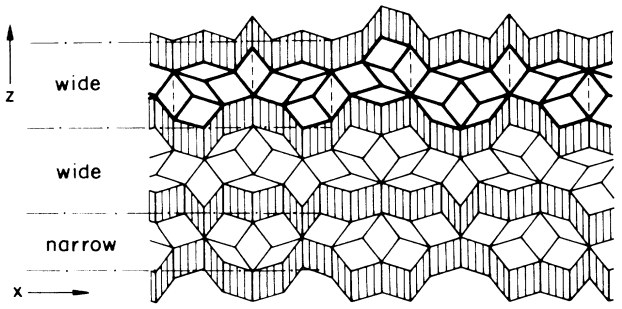

FIG. 1. Part of two-dimensional Penrose tiling showing three "lanes" (two wide and one narrow). Any path which always moves to the right and does not cross the shaded strips is a ground-state interface; the union of these paths is shown bold in the first lane. The vertical dashed lines in the first lane show how it breaks up into two kinds of units, repeated quasiperiodically.

reflects the reduction in entropy due to the constraint that a hop must start from the edge of a lane.

Thus, the interface should look rough with an exponent behaving like (12) as $T \to 0$. However, there is evidence that $s_{\text{lane}}(y)$ [and the analogous envelope function for $t(z,z+1)$] is not exactly piecewise constant. We speculate that this may lead to a crossover to a roughening transition at very low T [the exponents would differ from (13) since $s_{\text{lane}}(y)$ is nonanalytic.]

In other, more generic 2D models (e.g., with J_{ij} depending on local environment,[14] or with farther-neighbor interactions), we would expect the effective potential to have a continuum of values (and include energy terms, not just entropy terms). In this case, $\tilde{V}(z)$ might better be approximated by Harper's equation (9), which implies a roughening transition.

We have not analyzed the case of $d=3$ here; clearly, a quasiperiodic $V(z)$ in the interface normal direction will increase the tendency of the interface to be localized. In fact, an argument based on the functional renormalization group[15] suggests that the interface is *always* localized in $d=3$ dimensions.

We have also ignored the role of disorder, which seems to be universal in the real alloys.[2b,16] An important kind of disorder is "phason strain"[17] which involves rearranging tiles without introducing dislocations.[3b] A lattice-gas model on a fixed lattice with quenched "phason" disorder should exhibit a roughening due to effective random exchange as in Ref. 7.

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