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LETTER TO THE EDITOR

Localisation–delocalisation transition in a solid-on-solid model with a pinning potential

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Abstract. The influence of pinning forces on domain-wall fluctuations is studied in a continuous planar solid-on-solid model with a one-dimensional interface. The system is simple enough so that exact results can be obtained for a variety of pinning forces. The pinning of the interface is formally equivalent to the binding of a quantum mechanical particle in a temperature-dependent effective potential. In the case of a short-range pinning force applied a finite distance from the edge of the system, there is a localisation–delocalisation transition at a finite temperature. The transition is qualitatively similar to that studied in the $d=2$ Ising model by Abraham.

Recently Abraham (1980) reported some results for a two-dimensional Ising model in which a transition associated with a domain wall occurs at a temperature below the bulk critical temperature. Along one edge of the system there is a ladder of weaker bonds where it is energetically favourable for a domain wall to pass. Below the transition temperature the domain wall is bound by the ladder. Its mean distance $\langle x\rangle$ from the edge of the system is finite, and it is smooth, i.e. $\langle(x-\langle x\rangle)^2\rangle$ is finite. Above the transition temperature but below the bulk critical temperature the domain wall is no longer bound and is rough. Both $\langle x\rangle$ and $\langle(x-\langle x\rangle)^2\rangle$ are infinite. On approaching the critical temperatuie $T_{\rm D}$ of the domain-wall transition from below, $\langle x\rangle$ diverges as $(T_{\rm D}-T)^{-1}$. At $T_{\rm D}$ the specific heat of the domain wall is discontinuous.

Abraham's model differs from conventional models for the roughening transition (see, for example, Leamy *et al* (1975), van Beijeren (1977)) in an obvious but important respect. The ladder of special bonds breaks the translational symmetry and in binding the domain wall also reduces its width. In the translationally invariant case the domain wall of the $d=2$ Ising model is always rough except at zero temperature.

In this Letter a simple soluble model is discussed which exhibits a localisation–delocalisation transition with all of the qualitative characteristics of Abraham's model mentioned above. The model, which is indicated schematically in figure 1, is a solid-on-solid (SOS) model (Temperley 1952, Leamy *et al* 1975) with a pinning potential which favours a flat bound interface energetically. The Hamiltonian is given by

$$\mathscr{H}=J\sum_{i=1}^{N-1}|x_{i+1}-x_i|+\sum_{i=1}^{N}U(x_i) \tag{1}$$

where x_i denotes the perpendicular distance of the interface from point i on the lower horizontal edge. The x_i vary continuously in the interval $0<x_i<\infty$. The case of an integer spectrum for the x_i (Hilhorst and van Leeuwen 1980, Chui and Weeks 1980,

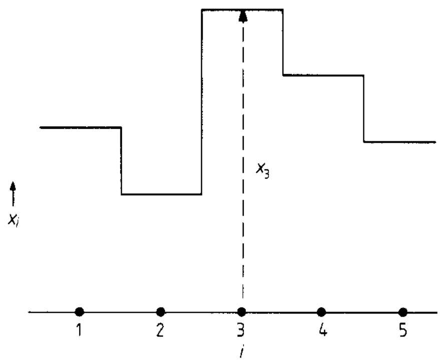

Figure 1. The solid-on-solid model.

Kroll 1980) can also be treated exactly, but will not be discussed here, as the phase transition is qualitatively the same. The energy contribution from the first sum in (1) is proportional to the extra length of an interface which is not flat and horizontal. The second sum is the pinning potential which localises the interface below the transition temperature. The case of a square-well potential is considered explicitly below.

Since the SOS model is a special case of the Ising model in the limit of infinite anisotropy (Temperley 1952, Leamy *et al* 1975), results for the discrete SOS model with a particular pinning potential are contained in Abraham's work. Dealing directly with the SOS rather than the Ising model permits one to obtain exact results for a large variety of pinning potentials, since the transfer matrix is that of a one-dimensional instead of a two-dimensional system, which simplifies the mathematics enormously. A useful equivalence between the pinning of the interface and the binding of a quantum mechanical particle in a potential well related to the pinning potential emerges from the analysis of the transfer matrix corresponding to (1). The equivalence allows one to make qualitative statements about the nature of the transition for different types of pinning potentials. In particular, one sees that the interface generally remains smooth and localised at all finite temperatures if the pinning force is applied at an infinite rather than a finite distance from the edge of the system.

The transfer matrix (Kramers and Wannier 1941, Huang 1963) corresponding to (1) is given by

$$\langle x|T|y\rangle = \exp(-V(x)/2 - K|x-y| - V(y)/2) \tag{2}$$

where $K = J/k_BT$ and $V(x) = U(x)/k_BT$. Its eigenfunctions $\phi(x)$ satisfy the integral equation

$$\int_0^\infty dy\, \langle x|T|y\rangle\phi(y) = \lambda\phi(x). \tag{3}$$

In the thermodynamic limit the free energy of the system is proportional to the logarithm of the largest eigenvalue λ for which (3) has a well behaved solution.

With the substitution $\psi(x) = e^{V(x)/2}\phi(x)$, equation (2) takes the form

$$\int_0^\infty dy\, \exp(-K|x-y| - V(y))\psi(y) = \lambda\psi(x). \tag{4}$$

Using $(-\mathrm{d}^2/\mathrm{d}x^2+K^2)\,\mathrm{e}^{-K|x-y|}=2K\delta(x-y)$ in (4), one finds that $\psi(x)$ satisfies the Schrödinger equation

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}-\frac{2K}{\lambda}\,\mathrm{e}^{-V(x)}+K^2\right)\psi(x)=0 \tag{5}$$

with the boundary condition

$$\psi'(0)/\psi(0)=K \tag{6}$$

which is implied by (4). From the transfer-matrix formalism it follows that the probability density $P(x)$ for finding the interface at a distance x from the edge of the system is given by

$$P(x)\propto \mathrm{e}^{-V(x)}|\psi(x)|^2 \tag{7}$$

where $\psi(x)$ is the eigenfunction of (5) and (6) corresponding to the largest value of λ. One sees from (7) that the interface probability density is more concentrated in regions of lower potential energy than the quantum mechanical probability density $|\psi(x)|^2$.

From elementary quantum mechanics (Schiff 1968) one knows that (5) and (6) have scattering solutions with the asymptotic form $\psi(x)\approx A\sin(qx+\delta)$, $x\to\infty$ and eigenvalue $\lambda(q)=2K/(K^2+q^2)$ for potential wells $U(x)$ which tend to zero rapidly enough in the limit of large x. If the potential well is sufficiently attractive, there may be one or more bound states. The bound states have the asymptotic form $\psi(x)\approx B\,\mathrm{e}^{-px}$, $x\to\infty$, with eigenvalues $\lambda_p=2K/(K^2-p^2)$. From the expressions for $\lambda(q)$ and λ_p it is clear that the largest λ for which (5) and (6) can be solved corresponds to the bound state with the largest value of p (the most tightly bound) or, in the absence of bound states, the $q=0$ scattering state. From (7) one sees that these two types of states correspond to bound and unbound interfaces, respectively. The system exhibits a localisation–delocalisation transition at temperatures where the eigenvalues corresponding to the two types of states become degenerate.

We now consider the square well potential $U(x)=-U_0$ for $0<x<R$, $U(x)=0$ otherwise, which corresponds to a short-range pinning force applied near the edge of the system. The function $\psi(x)$ corresponding to the most tightly bound state is shown in figure 2(a). For $0<x<R$, $\psi(x)=A\sin kx+B\cos kx$ and for $x>R$, $\psi(x)=C\,\mathrm{e}^{-px}$.

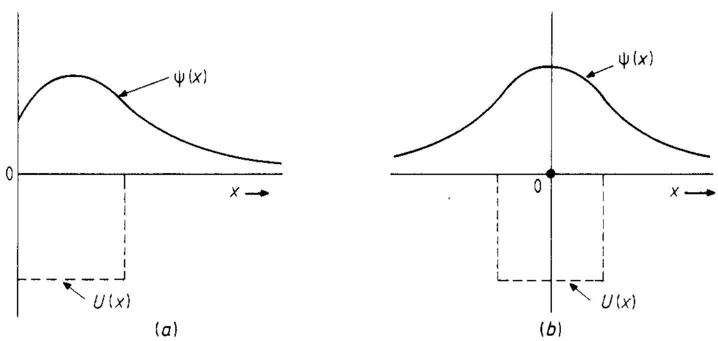

Figure 2. (a) Bound-state solution $\psi(x)$ for a square-well pinning potential at the edge of the system. The boundary condition is $\psi'(0)/\psi(0)=K$. (b) Bound-state solution $\psi(x)$ for a square-well pinning potential infinitely far from the edge of the system. The boundary condition is $\psi'(0)=0$.

The eigenvalue λ is determined by

$$k^2-(2K/\lambda)\,e^{V_0}+K^2=0, \tag{8}$$

$$-p^2-2K/\lambda+K^2=0, \tag{9}$$

$$K=k\frac{\sin kR-(p/k)\cos kR}{\cos kR+(p/k)\sin kR}, \tag{10}$$

where $V_0=U_0/k_BT$. Equations (8)–(10) follow from (5) and (6) and the continuity of $\psi(x)$ and $\psi'(x)$ at $x=R$. The bound state and the $q=0$ scattering state become degenerate when $p=0$. Combining this condition with equations (8)–(10), one finds the critical line

$$KR=(e^{V_0}-1)^{-1/2}\tan^{-1}(e^{V_0}-1)^{-1/2} \tag{11}$$

which is plotted in terms of the variables $t=k_BT_D/JR$ and $u=U_0/JR$ in figure 3. $u\approx\pi^2t^3/4$ for $t\ll 1$ and $u\approx t\ln t$ for $t\gg 1$.

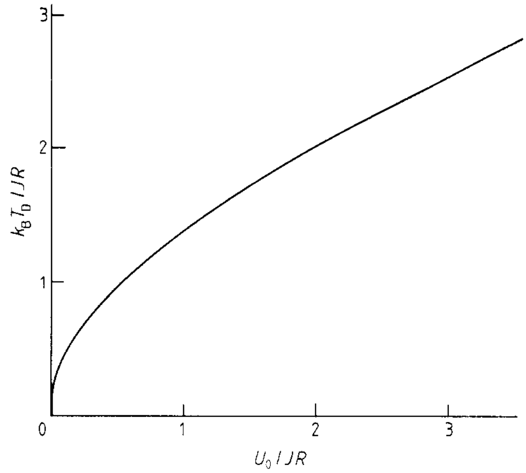

Figure 3. Critical line of localisation–delocalisation transitions for a square-well pinning potential at the edge of the system.

Equations (8)–(10) imply that p vanishes as T_D-T on approaching the delocalisation temperature T_D from below at constant J and $U(x)$. Since the gap between the eigenvalues $\lambda_p=2K/(K^2-p^2)$ and $\lambda(0)=2/K$ of the bound state and the $q=0$ scattering state varies as $p^2\propto(T_D-T)^2$, the specific heat is discontinuous at the transition. From (7) one sees that the mean distance $\langle x\rangle$ of the interface from the wall and the root-mean-square width $[\langle(x-\langle x\rangle)^2\rangle]^{1/2}$ diverge as $(T_D-T)^{-1}$. Qualitatively similar behaviour is found in Abraham's model. The height–height correlation function $\langle(x_n-x_0)^2\rangle$ of the SOS model may also be readily calculated. It approaches its $n\to\infty$ limit $2\langle(x-\langle x\rangle)^2\rangle$ with an exponential tail of the form $\exp(-\text{constant}\times n(T_D-T)^2)$ for $T\leqslant T_D$. For $T>T_D$, $\langle(x_n-x_0)^2\rangle\propto n$, $n\to\infty$, as in the translationally invariant SOS model without a pinning potential.

Let us now consider the case in which the square well is infinitely far from the edge of the system. It is convenient to measure the coordinate x from the midpoint of the well, i.e. $U(x) = -U_0$ for $-R/2 < x < R/2$, and $U(x) = 0$ for $R/2 < x < \infty$ or $-\infty < x < -R/2$. Equation (5) still applies, but not the boundary condition (6). The most tightly bound state is the even-parity solution with no nodes sketched in figure 2(*b*). Inside the well $\psi(x) = A \cos kx$, and outside $\psi(x) = B\, e^{-p|x|}$. The eigenvalue λ is determined by (8), (9) and the continuity condition

$$k \tan(kR/2) = p. \tag{12}$$

The properties of this set of equations are well known from elementary quantum mechanics (Schiff 1968). There is a bound state for every $V_0 > 0$. Thus an arbitrarily weak square-well potential localises the interface at all finite temperatures.

The system described by (8), (9) and (12) does, of course, exhibit a localisation–delocalisation transformation as $U_0 \to 0$ at constant J, R and T. In this limit p vanishes as U_0. The gap between the eigenvalues of the bound state and the even-parity $q = 0$ state varies as U_0^2. It follows from (7) that the root-mean-square width $[\langle (x - \langle x \rangle)^2 \rangle]^{1/2}$ of the interface diverges as U_0^{-1}.

Obviously the qualitative characteristics of the transition described above do not depend on the details of the pinning potential. For a large class of potentials with asymptotic bound and scattering states one expects similar behaviour. In the case of a potential well at a finite distance from the edge of the system, equation (6) requires that $\psi(x)$ have a positive slope at the edge, as shown in figure 2(*a*). Unless the well exceeds a certain critical depth, the wavefunction does not turn over in the well, and there is no bound state. Since $V(x)$ varies as T^{-1} it is clear that the critical depth corresponds to a finite temperature, in general. In the case of a well infinitely far from the edge of the system, the appropriate solution $\psi(x)$ has slope zero at some point in the well. Even an infinitesimally attractive potential turns $\psi(x)$ downward to produce a bound state.

Thus far, only short-range pinning forces have been considered. These forces vanish rapidly enough as $x \to \infty$ so that $U(x)$ approaches a constant, implying that (5) has scattering and perhaps bound-state solutions. For long-range forces corresponding to potentials with the behaviour $U(x) \to \infty$, $x \to \infty$ (for example, potentials such as $U(x) = cx^s$, $c > 0$, $s > 0$), the solutions of (5) are seen to have the asymptotic form $\psi(x) \approx A\, e^{-Kx}$, $x \to \infty$. Thus for these forces (5) only has bound-state solutions, i.e. the interface remains pinned for all finite temperatures. The long-range force $U(x) = F_0 x$ is of special interest, since it corresponds to a constant (gravitational) force. Hilhorst and van Leeuwen (1980) have considered several long-range pinning forces in the discrete SOS model in more detail.

That a short-range pinning force is less effective in localising the interface the closer it is applied to the edge of the system is intuitively clear. In the case of a pinning force far from the edge, the interface can make large excursions to both sides of the well. The number of interface configurations which profit from the lower energy in the well decreases as the well is moved closer to the edge. The interface is repelled at the edge since a point on the interface is pulled away from the edge by neighbouring points. The pinning force must overcome this repulsion in order to bind the interface. Equations (6) and (7) make a quantitative statement about the repulsion. They imply

$$P'(0)/P(0) = (F(0) + 2J)/k_B T \tag{13}$$

where $F(x) = -dU(x)/dx$ is the pinning force. In the absence of a pinning force at the edge or for weak pinning forces $F(0) + 2J > 0$, $P'(0)$ is positive, i.e. the probability density decreases on approaching the edge.

The class of models with one-dimensional interfaces which exhibit localisation–delocalisation transitions which are qualitatively similar to Abraham's Ising transition is presumably quite large. So far the class is known to include the continuous and discrete SOS models and a model with Gaussian interactions investigated by Lajzerowicz and Vallade (1980). In closing, we note that some but not all of the quantitative characteristics discussed above are found in a simple mean-field theory in which one calculates the mean position $\langle x \rangle$ of a point on the interface self-consistently with the distribution

$$P(x) \propto \exp(-V(x) - 2K|x - \langle x \rangle|) \tag{14}$$

which neglects fluctuations in the positions of the two neighbouring points of the interface. The mean-field theory predicts a smooth localised interface at all finite temperatures for long-range pinning forces and for short-range forces applied infinitely far from the edge. In the case of a short-range pinning force near the edge (a square-well potential was considered explicitly), $\langle x \rangle$ is found to diverge as $(T_D - T)^{-1}$ on approaching a finite temperature T_D from below, as in the exact solutions of the models mentioned above. However, the mean-square width $\langle (x - \langle x \rangle)^2 \rangle$ calculated with (14) remains finite for $T > T_D$. Thus the mean-field theory predicts the delocalisation transition but not the roughening transition.

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Note added in proof. In an improved mean-field theory, which perhaps is qualitatively correct in high dimensions, (14) is replaced by $P(x) \propto \exp(-V(x) - 2K \int_0^\infty dy|x - y|P(y))$ and solved selfconsistently. In the case of a square-well pinning potential at the edge of the system, one finds a localisation–delocalisation transition in which the interface remains smooth. The mean distance of the interface from the edge diverges as $-\ln(T_D - T)$, and there is a discontinuity in the specific heat at the transition.

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