Pinning and roughening of one-dimensional models of interfaces and steps

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We show that an external pinning potential located along a single row will at all temperatures localize the interface in a one-dimensional solid-on-solid model unless the pinning row is located near a boundary. Then there arises a simple example of the roughening transition found by Abraham, with a localized interface possible only for sufficiently large potential strengths. We suggest this transition may be observed experimentally on a stepped semiconductor surface.

Thermal fluctuations play an important role in determining the properties of an interface, particularly in a system of low dimensionality. Indeed these fluctuations are sufficient at any nonzero temperature to cause the interface between oppositely magnetized phases in a two-dimensional (2D) Ising model to wander arbitrarily far from its straight $T=0$ location.[1] Similar wandering or "roughening" behavior is found for models of a step on a crystal surface.[2]

Abraham[3] recently showed that interesting new behavior can arise from the addition of an attractive "pinning" potential which favors locating the interface in a semi-infinite 2D Ising model along a row near the boundary of the system. At sufficiently low temperatures the interface is pinned or localized near the attracting row. However there is a "roughening temperature" T_R (which tends to zero as the pinning potential tends to zero) above which the interface wanders arbitrarily far from the boundary.[3] Abraham's solution makes use of detailed properties of transfer matrices for the semi-infinite 2D Ising model and represents a true mathematical *tour de force.*

However the nature of the roughening transition does not change even in the limit of a small but finite pinning potential, for which there is a small T_R. This suggests that the main features of the transition can be found more simply by suppressing bulk heretophase fluctuations by a "no-overhang" or "solid-on-solid" (SOS) condition.[4,5] We provide such an analysis below.[6]

The positions of the interface (or step edge) in a SOS model are given by the set of integer heights $\{h_i\}$ of a 1D array of N columns. Here h_i gives the height of the ith column ($1 \leq i \leq N$) from the fixed reference level with all $h_i=0$. The energy of a particular configuration is

$$E(\{h_i\}) = \sum_{i=1}^{N} [f(|h_i - h_{i+1}|) + V(h_i)] \ , \qquad (1)$$

where the intercolumn interaction energy $f(h)$ is some increasing function of the absolute value of h with $f(0)=0$ and $V(h)$ is a single-column pinning potential. At low temperatures the essential physics should be independent of the form of $f(h)$ for $h > 1$.[5] Particular choices for f and V will be discussed later. We assume cyclic boundary conditions $h_1 \equiv h_{N+1}$ and take the limit $N \to \infty$. At a reduced temperature $k_B T \equiv \beta^{-1}$ the free energy A and partition function Z are given by

$$Z \equiv \exp(-\beta A) = \sum_{\{h_i\}} \exp[-\beta E(\{h_i\})] \ , \qquad (2)$$

where the summation is over all possible integer heights of each column.

If we define the "transfer matrix" T using Eq. (1) as

$$T(h',h) \equiv \exp[-\beta f(|h'-h|)] \exp[-\beta V(h)]$$
$$\equiv T_0(h',h) \exp[-\beta V(h)] \ , \qquad (3)$$

with T_0 the "zero-field" transfer matrix, it is easy to see that Eq. (2) can be rewritten as the trace of the Nth power of T. Representing the eigenvalues and eigenfunctions of T as

$$\sum_h T(h',h)\phi(h) = \epsilon\phi(h') \qquad (4)$$

we find in the usual way[7] that the free energy in the limit $N \to \infty$ is given by

$$\frac{\beta A}{N} = -\ln\epsilon_m \ , \qquad (5)$$

where ϵ_m is the largest eigenvalue of Eq. (4). Similarly the probability of finding a particular column at some height h is

$$P(h) = c\,\phi_m^2(h) \qquad (6)$$

with $\phi_m(h)$ the corresponding eigenfunction and c a normalization constant.

In this paper we consider only the special case suggested by Abraham[3] of a single pinning row located at $h=0$. Then V has the form $V(h) = -B\delta_{h,0}$. Thus a column with height $h=0$ gains an extra energy $-B$ over other positions of the column and the flat interface with all $h_i=0$ is favored. This pinning field can

be located near a boundary by considering a semi-infinite system with $0 \leq h \leq \infty$.

We can exploit this simple form for V by defining $\psi(h) \equiv \exp(b\delta_{h,0})\phi(h)$ with $b \equiv \beta B$. Using Eq. (3), the eigenvalue problem Eq. (4) can then be rewritten

$$\sum_h T_0(h',h)\psi(h) = \epsilon\psi(h'), \quad h' \neq 0 \tag{7}$$

with the special case

$$\sum_h T_0(0,h)\psi(h) = \epsilon e^{-b}\psi(0) \ . \tag{8}$$

Thus the modified eigenfunctions $\psi(h')$ for $h' \neq 0$ in Eq. (7) must be closely related to those of the zero-field matrix T_0 and Eq. (8) represents a boundary condition created by the pinning field which $\psi(0)$ must obey.

The eigenfunctions of T_0 are easy to find for an infinite system with $-\infty < h < \infty$. Clearly Eqs. (7) and (8) with $b = 0$ can be satisfied by an eigenfunction of the form

$$\psi(h) = t^h \tag{9}$$

and to obtain finite probabilities as $h \to \pm\infty$ from Eq. (6) we must have t pure imaginary. Thus we find a band of eigenfunctions $\psi(h) = e^{ikh}$ $(-\pi \leq k \leq \pi)$. The maximum eigenvalue ϵ_0 in Eq. (8) occurs for $k = 0$:

$$\epsilon_0 = 1 + 2\sum_{h=1}^{\infty} T_0(0,h) \tag{10}$$

and from this the free energy can be calculated using Eq. (5).

The simplest column model we study, the "restricted" or RSOS model, permits at most a height difference of unity between neighboring columns. This restriction should be unimportant at low temperatures. The only nonzero matrix elements of T_0 are then

$$T_0(h',h) = \begin{cases} e^{-\beta J} \equiv R, & |h-h'| = 1 \\ 1, & h = h' \end{cases} \ . \tag{11}$$

Here J is the cost in energy to move nearest-neighbor columns one unit apart and is proportional to the spin-flip energy in the unconstrained Ising model.

T_0 is a tridiagonal matrix and hence is linearly related to the matrix K representing a finite-difference approximation to the kinetic energy operator $-\frac{1}{2}\nabla^2$. Thus finding the eigenfunctions of the transfer matrix T_0 is equivalent to finding the eigenfunctions of the (finite difference) kinetic energy matrix K. The maximum eigenvalue $\epsilon_0 = 1 + 2R$ arising from Eqs. (11) and (10) in the infinite unpinned case corresponds to the zero kinetic energy solution. The pinning field at $h = 0$ then gives a localized attractive potential which produces a boundary condition Eq. (8) which the "wave function" ψ must obey.

We first consider the case where the pinning field at $h = 0$ is located far from the boundaries of an infinite system with $-\infty < h < \infty$. In the quantum-mechanical analogy we seek a bound-state solution induced by the attractive potential. A solution of even parity of the form of Eq. (9) satisfying boundary conditions at $h = \pm\infty$ is $\psi(h) = t^{|h|}$ $(t \leq 1)$. As will become evident immediately, this solution satisfies both Eq. (7), which can be written after division by $t^{h'}$ as

$$Rt + 1 + Rt^{-1} = \epsilon \quad (h' > 0) \tag{12}$$

and the boundary condition, Eq. (8),

$$Rt + 1 + Rt = \epsilon e^{-b} \tag{13}$$

for an appropriate choice of t. Note from Eq. (12) that $\epsilon > \epsilon_0 = 1 + 2R$ for any $t < 1$ and that $\epsilon \to \epsilon_0$ as "critical binding" is achieved and $t \to 1$. Dividing Eq. (13) by Eq. (12) we find that t must satisfy

$$e^{-b} = \frac{t(1+2Rt)}{t + R(t^2+1)} \ . \tag{14}$$

This quadratic equation for t has a unique solution $t < 1$ for *any* $b > 0$. Hence we always get a "bound state" and exponential decay of $P(h)$ in Eq. (6). The interface remains pinned for any nonzero b and a roughening transition to free behavior does not occur. This is simply an example of the well-known fact that in one dimension a symmetric square-well attractive potential will always support a bound state.[8] Similar conclusions have been reached by Burkhardt and by van Leeuwen and Hillhorst.[6]

The semi-infinite case with heights restricted to $0 \leq h < \infty$ has very different behavior since the pinning potential at $h = 0$ is located next to a "hard wall." Such an unsymmetric potential can support a bound state only if the well is sufficiently deep.[8] Equation (7) still gives Eq. (12) as before for $h' > 0$ but now rather than Eq. (13) the boundary Eq. (8) is $Rt + 1 = \epsilon e^{-b}$ since negative heights are not permitted. These equations combine to give

$$e^{-b} = \frac{t(1+Rt)}{t + R(t^2+1)} \ . \tag{15}$$

This quadratic equation for t has bound-state solutions $t < 1$ only for sufficiently large b. The minimum value b_c produces "critical binding" with $t = 1$ and is, from Eq. (15),

$$e^{-b_c} = (1+R)/(1+2R) \ . \tag{16}$$

As $b \to b_c$, $t \to 1$, and the exponential decay of $P(h)$ in Eq. (6) becomes weaker and weaker. For $b < b_c$ the interface is unpinned and delocalized; the probability of finding the interface at any particular height h is zero.

At low temperatures $R \equiv e^{-\beta J} \to 0$; hence from Eq. (16) $b_c \equiv \beta B_c \to 0$. Thus for fixed pinning poten-

tial strength B there is always a T small enough that $B > B_c(T)$ and a bound state or localized interface arises. As T becomes large however we have from Eq. (16) that $B_c(T) \propto T$. At sufficiently high temperatures then, the interface becomes unpinned and moves far from the boundary. This is the roughening transition found by Abraham.[3]

These same methods suffice to treat the usual ASOS model[4,5] where the matrix T_0 is now

$$T_0(h,h') = R^{-|h-h'|} \quad . \tag{17}$$

This model is a special case of the general anisotropic Ising model considered by Abraham[3] which arises when the vertical coupling strength $J_\perp \to \infty$. Since no new physics arises from the possibility of multiple height jumps between nearest-neighbor columns permitted in Eq. (17) we will be brief in our discussion.

Considering first the infinite unpinned system with $b=0$, we have from Eqs. (17) and (10) the maximum eigenvalue $\epsilon_0 = (1+R)/(1-R)$. A pinning potential at $h=0$ may induce a bound state with wave function of even parity

$$\psi(h) = \begin{cases} t^{|h|}, & h \neq 0 \\ \psi_0, & h = 0 \end{cases} , \tag{18}$$

where we must now explicitly choose an approximate ψ_0 as well as t to ϵ to satisfy Eqs. (7) and (8). Substituting Eq. (18) into Eq. (7) we find after division by $t^{h'}$,

$$(R/t)^{h'}[\psi_0 + Rt/(1-Rt) - t/(t-R)] + 1/(1-Rt) + R/(t-R) = \epsilon \quad . \tag{19}$$

If we choose $\psi_0 = t/(t-R) - Rt/(1-Rt)$ so that the term in square brackets vanishes, we find from Eq. (19) an expression for ϵ independent of h':

$$\epsilon = 1/(1-Rt) + R/(t-R) \tag{20}$$

and we note that $\epsilon > \epsilon_0$ for $t < 1$. These choices must be consistent with Eq. (8) which becomes $\psi_0 + 2Rt/(1-Rt) = \epsilon e^{-b}\psi_0$. Combining these results we find t must satisfy

$$e^{-b} = \frac{(1-Rt)(t-R)}{t(1-2Rt+R^2)} \quad . \tag{21}$$

This quadratic equation always has a bound-state solution $1 \geq t \geq R$ as b varies from zero to infinity. As $b \to 0$, ϵ in Eq. (20) tends smoothly to ϵ_0.

In the semi-infinite or hard-core case $0 \leq h < \infty$ the terms arising from negative heights are missing. Instead of Eq. (21), we find $\exp(-b) = (t-R)/t$ and a bound-state $t < 1$ solution is possible only for $b > b_c = -\ln(1-R)$. This requirement is a special case of the general expression [his Eq. (8)] found in Abraham's paper.[3] Again the hard-core condition will induce a roughening transition from localized to delocalized behavior of the interface.

A physical realization of this transition may be found by considering the behavior of steps on a crystal surface cut at a small angle to a close-packed plane.[9] In the simplest case which probably applies to metallic surfaces we expect the equilibrium vicinal surface to consist of single steps separated by terraces whose average width is determined by the angle of the original cut. Thermal fluctuations will occasionally cause the steps to wander[10] close to one another but it is clearly unfavorable for the lower step to pass beyond the position of the upper step, though two step edges can coincide and form a double height step. This noncrossing requirement produces a "hard-core" repulsion between the steps. To achieve the maximum entropy of wandering the steps will on average be as far apart as possible just as the unpinned interface discussed before is found far from the system's boundaries.

However for certain (probably covalent) materials it may be energetically more favorable to form multiple-height steps or step bunches (risers) rather than separated monoatomic steps. These are in fact observed on vicinal semiconductor surfaces.[11,12] The terraces undergo covalent reconstruction and the wider terraces that result from step bunching allow additional reconstruction.[13] The bunched steps themselves may be stabilized by some similar kind of reconstruction, though impurities could also play an important role.[12] This difference in energy produces a pinning mechanism which must dominate the entropy-driven repulsion between steps at sufficiently low temperatures. However since the pinning is associated with a hard core from the noncrossing condition, at high temperatures the risers should break apart in a roughening phase transition with widely separated single steps favored. Indeed after laser annealing, when the Si surface is raised to very high temperatures, single steps are found[11,14] on the fast-quenched surface, though this is not necessarily the equilibrium situation. In addition, impurities could complicate this simple picture.

It would be very interesting to study the equilibrium properties of these vicinal semiconductor surfaces as a function of temperature. If our ideas are correct the risers will break apart at a given temperature T_R whose magnitude depends on the pinning or reconstruction energy B. Thus information both about the phase transition and the pinning energy could be obtained from these experiments.

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