Singularities in correlation functions for systems with defect lines and walls

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We consider a system consisting of a continuous solid-on-solid interface between two parallel defect lines in the bulk and calculate its free energy and longitudinal (i.e., parallel to the defect lines) correlation length. We find a *nonthermodynamic* singularity in the longitudinal correlation function, which was also found to be present for an interface confined to a strip of finite width.

Statistical mechanics of systems with surfaces and defect lines (planes) has generated much interest in the last decade or so. Two-dimensional systems have proven to be particularly accessible to such studies.[1] Fisher and Ferdinand[2] made an extensive study of two-dimensional Ising models containing a defect line. It was later shown by Abraham[3] that an interface bound to a defect line in the bulk never depins although he previously demonstrated the existence of a pinning-depinning (wetting) transition if a row of weakened bonds is placed along the edge of a semi-infinite Ising model.[4] Defect lines also exhibit unusual properties at the bulk critical point; in particular McCoy and Perk[5] discovered nonuniversal asymptotic behavior for the pair-spin correlation function along the defect line.

Interface models, which ignore bulk fluctuations, have also proven to be useful in the study of pinning-depinning phenomena. In particular, the solid-on-solid (SOS) model[6] was found to mirror much of the behavior derived through exact calculations of the two-dimensional Ising model.[4,7,8]

In this paper, we consider an SOS interface in a system with two parallel defect lines in the bulk separated by a distance R (see Fig. 1). The Hamiltonian, $\mathcal{H}$, is given by

$$\beta\mathcal{H}\{x\}=K\sum_{j=-N}^{N-1}|x_{j+1}-x_j|+\sum_{j=-N}^{N}V(x_j)\ , \tag{1}$$

where x_j is the height of the jth column (see Fig. 1) and is taken to vary continuously in the interval $-\infty<x_j<\infty$ with fixed end conditions $x_{-N}=x_N=0$. As usual, β is the inverse temperature, $\beta=1/k_BT$. The effect of the defect lines is embodied in $V(x)$ which is a symmetric double-well potential with wells situated at $x=\pm R/2$ (in this paper we shall always take the pinning potential to be the same for both defect lines). The wells are assumed to be sufficiently short ranged with $V(x)\to 0$ as $|x|\to\infty$. Since the defect lines are situated in the bulk, one expects, from previous results,[3,7] that the interface will always be localized to the vicinity of the defect lines so that there is no pinning-depinning transition.

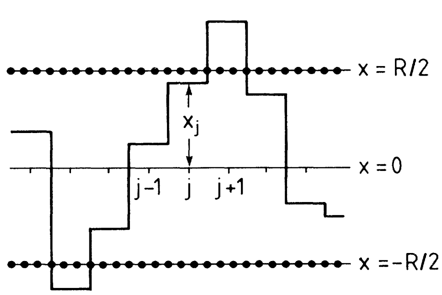

FIG. 1. A typical SOS configuration. The dots represent the defect lines.

The probability that an interface, described by Eq. (1), which is fixed at $(-N,0)$ and $(N,0)$, passes through $(0,x)$ is given by

$$p_N(x,0)=\frac{Z_N^2(x)e^{-V(x)}}{Z_{2N}(0)}\ , \tag{2}$$

where $Z_N(x)$ is the partition function for an interface fixed at (0,0) and (N,x). This can be expressed in terms of transfer integral operators[8] in the following inner product:

$$Z_N(x)=(\delta_x,(T_1T_2)^{N-1}T_1\delta_0)\ , \tag{3}$$

with

$$(T_1f)(x)=\int_{-\infty}^{\infty}e^{-K|x-y|}f(y)dy\ , \tag{4a}$$

$$(T_2f)(x)=e^{-V(x)}f(x)\ , \tag{4b}$$

and δ_x is the Dirac δ distribution centered on x.

By applying the usual methods for treating SOS models, as described, for example, in Ref. 8, which exploit the fact that $\exp(-K|x-y|)$ is the Green's function for a free Schrödinger equation, Eq. (3) can be written

$$Z_N(x)=\sum_{n=0}^{\infty}\psi_n(0)\psi_n(x)\lambda_n^{N-1}\ , \tag{5}$$

where $\psi_n(x)$ is an eigenfunction, with eigenvalue λ_n, of the transfer integral operator; that is, $T_1T_2\psi_n=\lambda_n\psi_n$. These are eigenstates of the following Schrödinger equation:

$$\left[-\frac{d^2}{dx^2}-\frac{2K}{\lambda_n}e^{-V(x)}+K^2\right]\psi_n(x)=0\ . \tag{6}$$

It follows that $-\exp[-V(x)]$ also has a double-well structure, so we can now discuss the system in terms of a one-dimensional quantum mechanical particle moving in

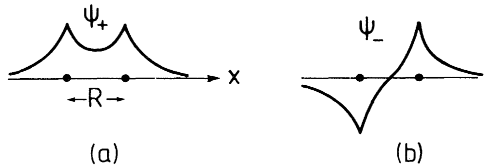

FIG. 2. Wave functions for the two lowest-lying states of a $H_2{}^+$-like system including (a) the bonding state, $\psi_+(x)$, and (b) the antibonding state, $\psi_-(x)$. The dots represent the nuclei and clearly, in this case the potential is singular at the nuclear centers.

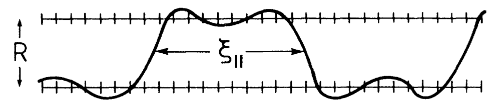

FIG. 3. Schematic illustration of how the SOS string might typically pin to the defect lines (rows of vertical bonds).

a double-well potential with wells separated by distance R. This is a familiar problem particularly in the context of (one-dimensional) models for the electronic states of diatomic molecules such as the hydrogen molecule ion, $H_2{}^+$. For such a system, we expect to find at least two (lowest-lying) bound states, $\psi_\pm$, with typical examples shown in Fig. 2. The lowest state, $\psi_+(x)$ [Fig. 2(a)], which is symmetric and has eigenvalue λ_+, can be thought of as the bonding state in the $H_2{}^+$ analogy and the next lowest, $\psi_-(x)$ [Fig. 2(b)], which is antisymmetric and has eigenvalue λ_-, corresponds to the antibonding state. One should remember that increasing λ is equivalent to decreasing energy in the quantum mechanical analogue.

The free energy per column, F, is given by

$$\beta F = -\lim_{N\to\infty}[\ln Z_{2N}(0)/2N] = -\ln\lambda_+ \ . \tag{7}$$

We are also interested in the longitudinal correlation length, $\xi_\parallel$, (characteristic length running parallel to the defect lines). This might correspond to the expected length which the interface stays bound to one defect line before it jumps to the other (see Fig. 3). Since the matrix element $\int_{-\infty}^{\infty}\psi_-^*(x)x\psi_+(x)dx$ is clearly nonzero, it follows that $\xi_\parallel$ can be expressed as

$$1/\xi_\parallel = \ln(\lambda_+/\lambda_-) \ . \tag{8}$$

Returning to the quantum mechanical $H_2{}^+$ analogy, for large internuclear distance R, the bonding-antibonding states can be understood as resulting from tunneling between single atom states. On heuristic grounds, such tunneling might typically lead to the following asymptotic degeneracy:

$$\lambda_\pm \approx \lambda_\infty \pm \mathcal{E}_\pm e^{-\sigma R} + \cdots \quad \text{as } R\to\infty \ , \tag{9}$$

for *sufficiently short-ranged* potentials, where $\mathcal{E}_\pm > 0$ and $\frac{1}{2}\lambda_\infty$ is the eigenvalue for the lowest bound state of a single isolated well (atom). If the pinning potentials are sufficiently long ranged, then the exponential in (9) may be replaced by an inverse power law but we shall not discuss this case any further in this Brief Report.

From (7), it follows immediately that

$$\beta F \approx -\ln\lambda_\infty - \frac{\mathcal{E}_+}{\lambda_\infty}e^{-\sigma R} \quad \text{as } R\to\infty \ , \tag{10}$$

showing that the interface induces an exponential attraction between the defect lines. Equation (8) implies that

$$\xi_\parallel \approx \frac{\lambda_\infty}{(\mathcal{E}_+ + \mathcal{E}_-)}e^{\sigma R} \quad \text{as } R\to\infty \ , \tag{11}$$

which is the expected form and, in fact, similar to the results of Privman and Švrakić[9] in the "nonwet" regime.

Let us now consider the exact results for the following choice of potential:

$$e^{-V(x)} = 1 + a\delta(x-R/2) + a\delta(x+R/2) \ . \tag{12}$$

This would be appropriate if the SOS interface represented the long low-temperature contour in an Ising model (with nearest-neighbor couplings $K/2$) with two rows of weakened vertical bonds (see Fig. 3) with couplings $K_d/2$ and the rows separated by distance R. In this case, we should put $a=\exp(K-K_d)-1$ and clearly $a>0$ since $K_d<K$. Hence, for $x\neq\pm R/2$, Eq. (6) becomes

$$\left[-\frac{d^2}{dx^2} - \frac{2K}{\lambda_n} + K^2\right]\psi_n(x) = 0 \ , \tag{13}$$

where the wave function $\psi_n(x)$ is continuous at $x=\pm R/2$ but

$$\psi_n^{(1)}\left[\pm\frac{R}{2}+\right] - \psi_n^{(1)}\left[\pm\frac{R}{2}-\right] = -\frac{2Ka}{\lambda_n}\psi_n\left[\pm\frac{R}{2}\right] \ . \tag{14}$$

The eigenvalue spectrum for this system is shown schematically in Fig. 4. There is a continuous spectrum of "scattering" states with $0<\lambda<2/K$ and only two bound states $\psi_\pm$, with $\lambda_+>\lambda_->2/K$ which are solutions of

$$\lambda_\pm\kappa_\pm = Ka[1\pm\exp(-\kappa_\pm R)] \ , \tag{15}$$

where $\kappa_\pm = [K(K-2/\lambda_\pm)]^{1/2}$. For $x\geq R/2$, the bound-state eigenfunctions are of the form

$$\psi_\pm(x) \propto \exp(-\kappa_\pm x) \ . \tag{16}$$

Note that although λ_+ (bonding state) is always present for $R\geq 0$, the second solution of (15), λ_- (antibonding state), exists only for $R>R_c=2/K^2a$). This is interesting, since it implies that the longitudinal correlation function is singular at $R=R_c$. This singularity will show up as a jump discontinuity in $\partial^2\xi_\parallel/\partial R^2$ at R_c with

$$\lambda_- - 2/K \approx \tfrac{1}{2}K^5a^4(R-R_c)^2 \quad \text{as } R\to R_c+ \ , \tag{17}$$

although it has no thermodynamic consequences since

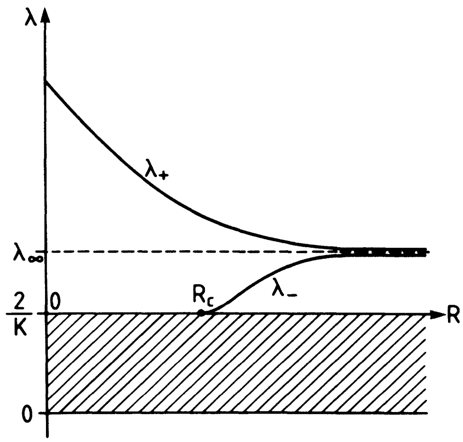

FIG. 4. Schematic representation of the eigenvalue spectrum λ plotted as a function of defect-line separation R. The hatched region represents the continuum of scattering states with $0<\lambda<2/K$.

λ_+ (and hence the free energy) remains analytic. This rather novel feature of these systems appears not to have been noted before although it is reminiscent of behavior found elsewhere.[14]

In fact, a similar singularity is also present when a *continuous* SOS interface is confined between two *walls* separated by distance R. In this case, Hamiltonian (1) is used but now x_j is constrained to vary continuously in the interval $-R/2 \le x_j \le R/2$. With $V(x)$ given by Eq. (12), the eigenfunctions, $\psi_n(x)$, of the transfer operator obey the same Schrödinger equation (13) but with different boundary conditions given by $\lambda_n \psi_n^{(1)}(\pm R/2) = \pm(2a-\lambda_n)K\psi_n(\pm R/2)$. For $R\to\infty$, one finds the usual depinning transition[4] at $a=a_c=1/K$. For $a>a_c$ (nonwet regime) and R finite, there are at most two bound states whose eigenvalues ($\lambda_+>\lambda_->2/K$) are solutions of

$$[\lambda_\pm \kappa_\pm - K(2a-\lambda_\pm)]\exp(\kappa_\pm R) = \pm[\lambda_\pm\kappa_\pm + K(2a-\lambda_\pm)] \ , \quad (18)$$

where $\kappa_\pm$ is defined as before. Again, although λ_+ exists for all $R\ge 0$ (provided that $a>a_c$, λ_- occurs only for $R>R_c'=2/[K^2(a-a_c)]$, leading to a similar singularity in the longitudinal correlation function at $R=R_c'$. Note that $R_c'\to\infty$ as the (semi-infinite system) wetting transition is approached, i.e., as $a\to a_c+$.

We now return to the system with two defect lines in the bulk. Taking $R\to\infty$ in Eq. (15), we arrive at Eq. (9) with

$$\lambda_\infty = \frac{1+(1+a^2K^2)^{1/2}}{K} \ , \quad (19a)$$

$$\mathcal{E}_+ = \mathcal{E}_- = \frac{Ka^2\lambda_\infty}{Ka^2+\lambda_\infty} \ , \quad (19b)$$

and

$$\sigma = Ka/\lambda_\infty \ . \quad (19c)$$

Hence, we do indeed find exponential attraction between the defect lines and exponential divergence of $\xi_\parallel$ as $R\to\infty$.

Since, from (2), $p_N(x,0)\propto\psi_+^2(x)$ for $x\ne\pm R/2$, then Eq. (16) implies that $p_N(x,0)\sim\exp(-2\sigma x)$ as $R\to\infty$ for $x>R/2$. This would suggest that we can identify $1/2\sigma$ as some characteristic length scale (transverse correlation length) and hence put $\xi_\perp=1/2\sigma$. Therefore, as $R\to\infty$, $\xi_\parallel\sim\exp(R/2\xi_\perp)$ which is similar to the finite-size scaling result found by Privman and Švrakić[9] in their model (in the nonwet regime) which was itself in accord with general expectations.[10] Also, as $a\to 0+$ (i.e., $K_d\to K-$), where there are transverse fluctuations in the interface across large distances, $\xi_\perp\approx 1/(K^2a)=R_c/2$. This then leads to a simple scaling argument to account for the singularity in the longitudinal correlation function;[11] the singular behavior results from the onset of transverse fluctuations spanning the distance between the defect lines which occurs when $R=2\xi_\perp$.

A similar argument accounts for the analogous singularity found for the interface confined to a strip of finite width except here we find that $R_c'\approx 4\xi_\perp$. We may conclude that this singularity is a general feature of systems containing walls and defect lines.

If, on the basis of comparing (11) to results obtained by Fisher,[12] we make the identification $\sigma=\Sigma(T)/k_BT$ where $\Sigma(T)$ is the "interfacial tension," we have $\xi_\perp(T)\Sigma(T)/k_BT=\frac{1}{2}$ which is, in fact, exact for the two-dimensional Ising model for all subcritical temperatures.[2,13] Note, however, that this comparison with Fisher[12] is strictly valid only for $K_d=0$ (or $a=e^K-1$), where a strip of finite width decouples from the rest of the system; otherwise, $\Sigma(T)$ would *not* be the interfacial tension. In general, both σ and $\xi_\perp$ depend on "a" (and therefore K_d) although, interestingly, one still has the invariant relation

$$\sigma(T,K_d)\xi_\perp(T,K_d)=\tfrac{1}{2} \ , \quad (20)$$

which also holds for the continuous SOS interface confined between two walls.

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