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Unusual Wetting Transitions in Two-Dimensional Quasi-Crystals.

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Abstract. – A model for wetting in a 2*d* ideal Penrose tiling is presented. The exponents and the nature of the wetting transition for long-ranged potentials are determined by an approximate renormalization group approach and confirmed numerically. The wetting shows unusual features due to the self-similarity of the quasi-periodic lattice. For short-ranged potentials a new universality class of transitions is established and the critical behaviour is determined.

Interfaces in ideal quasi-crystals exhibit very unusual fluctuations. They are genuinely less rough than their crystalline counterparts. In the case of two dimensions, where interfaces in crystals are rough for all finite temperatures T with a universal roughness exponent $\zeta = 1/2$, interfaces in quasi-crystals can exhibit a roughening transition at finite T or, in an alternative model, a roughness exponent $\zeta < 1/2$ that depends continuously on T [1-4]. This critical behaviour could possibly be observed in the edge melting of domains of an adsorbed monolayer on the facets of decagonal (T-phase) quasi-crystals, as the edge of the monolayer should feel the quasi-periodic modulation of the underlaying substrate.

New critical phenomena arise when the interface is bound to a second surface. Consider, *e.g.*, the experimental situation where a quasi-crystalline layer is grown from the melt on a flat crystalline substrate (1). The thickening of the layer depends primarily on the wetting properties of the system, which can be understood in terms of the effective interaction between the two interfaces bounding the layer. The different character of the interfacial fluctuations in

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(1) In our model we consider the interface between two domains within a *fixed* quasi-crystalline lattice. This describes, *e.g.*, the boundary between magnetic domains. By analogy to the periodic crystal it is plausible to assume that the same model applies to the surface of a quasi-crystal in contact with a fluid phase. Thus, we do not address the subtleties of the aggregation mechanism at the surface of quasi-crystals.

quasi-crystals is expected to alter the critical behaviour at wetting transitions. This is indeed what we find for the two-dimensional model we consider.

Using an approximate renormalization (RG) group we determine the exponents and the nature of the wetting transition analytically for long-ranged potentials. The wetting proceeds by an almost discontinuous addition of layers whose thickness increases exponentially. For short-ranged potentials, numerical solution of the transfer matrix equation reveals that the critical exponent $\nu_{\parallel}$ goes to 1 for large $\tau = 1/\zeta$ in contrast to the behaviour of Gaussian models. The dependence of the exponents on τ is found to be approximately given by a generalized necklace model.

To be more specific consider a free interface in a lattice gas model on an ideal $2d$ Penrose tiling. It was shown previously that this model can be represented, at least for low T, by an effective interface model on a $2d$ square grid with Hamiltonian

$$\mathcal{H}\{z\}/T = \sum_x \frac{J}{T}\,|z_{x+1} - z_x| + V_\sigma(z_x), \tag{1}$$

where x and z_x are integers (*i.e.* the lattice spacing is taken to be unity) [1, 2]. The variable z_x measures the distance of the interface to a line of reference and V_σ is an (entropic) Fibonacci potential

$$V_\sigma(z) = \begin{cases} 0 & \text{for } 0 < z + z_0 \leq 1 \pmod{\sigma}, \\ \Delta S & \text{for } 1 < z + z_0 \leq \sigma \pmod{\sigma}. \end{cases} \tag{2}$$

The parameter z_0 is a free phase which depends on the choice of the z-origin in the tiling, $\sigma = (1 + \sqrt{5})/2$ is the golden mean, J the coupling between neighbouring spins in the original tiling and ΔS the difference in entropy per projected length between the wide and the narrow tracks of the Penrose tiling. For low T the equilibrium properties are given by the ground-state solutions of the discrete Schrödinger equation

$$E\psi(z) = U(z)\,\psi(z) - t(z-1, z)\,\psi(z-1) - t(z, z+1)\,\psi(z+1) \tag{3}$$

with

$$U(z) = 1 - \exp[-V_\sigma(z)] \quad \text{and} \quad t(z, z') = \exp[-J/T - (V_\sigma(z) + V_\sigma(z'))/2].$$

The roughness exponent ζ has been deduced from the scaling of the integrated density of states [1] which is known from an exact RG treatment of the Schrödinger equation (3) [5]. The result is exact and valid for all temperatures but cannot easily be extended to incorporate an additional binding potential. Alternatively one can use an approximative RG [2] which gives a very intuitive picture of the scaling of the wave function and the spectrum [6]. We shall extend the second approach and incorporate an external potential.

The RG consists of a successive elimination of sites with locally higher energy. In each RG step, the weaker hopping terms are ignored, the ground state is calculated and the weak couplings are then reintroduced perturbatively. The first step reduces the general Schrödinger equation to a pure hopping model with hopping constants $t_s^{(0)}$ and $t_w^{(0)}$. They form a Fibonacci sequence and their ratio is given by

$$q = t_w^{(0)}/2t_s^{(0)} = \exp[-J/T]\,\frac{1 - U_0}{2(\exp[-J/T] + U_0)} \tag{4}$$

with $U_0 = 1 - \exp[-\Delta S]$.

The lowest-lying states of the n-th RG step, corresponding to the strongly coupled pairs of sites, shall be called «molecules of n-th order». The energy $E(n)$ of such a state can be calculated exactly by summing up the contributions from all RG steps (including the energy shifts). In this way, we arrive at

$$E_0(n) = E_0 + G(n) \qquad \text{with} \qquad G(n) = \exp[-J/T]\,\frac{1+2q}{1-q}\,q^{n+1} \tag{5}$$

with the ground-state energy

$$E_0 = -\exp[-J/T](1+2q)(1-q+q^2)/(1-q)\,. \tag{6}$$

In each RG step the lattice is rescaled by a factor σ^2. Hence the size $\xi_\perp$ of the molecule of n-th order scales as σ^{2n}. The lateral coherence length $\xi_\parallel$ of a state superimposed from eigenfunctions with energies between E and E_0 is of the order $1/(E - E_0)$, which is $1/G(n)$ for the n-th order molecule. Comparison with the scaling relation $\xi_\perp \sim \xi_\parallel^\zeta$ leads to the roughness exponent

$$\zeta = 2\ln\sigma/(-\ln q)\,, \tag{7}$$

where ζ depends continuously on T according to (4).

We have determined E_0 numerically for several values of J/T i) by diagonalizing the transfer matrix in a finite range of z and subsequent finite-size scaling and ii) by direct iteration of the transfer matrix. The numerical values for E_0 compare favourably with the predictions of eq. (6), which can thus be used in the exact expression for ζ (eqs. (10) and (11) of ref. [1]), where E_0 enters as a parameter. In this way one obtains an excellent fit to the values as determined numerically for all J/T. The approximate expression (7), on the other hand, represents the behaviour for small T fairly accurately, with an error of less than two percent for $J/T \gtrsim 4$ or $\tau = 1/\zeta \gtrsim 3$.

Consider now a semi-infinite geometry where the fluctuating interface is excluded from the half-space with $z < 0$ and an interaction potential $V(z)$ is added to the effective Hamiltonian (1). This models the presence of a second interface or surface interacting with the fluctuating one. The interface can now undergo a wetting or unbinding transition from a bound state, for which it is confined to small values of z, to an unbound state where it makes arbitrarily large excursions in z.

The critical behaviour depends strongly on the behaviour of the binding potential $V(z)$ for large z. The inhibition of fluctuations over the boundary at $z = 0$ induces an effective repulsion $V_{\mathrm{fl}}(z)$ of the surface which decays as $z^{-\tau}$ for large z with $\tau = d_\parallel/\zeta = 1/\zeta$ [7-9]. For the potentials that decay more slowly than V_{fl} the interface is expected to be found for arbitrarily small amplitude of the potential. Its mean position may be estimated from the minimum of the effective interaction $V + V_{\mathrm{fl}}$. For power law potentials $V(z) \approx -W(z^{-s}+1)/s$ for large z, with $s < \tau$, this yields

$$\langle z\rangle \sim W^{-\psi} \qquad \text{with} \qquad \psi = 1/(\tau - s)\,. \tag{8}$$

Note that the expression is valid for all $s < \tau$, *i.e.* for s negative. This includes the cases $s = -1$ and $s > 0$, conventionally termed complete and critical wetting, respectively.

The approximate RG confirms this result and gives a more detailed account of the unbinding transition. As the strength of the potential for large z will limit the spread of the probability distribution we expect it to be localized on the «molecule», say of order n, which is closest to the wall at $z = 0$. The contribution to the free energy from the quasi-periodic potential, $E_0(n)$, is smaller for large n, while the contribution from the potential energy increases, because the mean distance $\bar{z}(n)$ of the first molecule of n-th order from the wall grows with n. We estimate the potential energy by $V(\bar{z}(n))$ and observe that $\bar{z}(n)$ scales like the size of the molecule, namely $\bar{z}(n) \sim \sigma^{2n}$. Minimization of the total free energy $F(n) = E_0(n) + V(\bar{z}(n))$ with respect to n

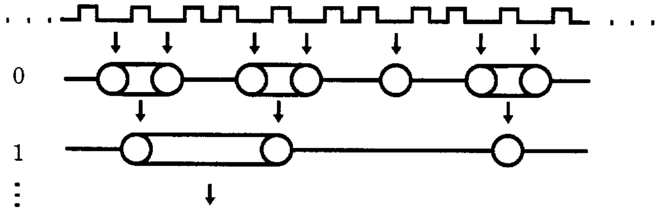

Fig. 1. – Scheme of the renormalization group. Only the sites of lowest energy are retained. The double valleys of the Fibonacci potential couple over the intermediate sites, thus forming strongly coupled «molecules» (double lines) and weakly coupled «atoms» (single lines). They couple again to «molecules» of successively higher order.

gives $n \approx -\ln W/[2(\tau - s)\ln\sigma]$ for small W where (5) and (7) have been used. Insertion into $\bar{z}(n) \sim \sigma^{2n}$ yields eq. (8). In addition, $\xi_\parallel \sim 1/G(n)$ leads to

$$\xi_\parallel \sim W^{-\nu_\parallel} \quad \text{with} \quad \nu_\parallel = \tau/(\tau - s). \qquad (9)$$

The transition from n-th order molecule to the $(n+1)$-st order molecule can i) be smooth, if the two molecules overlap, or ii) abrupt, if they do not, because the two molecules are then separated by a region of higher average potential (see fig. 1). Thus, on a double logarithmic scale, $\xi_\parallel$ *vs.* W will exhibit rounded or sharp steps whose average height is $\ln\bar{z}(n+1) - \ln\bar{z}(n) = 2\ln\sigma$.

The unbinding has been studied by numerical diagonalization of the Schrödinger equation (3) for a variety of algebraic potentials and several values of τ. The results for ψ are shown in fig. 2. The divergence of the exponents as s approaches τ from below can be seen clearly. The agreement between measured and predicted exponents lies within five percent. An equally good agreement is observed for $\nu_\parallel$.

Figure 3 shows the details of the unbinding process for $s = -1$. The distribution depicted in fig. 3*b*) is indeed localized on the molecules of successively higher order, as is apparent from its self-similar structure in comparison with fig. 1. Figure 3*a*) shows clearly the predicted steps in $\langle z\rangle$ and $\xi_\perp$ and cusps of $\xi_\perp$ at the transition points, thus resembling a layering transition. We emphasize again that the thickness of the added layers increases exponentially with diminishing W. This unusual behaviour is a direct consequence of the self-similarity of the potential V_σ and a similar effect should be observed in wetting transitions in other self-similar structures.

If the direct interaction $V(z)$ decays faster than V_{fl} for large z, the simple scaling picture breaks down. The Schrödinger equation has been diagonalized numerically for several values of τ and a wide variety of short-range potentials V. The results are consistent with the expecta-

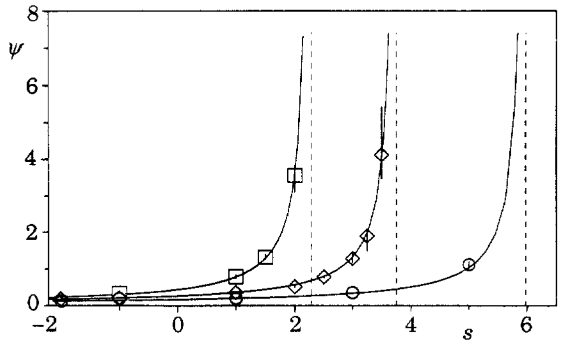

Fig. 2. – Critical exponent ψ for long-ranged potentials. The dashed lines indicate the limit $s = \tau$. □ $\tau = 2.28$, ◇ $\tau = 3.75$, ○ $\tau = 5.97$.

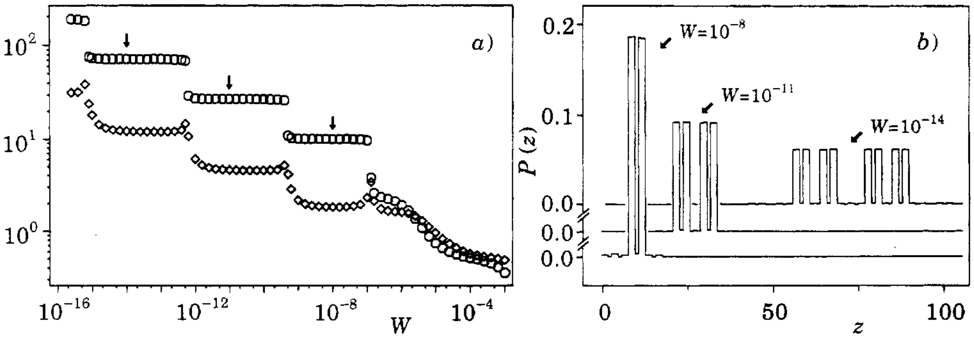

Fig. 3. – Details of the wetting transition for long-ranged potential for the case $V(z) = Wz$, $z_0 = 0$. *a*) $\langle z\rangle$ (○) and $\xi_\perp$ (◇) grow in a stepwise manner as W diminishes. *b*) Normalized probability distributions for the W-values indicated by arrows in *a*). They are localized on the sites of the «molecules» of the Fibonacci potential and show their self-similar structure.

tion that the critical exponents of the unbinding depend only on τ but not on the detailed shape of the potential. Very accurate scaling $\langle z\rangle \sim (W - W_{\text{crit}})^{-\psi}$ is observed, with W_{crit} finite. The results for a square-well potential at the wall are shown in fig. 4. Both $\nu_\parallel$ and ψ decrease with increasing τ. Apparently ψ approaches 0 and $\nu_\parallel$ approaches 1 for large $\tau = 1/\zeta$ or small T, see (7). This is plausible, as the interface is flat at $T = 0$ and the transition is therefore of first order.

The critical exponents can be reproduced quite accurately by a generalized necklace model: in ref. [10] it was shown that $\nu_\parallel = 1/(1-\gamma)$ if the probability of return of the freely fluctuating interface to the wall scales as $x^{-\gamma}$. Now, let $P_x(z)$ be the probability distribution for the position of the interface at x. If $\langle z^2(x)\rangle \sim x^{2\zeta}$ holds for large x and if the shape of the distribution does not change with increasing number of steps x, then one has $P_x(z) \sim x^{-\zeta}\chi(z/x^\zeta)$ with some normalized shape function χ and the probability of return to the origin after x steps, $P_x(0)$, scales as $x^{-\zeta}$ [11, 8]. Hence

$$\psi = 1/(\tau - 1), \qquad \nu_\parallel = \tau/(\tau - 1), \qquad \text{with} \qquad \tau = 1/\zeta. \tag{10}$$

This gives the correct limit for large τ. The values agree quite well with the numerical values as shown in fig. 4 although the deviations exceed the numerical error. The discrepancy might be due to the fact that the shape of P_x as observed numerically is only approximately independent of x.

It should be noticed that the standard effective Gaussian model for an interface with (contin-

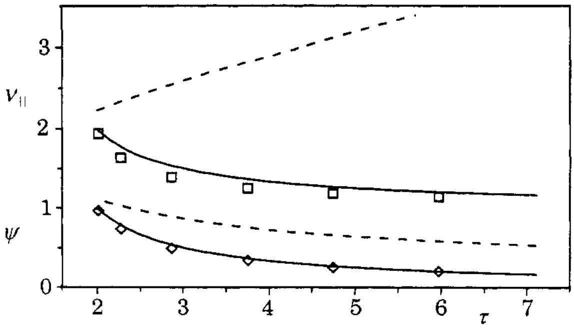

Fig. 4. – Critical wetting exponents for short-ranged potential. The numerical results (□ $\nu_\parallel$, ◇ ψ) are compared with the predictions of the necklace model (NM) (——) and of the functional renormalization group treatment of an effective Gaussian model (FRG) (- - -).

uous) Hamiltonian [9]

$$\mathscr{H}\{z\} = \int \frac{\mathrm{d}^{d_\parallel} q}{(2\pi)^{d_\parallel}} \frac{\tilde{\Sigma}}{2} q^{2-\eta} |\hat{z}(\boldsymbol{q})|^2 + \int \mathrm{d}^{d_\parallel} x V(z(\boldsymbol{x})) \tag{11}$$

behaves rather differently. Since $\zeta = (2 - d_\parallel - \eta)/2$, the free interface in this model shows for $d_\parallel = 1$ and $\eta = 1 - 2\zeta$ exactly the same scaling as the free interface in the lattice model with a Fibonacci potential, namely the same ζ. However, when the effect of the potential V is studied by functional renormalization (FRG), the critical exponent $\nu_\parallel$ is found to increase with increasing τ and to diverge for large τ [7, 12, 13]. The values obtained numerically from a FRG with infinitesimal rescaling factor are shown for comparison in fig. 4 [12]. However, the general fixpoint structure of the FRG, with ψ depending only on τ, is conserved (2).

The difference between the quasi-periodic lattice model and the effective Gaussian model can be understood if the kinetic term in (11) is written as an interaction term in real space. For $d_\parallel = 1$ and $\eta \geqslant 0$, one then has $\mathscr{H}\{z\} = \int \mathrm{d}x\, \mathrm{d}y\, z(x)\, W(|x - y|)\, z(y)$, where $W(r) \sim r^{-(2+\sigma)}$. For $\sigma > 1$ the exponents $\eta = 0$ and $\zeta = 1/2$ are universal, while for $1 > \sigma > 0$ one has $\eta = 1 - \sigma$ and $\zeta = \sigma/2$. The borderline case $\sigma = 1$ separates short-ranged interactions from long-ranged ones [14]. For the values of ζ which apply to the quasi-periodic system, $0 < \zeta < 1/2$, the Gaussian model is thus in the regime of long-ranged lateral interactions. This has to be confronted with the lattice model itself, which includes only nearest-neighbour interactions. The necklace model, on the other hand, is based on the concept of a random walk with x as the time and is hence a Markov process with no long-ranged interaction in x-direction. This explains why it is more appropriate for the model at hand than the effective Gaussian model.

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(2) In recent work on FRG additional fixpoints have been postulated for large values of τ [12, 13]. We have not found evidence for these fixpoints in simulations with appropriately shaped potentials. However, an analytical solution in the periodic case indicates that strong crossover effects hide the postulated transitions for system sizes that are numerically manageable.

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