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LETTER TO THE EDITOR

Wetting of random substrates

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Abstract. Using a position-space renormalisation group (RG) we analyse the phase diagram for wetting of the substrate interacting randomly with the Ising system. The critical probability p_c for the onset of wetting is calculated as a function of temperature. We expect that numerical values obtained for the two-dimensional system are quite accurate when compared with (non-existent) exact results. Results for a three-dimensional system are expected to be qualitatively correct.

The phenomenon of substrate wetting has been the subject of much recent interest (Cahn 1977, Abraham 1980, 1981, Pandit *et al* 1982, Pandit and Fisher 1983). In particular, a considerable amount of work was devoted to questions of substrate wetting in substrate-vapour systems: it is known that many such systems always wet, and others never wet, and that some systems may wet at higher temperatures and cease to do so as the temperature is lowered. It is generally believed that the main source of this kind of behaviour is to be found in the nature of the substrate-vapour interaction. This interaction, if sufficiently weak or long-ranged, can interfere with wetting and, in some cases, suppress it completely (Nightingale *et al* 1983).

Theoretical studies of the subject have mostly relied on lattice-gas or Ising model systems (Oliveira and Griffiths 1977, Abraham 1980, Pandit *et al* 1982) in which the substrate is taken as ideal, chemically inert, and uniform. The purpose of the present letter is to analyse the phenomenon of wetting of non-ideal substrates, a situation much more likely to be encountered in real experiments. Our study will be based on the appropriately modified version of Abraham's (1980) archetypal model for wetting in two-dimensional Ising systems.

Let us then consider a two-dimensional Ising model with periodic boundary conditions in one direction and antiperiodic in the other, with the seam of 'defect' couplings (of strength J_d) orthogonal to one surface, as shown in figure 1. Defect couplings in the original version of this model (Abraham 1980) are assumed weaker than those in the bulk so that the interface (created by the boundary conditions) will be bound to the defect at sufficiently low temperatures. When the temperature T is increased above a certain value $T_R(J_d)$, the interface unbinds from the defect and the interface specific heat exhibits a jump discontinuity. It is said that a wetting (unbinding, depinning) transition takes place at $T = T_R$. The functional dependence of the wetting transition temperature T_R on the defect coupling strength J_d (the phase diagram) is shown in figure 2. The phase diagram is obtained as the non-trivial solution of the (exact) equation (Abraham 1980, equation (8))

$$\tanh^2(K_d) = \tanh(K) \tanh(K - K^*) \quad (1)$$

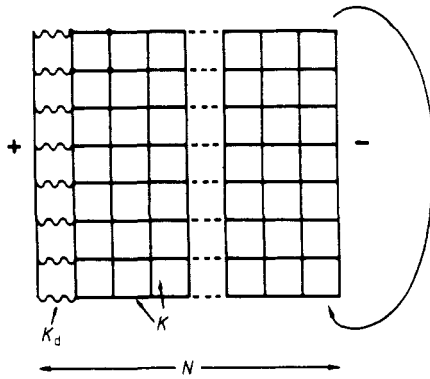


Figure 1. Schematic drawing of the model used in our calculation. Periodic boundary conditions are taken in the direction indicated. Couplings K_d and K are shown by wavy and full lines respectively.

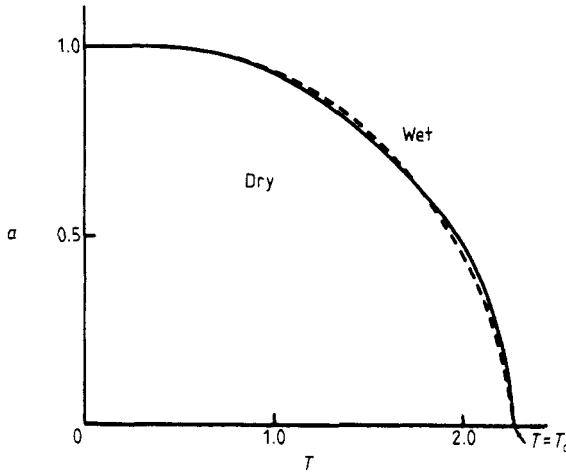


Figure 2. The wetting transition phase diagram (Abraham 1980) as a function of parameter $a = K_d/K$. Full curve: exact result obtained from (1). Broken curve: RG result obtained from (2).

where $K_d = J_d/k_B T$, $K = J/k_B T$, and K^* is the dual coupling defined by $\tanh(K^*) = \exp(-2K)$. (Note that the original equation of Abraham (1980, equation (8)) differs from (1) but we have kept this form for future convenience; otherwise, equation (1) above and equation (8) of Abraham (1980) are equivalent.) Defect couplings J_d are parametrised as $J_d = aJ$ ($0 \leq a \leq 1$), where the parameter a measures the amount by which defect couplings are weaker than those in the bulk. We note that defect couplings all have the same value J_d indicating that the substrate is uniform. In order to study wetting of non-uniform substrates we shall modify the model just described by appropriately changing the value of J_d .

In order to model a non-uniform substrate we shall take defect couplings to have value J_1 with probability p , and a value J_2 with probability $(1 - p)$. Coupling strengths J_1 and J_2 can in principle have arbitrary values but the most interesting choice is when,

for a given temperature, coupling J_1 , say, binds the interface, while J_2 does not. The result of the competition between binding (J_1) and unbinding (J_2) tendencies of the substrate will depend on the value of probability p and there clearly must exist some critical probability p_c at which the corresponding transition takes place. A quantitative analysis of this problem is the subject of the rest of this letter.

We propose to study the model just described by using a position-space renormalisation-group (RG) method applied earlier (Švrakić 1983) to the original wetting problem of Abraham (1980). The method is based on the simple cumulant expansion approximation for RG recursion relations. In spite of the apparent simplicity of this approach the method is fully capable of capturing the essential physical features of a number of phenomena associated with interfaces. For example, the RG phase diagram for the wetting transition is obtained from the equation

$$K_d^2 = K(K - K^*) \quad (2)$$

which is just equation (12) of Švrakić (1983), and is shown as the broken curve in figure 2. At this point we should make a technical comment. First, equation (2) is *independent* of the particular approximation used; simply, any RG scheme will produce the result above. Second, both equation (2) and (the exact) equation (1) have the same limiting forms: $K_d = 0$ (or $a = 0$) when $K = K^*$, and $K_d = K$ (or $a = 1$) when $K^* = 0$ (or equivalently $T = 0$). Note also that equation (2) looks like the first-order expansion of equation (1). Third, one can go a step further by observing that $\sigma = 2(K - K^*) = 1/\xi$ from which it immediately follows (since $\sigma \propto K_d$, up to a multiplicative factor) that the *bound* interface fluctuates on the scale $\xi^{1/2}$. At and above the wetting transition temperature, interface fluctuations are scaled by ξ and these extra fluctuations are responsible for the jump in the interface specific heat (Abraham 1980). We emphasise that these remarks are relevant for RG approximation in general. The difference between various approximations comes in through a particular definition/numerical value of quantities like the interface tension or the correlation length, a difference which ultimately comes from the particular approximation for K^* . *Within RG scheme employed here* K^* is defined (calculated) from $K^* = K(1 - \prod_{n=0}^{N=\infty} \langle S^{(n)} \rangle^2)$ where the notation follows that of Švrakić (1983). A glance at figure 2 where RG result (broken curve and equation (2)) are compared with the exact result (full curve and equation (1)) reveals that the first-order approximation can accurately reproduce the exact wetting phase diagram. Moreover, if one substitutes in equation (2) the exact expression for the dual coupling ($\tanh(K) = \exp(-2K^*)$) instead of computing it from the RG equations then the results become graphically indistinguishable. This indicates that *forms* given by equations (1) and (2) are quite close to each other over the whole temperature range, or that first-order expansion is sufficient in dealing with wetting problems. (To use a different language, higher-order diagrams cancel out.) Now we are in the position to address the problem of random defect couplings.

The calculation of the random defect coupling recursion relation follows closely that of the non-random problem. One writes down the recursion relation for defect couplings and the recursion relation for bulk couplings (see equations (5) and (6) of Švrakić (1983)). One then equates the two and the result is

$$[pK_1 + (1-p)K_2]^2 = K(K - K^*) \quad (3)$$

where $K_i = 1/k_B T$ ($i = 1, 2$). Note that equations (3) and (2) are of the same form indicating that randomness enters the problem as some effective substrate coupling $K_d^{\text{eff}} = [pK_1 + (1-p)K_2]$ i.e. in a mean-field-like fashion. If this is correct then we

expect the phase diagram calculated from (3) to be quite accurate when compared with the (presently non-existent) exact one. The calculation of this phase diagram is now straightforward: one solves equation (3) for p and introducing $K_1 = aK$; $K_2 = bK$ (a and b parameters, K bulk coupling) obtains

$$p_c = [(\sigma/2K)^{1/2} - b]/(a - b) \tag{4}$$

where we have used $\sigma = 2(K - K^*)$. This result is shown in figures 3, 4 and 5. We have chosen values for parameters a and b so that binding/unbinding tendencies of the substrate are most pronounced. Depending on this choice, the wetting region increases/decreases on the phase diagram and, indeed, may be absent at some temperatures. Other similar features are apparent in the figures.

We wish to conclude with two comments. First, keeping in mind the discussion following equation (2), it comes as no surprise that equation (4) is also valid for the

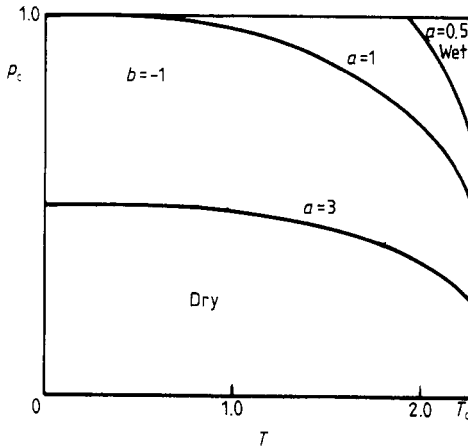


Figure 3. Critical probability for wetting of the random substrate as a function of temperature, calculated from (4). Parameter b is chosen so that couplings K_2 are binding for all temperatures.

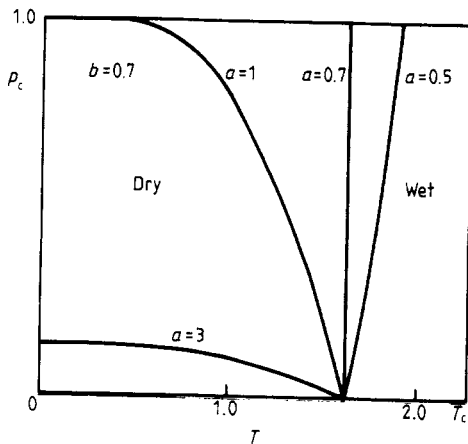


Figure 4. As figure 3 for K_2 partially binding.

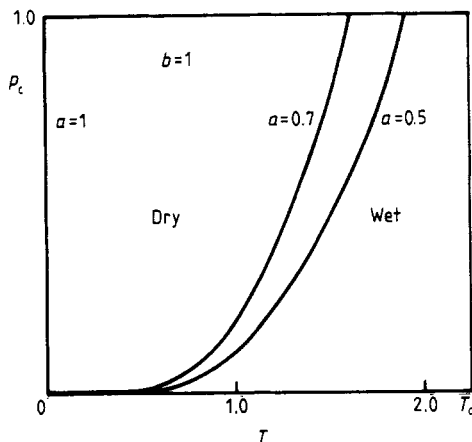


Figure 5. As figure 3 for K_2 unbinding for all temperatures.

three-dimensional problem with random substrate couplings (numerical values will, of course, depend on the accuracy of calculation of the interface tension in three dimensions). But the general form will stay with all its physical implications.

Second, we have chosen only one (probably the simplest) type of substrate irregularity. One can clearly introduce a number of different irregular substrate couplings but that would produce additional (quite difficult) problems in practical calculation.

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References

- Abraham D B 1980 *Phys. Rev. Lett.* **44** 1165
 — 1981 *Phys. Rev. Lett.* **47** 545
 Cahn J W 1977 *J. Chem. Phys.* **66** 3667
 Nightingale M P, Saam W F and Schick M 1983 *Phys. Rev. Lett.* **51** 1275
 Oliviera M J de and Griffiths R B 1978 *Surf. Sci.* **71** 678
 Pandit R, Schick M and Wortis M 1982 *Phys. Rev. B* **26** 5112
 Pandit R and Fisher M E 1983 *Phys. Rev. Lett.* **51** 1772
 Švrakić N M 1983 *J. Phys. A: Math. Gen.* **16** L171