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Interface tension of the square lattice Ising model with next-nearest-neighbour interactions

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Abstract – In a recent letter, Zandvliet (*Europhys. Lett.*, **73** (2006) 747) presented a simple derivation of an analytical expression for the interface free energy in the (10) direction of the Ising model on a square lattice with nearest- *and* next-nearest-neighbour couplings, reproducing the famous exact Onsager formula in the special case of only nearest-neighbour interactions. By comparing the resulting transition temperatures, determined as the point where the interface tension vanishes, with previous numerical results in the literature, support for the validity of the new analytical formula in the general case was claimed. Guided by the fact that Zandvliet's simple, but rather heuristic derivation neglects overhang configurations and bubble excitations completely, we show that his approach is equivalent to the classic solid-on-solid (SOS) approximation which is known to reproduce accidentally the exact interface tension along one of the two main axes in the case of only nearest-neighbour interactions. In the limiting situation where only next-nearest-neighbour interactions are considered, we prove analytically that such a coincidence no longer holds. To assess the accuracy of Zandvliet's formula for the general model we have performed a careful computer simulation study using multicanonical and cluster Monte Carlo techniques combined with finite-size scaling analyses. Our results for the hitherto unknown interface tension and the transition temperatures show that the analytical formula yields fairly good approximations but, in general, is not exact.

Introduction. – In a recent letter, Zandvliet [1] has derived an analytical expression for the interface free energy in the (10) direction of the Ising model on a square lattice with nearest- *and* next-nearest-neighbour interactions, being of experimental relevance for (001) surfaces of cubic crystals [2–5]. The temperature where the interface tension vanishes yields the transition temperature T_c, separating the ordered (ferromagnetic) from the disordered (paramagnetic) phase. The derivation presented in ref. [1] is heuristic and neglects overhang configurations of the interface between the plus and minus magnetized phase below T_c as well as bubble excitations in the two coexisting phases. While this can be expected to be an excellent approximation for very low temperatures $T \ll T_c$, it is *a priori* unlikely that with these approximations the correct behaviour can be captured when approaching the critical point, where fluctuations on all length scales become more and more important. Still, in the special case of *only* nearest-neighbour interactions (J_x, J_y), Zandvliet's general expression reproduces the famous exact Onsager formula [6–8], which *does* take into account also overhangs and bubble excitations. A similar observation was also made for the nearest-neighbour model on a triangular lattice, which is of experimental relevance for (111) FCC crystal surfaces [9]. In the general square lattice case with additional diagonal next-nearest-neighbour interactions (J_d), no exact solution for the interface tension was known before. Here, Zandvliet supports his analytical expression by comparing the transition temperature implied by the vanishing of the interface tension with approximate calculations [10] and numerical results based on high-temperature series expansions [11], extrapolations of transfer-matrix calculations [12][1] and

[1]Zandvliet [1] quotes in his ref. [11] work by Nightingale which is only remotely connected and does not contain estimates of the considered transition temperature. This quotation is thus apparently in error and should be replaced by our ref. [12], as is fairly obvious from the two data points referring to "ref. [11]" in fig. 2 of ref. [1].

Monte Carlo simulations [13]. When plotted over a relatively large range of coupling-constant ratios ($J_x/k_{\rm B}T = J_y/k_{\rm B}T$ *vs.* $J_{\rm d}/k_{\rm B}T$) as done in fig. 2 of ref. [1], the agreement with the numerical data looks indeed quite impressive. However, no numerical data for the primary quantity, the interface tension, was available for a direct comparison.

The purpose of this letter is to point out that Zandvliet's approach is equivalent to the classic solid-on-solid (SOS) approximation [14] which in the case of only nearest-neighbour interactions is well known to be exact for (10) interfaces due to "a delicate cancellation between overhang contributions and interactions between the interface and bubbles in the bulk" [4] (see also ref. [15]). A mathematical explanation was later discussed in ref. [16]. Being skeptical that such a delicate cancellation also happens in the general case, we first examined the comparison with previous numerical results for the transition temperature more carefully. While the first two or three digits indeed agree (which explains the very good fit in the plot of ref. [1]), it became also apparent that within the very small error bars of the numerical work [12], no real agreement can be claimed. In the limit where only next-nearest-neighbour interactions are considered we prove the deviation analytically. To assess the accuracy for the general model, we decided to perform an independent computer simulation study using state-of-the-art multicanonical Monte Carlo techniques in order to determine in particular also the hitherto unknown interface tension directly.

Analytical results. – The square lattice Hamiltonian used in ref. [1] has the form

$$\mathcal{H} = -J_x \sum_{\langle i,j\rangle} \sigma_i\sigma_j - J_y \sum_{\langle i,j\rangle} \sigma_i\sigma_j - J_{\rm d} \sum_{(i,j)} \sigma_i\sigma_j \,, \qquad (1)$$

where the spins can take the values $\sigma_i = \pm 1$, J_x and J_y denote the nearest-neighbour (nn) couplings in x- and y-direction, respectively, and $J_{\rm d}$ is the next-nearest-neighbour (nnn) coupling along the two diagonals. The corresponding pairs of spins are denoted by the brackets $\langle i,j\rangle$ and (i,j), respectively. We only consider the isotropic case $J_x = J_y \equiv J$, restrict ourselves to that region of the phase diagram where the ground states show ferromagnetic order ($J \geqslant 0$, $J_{\rm d} \geqslant -J/2$), and always assume periodic boundary conditions.

For the interface free energy per unit length in the (10) direction, that is along one of the two main coordinate axes, Zandvliet derived [1]

$$\begin{aligned} F_{(10)} \;&=\; -k_{\rm B}T \ln\left(Z_{(10)}\right) = 2J_y + 4J_{\rm d} \\ &\quad -k_{\rm B}T \ln\left(1 + \frac{2e^{-2J_x/k_{\rm B}T}}{1 - e^{-(2J_x+4J_{\rm d})/k_{\rm B}T}}\right). \end{aligned} \qquad (2)$$

By examining the general SOS approximation given by Burton *et al.* [14] for nn and nnn interactions and an interface at arbitrary angle, it is for the special case of an (10) interface relatively straightforward to verify that their expression agrees precisely with (2). For a recent more compact derivation of the general result including the explicit low-T solution, see ref. [2]. For vanishing diagonal couplings, $J_{\rm d} \equiv 0$, the expression (2) simplifies to $F_{(10)} = 2J_y + k_{\rm B}T \ln\left[\tanh(J_x/k_{\rm B}T)\right]$, which is indeed the famous exact Onsager formula [6–8]. For the nn model it is also easy to show that, by identifying Zandvliet's kink variables n_i with the gradient ∇h_i of interface height variables h_i, one ends up with the standard one-dimensional SOS model partition function $Z_{\rm SOS} = \sum_h \exp(-\beta_{\rm SOS} \sum_i |\nabla h_i|)$, where $\beta_{\rm SOS} = 2J_x/k_{\rm B}T$. Requiring $F_{(10)} = 0$, the critical temperature $T_{\rm c}$ follows from the transcendental equation[2]

$$\begin{aligned} &e^{-2J_x/k_{\rm B}T_{\rm c}} + e^{-2J_y/k_{\rm B}T_{\rm c}} \\ &+ e^{-2(J_x+J_y)/k_{\rm B}T_{\rm c}} \left(2 - e^{-4J_{\rm d}/k_{\rm B}T_{\rm c}}\right) = e^{4J_{\rm d}/k_{\rm B}T_{\rm c}} \,. \end{aligned} \qquad (3)$$

In the special case $J_{\rm d} \equiv 0$, the usual self-duality relation for the square lattice Ising model is recovered, $\sinh(2J_x/k_{\rm B}T_{\rm c})\sinh(2J_y/k_{\rm B}T_{\rm c}) = 1$, which further simplifies in the isotropic case $J_x = J_y \equiv J$ and yields the well-known critical temperature of the isotropic square lattice Ising model, $k_{\rm B}T_{\rm c}/J = 2/\ln\left(1+\sqrt{2}\right) \approx 2.269$.

Another special case is $J = 0$, where the model (1) decouples into two independent nearest-neighbour Ising models with spins at the "even" or "odd" sites, respectively, interacting via an isotropic coupling $J_{\rm d}$. Clearly, also in this case $k_{\rm B}T_{\rm c}/J_{\rm d} = 2/\ln\left(1+\sqrt{2}\right)$. Setting $J = 0$, it is easy to derive from (3) the explicit relation $\cosh(4J_{\rm d}/k_{\rm B}T_{\rm c}) = 2$ or $k_{\rm B}T_{\rm c}/J_{\rm d} = 4/\ln(2+\sqrt{3}) \approx 3.037$, which is completely off the exact result ($> 30\%$). Furthermore, for each of these two subsystems, $F_{(10)}$ should now play the role of the *diagonal* interface tension of the standard isotropic nn model which is given, *e.g.*, by Baxter [8] as[3] $\sqrt{2}k_{\rm B}T \ln\sinh(2J_{\rm d}/k_{\rm B}T) = 2\sqrt{2}J_{\rm d} - \sqrt{2}\ln(2)k_{\rm B}T + \sqrt{2}k_{\rm B}T\ln(1-e^{-4J_{\rm d}/k_{\rm B}T})$. In the limit $T \to 0$, the last term vanishes exponentially fast. On the other hand, if one sets $J = 0$ in (2), one arrives at the quite different expression

$$\begin{aligned} F_{\rm diag} \;&=\; F_{(10)}(J=0)/\sqrt{2} = 2\sqrt{2}J_{\rm d} \\ &\quad -(k_{\rm B}T/\sqrt{2}) \ln\left(1 + \frac{2}{1 - e^{-4J_{\rm d}/k_{\rm B}T}}\right), \end{aligned} \qquad (4)$$

with a $T \to 0$ behaviour $\simeq 2\sqrt{2}J_{\rm d} - (\ln(3)/\sqrt{2})k_{\rm B}T + \ldots$. Here the $1/\sqrt{2}$ normalization takes into account that

[2] Note that by fixing $K_x = J_x/k_{\rm B}T_{\rm c}$, $K_y = J_y/k_{\rm B}T_{\rm c}$, this can be solved explicitly for $J_{\rm d}/k_{\rm B}T_{\rm c} = (1/4)\ln\left[\cosh(\Delta K)\, e^{-2\overline{K}} + e^{-4\overline{K}} \pm e^{-3\overline{K}}\sqrt{\sinh^2(\Delta K)\, e^{2\overline{K}} + 2\cosh(\Delta K) + e^{-2\overline{K}}}\right]$, where $\overline{K} = (K_x + K_y)/2$ and $\Delta K = K_x - K_y$. In the isotropic case $K_x = K_y = K$, this simplifies to $J_{\rm d}/k_{\rm B}T_{\rm c} = (1/4)\ln\left[e^{-2K} + e^{-4K} \pm e^{-3K}\sqrt{2 + e^{-2K}}\right]$.

[3] Notice that in ref. [8] lengths are measured in a taxi-cab metric while here we prefer to use the Euclidean metric in which the interface tension becomes isotropic in the vicinity of the critical point. This explains the different prefactor ($2 \to \sqrt{2}$) compared with ref. [8].

Table 1: Comparison of the analytical prediction (3) for the transition point $\beta_c \equiv 1/k_B T_c$ with numerical estimates for $\alpha = J_d/J = 1.0$ and 0.5 with $J_x = J_y = J = 1$.

	$\beta_c(\alpha = 1)$	$\beta_c(\alpha = 0.5)$
Zandvliet [1]	0.185 921 566 ...	0.260 518 128 ...
Nightingale and Blöte [12]	0.190 192 69(5)	–
Luitjen *et al.* [19]	0.190 1908(19)	–
Luitjen *et al.* [19]	0.190 1931(11)	–
Oitmaa [11]	–	0.262 808
this work	0.190 1923(10)	0.262 8174(16)

we measure the diagonals in the two (independent) nn Ising subsystems in a Euclidean metric. Only the trivial temperature-independent contribution agrees with the exact result, but already the first term proportional to T differs. This proves analytically that even for an $F_{(10)}$ interface the expression (2) cannot be exact in general[4]. Specializing the general SOS result of ref. [14] to only nn interactions and an 45° interface, one finds $F^{\mathrm{SOS}}_{(11)} = k_B T \ln\left[\left(e^{4J/k_B T} - 1\right)/4\right]/\sqrt{2} = 2\sqrt{2}J - \sqrt{2}\ln(2)k_B T + (1/\sqrt{2})k_B T \ln(1 - e^{-4J/k_B T})$. For arbitrary angles the SOS approximation is no longer exact (for the nn model, 45° is the worst case), but the deviation $F^{\mathrm{SOS}}_{(11)} - F^{\mathrm{exact}}_{(11)} = -(1/\sqrt{2})k_B T \ln(1 - e^{-4J/k_B T}) = (1/\sqrt{2})k_B T e^{-4J/k_B T} + (1/2\sqrt{2})k_B T e^{-8J/k_B T} + \ldots$ is exponentially small as $T \to 0$ and the relative deviation is bounded by 1.5% up to $T = T_c/2$. This uncovers an intrinsic inconsistency of the SOS approximation in the general case with additional nnn interactions.

Numerical results. – One source of comparison with numerical results used in ref. [1] is a transfer-matrix calculation ("phenomenological renormalisation") by Nightingale and Blöte [12] where the critical line of a so-called "eight-neighbour model" was estimated (see footnote [1]). Identifying their parameters $K \equiv J/k_B T$ and $L \equiv J_d/k_B T$ shows the equivalence of their Hamiltonian with our isotropic nnn Ising model of eq. (1). Nightingale and Blöte introduce the ratio $\alpha \equiv L/K \equiv J_d/J$ and give results for $\alpha = 1$ (see table 1) and $\alpha = -1/4$ (not considered here). A glance at the results for $\beta_c \equiv 1/k_B T_c$ in table 1 reveals for $\alpha = 1$ a deviation in the third significant digit which is far beyond the claimed error margin of ref. [12][5].

To prepare for our investigations of the interface tension, we first checked by Monte Carlo simulations which of the two results is valid. For the estimation of the critical temperature we used a single-cluster Wolff update [21], which can be expected to be the most efficient update algorithm close to criticality also for the general nnn model (1). To be on the safe side, the algorithm and the employed pseudo-random number generator were checked against complete enumerations of small lattices (up to linear size $L = 6$). We collected finite-size scaling (FSS) data for $\alpha = 0.5$ and $\alpha = 1.0$, working with linear lattice sizes $L = 10, 20, 40, \ldots, 640$ at the two different temperatures T_Z and T_{NB}, the infinite-volume critical temperature given by Zandvliet (Z) and by Nightingale and Blöte (NB), respectively (see table 1). As output of each simulation run we obtained time series for the energy $E = \mathcal{H}(\{\sigma_i\})$ and the magnetization $M = \sum_i s_i$. In a first step, we checked the integrated autocorrelation time τ_{int} (in units of $V = L^2$ single spin flips) and found for $\alpha = 1.0$ a weak power law behaviour $\tau_{\mathrm{int}} \propto L^z$ with $z = 0.134(3)$ at T_{NB}, but a rather constant value at T_Z (see fig. 1), being already indicative that the transition point must be close to T_{NB}. From this we decided to measure 50×10^6 cluster flips at T_{NB}. At T_Z, taking into account the smaller mean cluster size we measured there, the same number of measurements was taken but with 50 cluster flips without measurements in between. All statistical errors are estimated with the Jackknife method.

Next, by applying the reweighting technique (with at least 80% overlap of the energy histograms) we determined the maxima of the specific heat $c_V = \beta^2(\langle E^2\rangle - \langle E\rangle^2)/V$, the susceptibility $\chi = V(\langle m^2\rangle - \langle |m|\rangle^2)$, the derivative $\mathrm{d}U/\mathrm{d}\beta$ of the Binder parameter $U = 1 - \langle m^4\rangle/3\langle m^2\rangle^2$, and various derivatives of the magnetization density $m = M/V$, $\mathrm{d}\langle |m|\rangle/\mathrm{d}\beta$, $\mathrm{dln}\langle |m|\rangle/\mathrm{d}\beta$, and $\mathrm{dln}\langle m^2\rangle/\mathrm{d}\beta$. The scaling behaviour of the resulting specific-heat curves shown in fig. 2 unambiguously favours T_{NB} over T_Z. From fits of the FSS prediction for the maximal Binder-parameter derivative, $(\mathrm{d}U/\mathrm{d}\beta)_{\max} \propto L^{1/\nu}$, to our data in the range $L = 40$–640, we obtain the estimate $\nu = 1.0006(13)$. Assuming thus the exact value $\nu = 1$ according to the universality class of the two-dimensional Ising model, we can obtain estimates for β_c from linear least-square fits of the scaling behaviour of the various

[4] This fact was already known to Burkhardt [17], who also proposed an alternative SOS type approximation for the *diagonal* interface tension of the model (1). While in the general case this alternative SOS approximation cannot be solved in closed form, it does reproduce the exact result in both limiting cases, that is *only* nearest-neighbour couplings $J \neq 0$, $J_d = 0$ (*i.e.*, the usual nearest-neighbour diagonal tension) and *only* next-nearest-neighbour couplings $J = 0$, $J_d \neq 0$ (*i.e.*, the Onsager tension along the (10) direction of the two decoupled models), yielding the exact limiting points of the critical line (albeit with a different slope close to $J = 0$ [18]), to be discussed in more detail elsewhere.

[5] We thank one of the referees of our manuscript for pointing out to us that this discrepancy was already noticed by Zandvliet in an erratum [20] to ref. [1].

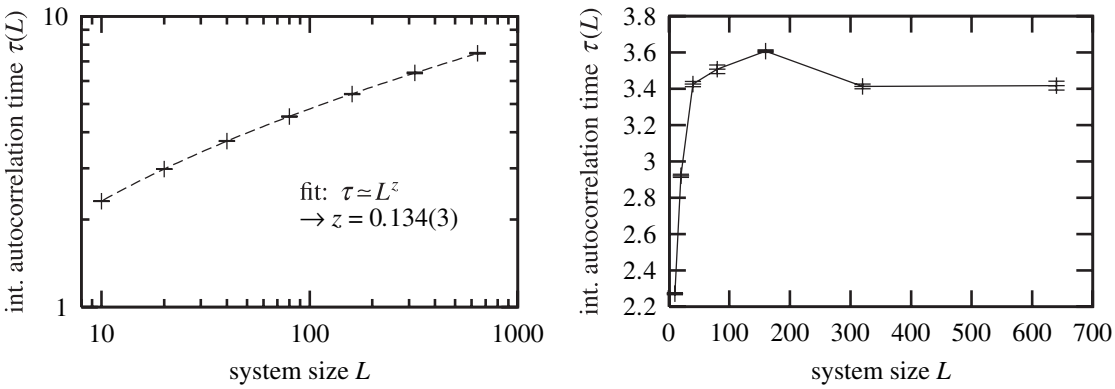

Fig. 1: Integrated autocorrelation time $\tau_{\rm int}$ for $\alpha = 1.0$ in dependence of the system size L in units of V single spin flips. Left: result of the simulations at $T_{\rm NB}$ on a log-log scale, with the dashed line showing the power law fit $\tau_{\rm int} = a + bL^z$. Right: result of the simulations at $T_{\rm Z}$ on a linear scale.

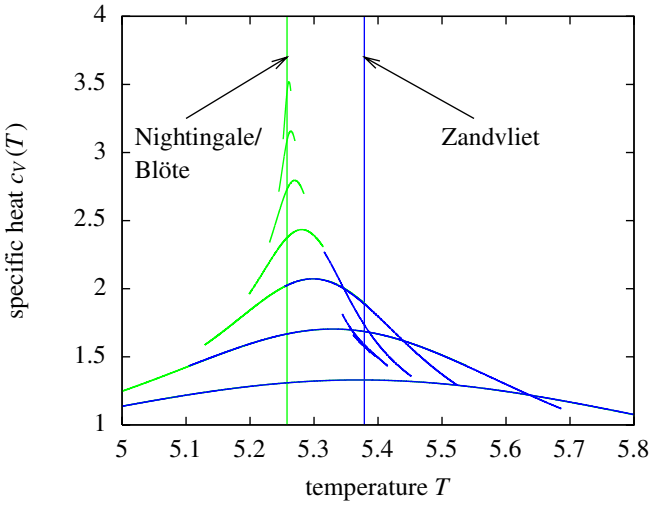

Fig. 2: Plot of the specific heat $c_V(T)$ for $\alpha = 1.0$ as a function of temperature T for different system sizes $L = 10, 20, 40, \ldots, 640$ from bottom to top. The light curves represent the reweighted data from the simulation at $T_{\rm NB}$ and the bold curves from the simulation at $T_{\rm Z}$. For the smaller system sizes, where the temperature reweighting range overlaps, the specific heat matches very well.

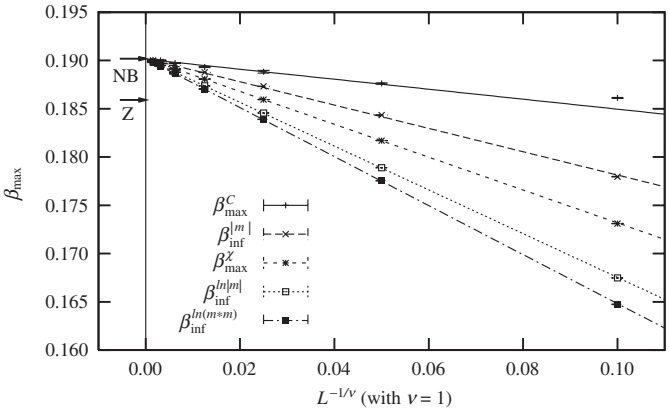

Fig. 3: FSS extrapolations of pseudo-transition points for $\alpha = 1.0$, assuming $\nu = 1$. The average of the extrapolations to infinite size yields $\beta_c = 0.190\,1923(10)$. The arrows indicate the numerical result of Nightingale and Blöte (NB) [12] and the analytical prediction of Zandvliet (Z) [1], respectively.

pseudo-critical point sequences, $\beta_{\rm max}(L) \propto L^{-1/\nu} = L^{-1}$, as shown in fig. 3. With such fits the combined estimate from the five sequences is $\beta_c = 0.190\,1923(10)$ for $\alpha = 1.0$, which is in perfect agreement with the numerical results of [12] and an independent Monte Carlo study [19], but clearly deviates from the analytic prediction of ref. [1] (by $\approx 2.2\%$, but about 400 standard deviations), cf. table 1. Table 1 also contains our estimate of β_c for $\alpha = 0.5$ from a similar analysis, which is more accurate than the compatible value from previous high-temperature series expansions [11]. Since for $\alpha \to 0$, eq. (3) becomes exact, here the deviation of Zandvliet's formula is smaller (less than 1%) but still significant (many standard deviations). For completeness we also checked the ratio of critical exponents γ/ν, using the FSS ansatz $\chi \propto L^{\gamma/\nu}$ for the susceptibility. From a (linear) least-square fit at $\beta_{\rm c}$, we find for $\alpha = 1.0$ that $\gamma/\nu = 1.750(2)$ is again in perfect agreement with the exact value $7/4$. For $\alpha = 0.5$ all exponent values turn out to be equally well determined.

Since already the aforementioned results strongly disagree with Zandvliet's conjecture (2), (3), it is clear that the expression (2) for the interface tension cannot be exact in general. For low temperatures $T \ll T_{\rm c}$, however, the interface width gets smaller and overhangs as well as bubble excitations are highly suppressed, such that one can expect that it yields in the low-temperature regime a good approximation of the true interface tension σ_0 also in the general case. To measure the interface tension below $T_{\rm c}$ we used a multimagnetical (multicanonical for the magnetization) simulation, the result of which is a double-peaked magnetization density $P(m)$. In the limit of large system sizes L, it holds in two dimensions [22]

$$\ln\left(\frac{P^{(L)}_{\rm max}}{P^{(L)}_{\rm min}}\right) = 2\beta\sigma_0 L\,, \qquad (5)$$

Table 2: Comparison of the analytical expression (2) for $F_{(10)}$ with the interface tension σ_0 obtained from fits of eq. (5) (supplemented with a correction term $(1+a/L)$) to the data of our multimagnetical simulations for $\alpha = J_\mathrm{d}/J = 1.0$ with $J_x = J_y = J = 1$.

T	4.00	4.25	4.5	4.75	5.00
T/T_c	0.7608	0.8083	0.8559	0.9034	0.9510
$F_{(10)}$	$2.237\,670\ldots$	$1.855\,163\ldots$	$1.461\,915\ldots$	$1.058\,308\ldots$	$0.644\,697\ldots$
σ_0	2.1357 ± 0.0009	1.7349 ± 0.0026	1.3157 ± 0.0018	0.8947 ± 0.0020	0.4504 ± 0.0014
$F_{(10)}/\sigma_0$	1.05	1.07	1.11	1.18	1.43

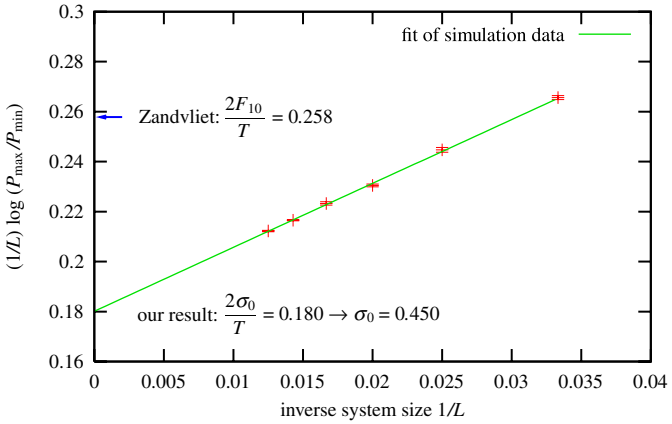

Fig. 4: Scaling of the interface-tension estimates from the histogram method for $\alpha = 1.0$, temperature $T = 5.0$ and system sizes $L = 30, 40, 50, 60, 70,$ and 80. The straight line shows the fit $\ln(P^{(L)}_\mathrm{max}/P^{(L)}_\mathrm{min})/L = 2\beta\sigma_0(1+a/L)$ with goodness-of-fit parameter $Q = 0.42$, yielding an interface tension estimate of $\sigma_0 = 0.4504 \pm 0.0014$. The arrow on the y-axis points to the analytical result of Zandvliet [1].

where $P^{(L)}_\mathrm{min}$ is the value of the density in the mixed phase region ($m \approx 0$) and $P^{(L)}_\mathrm{max}$ the value at its maxima ($m = \pm m_0$). Figure 4 shows the fit to our data for $\alpha = J_\mathrm{d}/J = 1.0$ at $T = 5.0$ according to eq. (5) (including the usual correction term of FSS [22]), and in table 2 our results from simulations at different temperatures T are collected. We see that close to criticality, Zandvliet's SOS approximation (2) clearly overestimates the numerically determined interface tension. Only for temperatures well below T_c, eq. (2) becomes a good approximation.

Let us finally add a few comments on simulations of the extreme, degenerate limit $J = 0$, *i.e.*, $\alpha \to \infty$, where the model (1) decouples into two independent nearest-neighbour models with spins defined on the even, respectively odd, sites and isotropic coupling J_d. Performing direct simulations below T_c one obtains triple-peaked magnetization densities: two peaks of equal height at about $\pm m_0$ and another one at $m = 0$ which is twice as high, resulting from the superposition of the two double-peaked densities of the two independent subsystems. Applying (5) to either of the two sides ($m \leqslant 0$ or $m \geqslant 0$) we obtain for $T = 1.45 \approx 0.64 T_\mathrm{c}$ the numerical interface tension estimate 1.270(3), in very good agreement with the exact expression for the diagonal interface tension, $\sqrt{2} k_\mathrm{B} T \ln \sinh(2J_\mathrm{d}/k_\mathrm{B}T) = 1.272\,785\ldots$.

Note that the temperature was chosen small enough to be able to clearly distinguish this value from the interface tension in the (10) direction (of the subsystems), $2J_\mathrm{d} + k_\mathrm{B}T \ln \tanh(J_\mathrm{d}/k_\mathrm{B}T) = 1.253\,880\ldots$. For comparison, the 45° SOS result is $k_\mathrm{B}T \ln\{[e^{4J_\mathrm{d}/k_\mathrm{B}T} - 1]/4\}/\sqrt{2} = 1.339\,919\ldots$ (+5.3%) and eq. (4) predicts $1.656\,774\ldots$ (+30%). The fact that the original (10) direction (respectively, the diagonal direction for the subsystems) is stable, even though the interface in this direction is the "most costly" one, can be traced back to our use of periodic boundary conditions when simulating the model (1). In fact, when extracting the two subsystems, their boundary conditions turn out to be of twisted type which enforces a diagonal interface. Direct simulations of these subsystems confirm our numerical estimate quoted above and configuration snapshots verify the expected orientation of the interface.

Conclusion. – To conclude we have i) pointed out that Zandvliet's analytic result in ref. [1] is equivalent to the classic solid-on-solid (SOS) approximation of ref. [14]. This suggests that his formula is only (and more or less accidentally) exact for the special case of only nearest-neighbour interactions (vanishing diagonal coupling J_d). By analytical reasoning we have ii) proved that his result cannot be exact in the limit $J_x = J_y = J \to 0$, $J_\mathrm{d} \neq 0$. Finally, by means of Monte Carlo simulations we have iii) demonstrated that also in all other cases, the analytical expressions (2) and (3) are *not* exact. For instance, for $J_x = J_y = J_\mathrm{d} = 1$ ($\alpha = 1.0$) and $T = 5.0 \approx 0.95 T_c$, the interface tension is overestimated by about 43%. From a comparison with our numerical results we find, however, that eq. (3) constitutes a fairly good approximation for $T_c(J_x = J_y, J_\mathrm{d})$ as long as $\alpha = J_\mathrm{d}/J$ is not too large and that the accuracy of the approximation (2) for the interface tension rapidly improves with decreasing temperature.

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