Interfacial Stiffness and the Wetting Parameter: The Simple Cubic Ising Model

Renormalization-group (RG) theory [1] for $d=3$ dimensions predicts that critical wetting transitions display strong *nonuniversality* controlled solely by the numerical parameter $\omega(T)=k_BT/4\pi\tilde{\Sigma}(T)\xi_\beta^2(T)$, evaluated at T_{cW}. Here $\tilde{\Sigma}$ is the stiffness of a rough interface separating coexisting bulk phases, while ξ_β is the correlation length of the phase β which wets the wall. However, Monte Carlo simulations for the simple cubic (sc) Ising model by Binder, Landau, and Kroll (BLK) [2] detected no nonuniversality. The initial results seemed consistent with classical theory as given by $\omega_{\rm fit}=0$. Later analyses [3], however, suggested that the data for $T_{cW}/T_c \simeq 0.6$–0.9 might be as well described by $\omega_{\rm fit}\simeq 0.25$ or 0.30. Note that T_c is the bulk critical point while the interfacial roughening temperature is $T_R \simeq 0.54_2 T_c$ [4]. BLK point out the difficulty of estimating ω (see also [3(b)]); but, quoting Ref. [5] for ξ_β and allowing for the (then) larger uncertainties in T_R, they found $\omega_R \equiv \omega(T\to T_R^+)\simeq 1.0\pm 0.2$, close to then current estimates $\omega_c \simeq 1.2\pm 0.3$. Thus the simulations disagree strongly with RG theory.

We have carefully reestimated $\omega(T)$ for the sc Ising lattice and conclude that the BLK estimates are *significantly too large*; see Fig. 1. Specifically, we find $\omega_R \simeq 0.51_2 \leq \omega(T>T_R)$ and $\omega_c \simeq 0.77_5$. The discrepancy factor, $\omega/\omega_{\rm fit}$, is thus reduced from 3–4 to 2–2.6 but remains unduly large.

The main ingredients in our ω estimates are the following: (a) recognition [2(b),6] that the length ξ_β required for RG theory is the *true correlation length* [5] which specifies the asymptotic exponential decay of correlations normal to the wall; (b) improved estimates of the sc interfacial tension $\Sigma a^2/k_BT \simeq K|t|^\mu$ with $\mu=2\nu\simeq 1.26_4$ and $K=1.58\pm 0.05$, as $t=(T-T_c)/T_c \to 0-$ [4,7,8]; concluding from RG theory, etc.,

$$\tilde{\Sigma}a^2/k_BT=\begin{cases}\Sigma(T)[1+qa^2/\xi_\beta^2+\cdots], & t\to 0-,\\ \frac{1}{2}\pi[1-c(t-t_R)^{1/2}+\cdots], & t\to t_R^+,\end{cases}$$

where (c) a mean-field theory [8] indicates $q\simeq\frac{1}{30}$ (close to $q=\frac{1}{24}$ for the square lattice), and (d) the *step free energy* $\sigma(T)$ *below* T_R [9] yields c via $\ln(k_BT/\sigma a)\simeq \pi/2c|\Delta t|^{1/2}$ [10]. For a (100) sc interface one finds $c=1.57\pm 0.07$ [8,9].

Conclusion (a) follows directly from a rederivation [6] of the effective wall-interface potential, $W(l)\sim e^{-l/\xi_\beta}$, entering the RG theory [1]. However, BLK [2(b)] used the *second-moment* correlation length, $\xi_1(T)$, which at T_c^- is only about 0.7% smaller than $\xi_\beta(T)$ [5]; but, the ratio ξ_1/ξ_β falls rapidly as T drops to T_R [11]. Accurate estimates for ξ_β follow from Refs. [5,8,12]. To compute ω these have been combined with two-point approximants for $\tilde{\Sigma}$ and Σ embodying (b)–(d). Figure 1 records the mean of various optimal approximants: confidence limits are about $\pm 4\%$ near T_c but fall to $\pm 1\%$ or less near T_R.

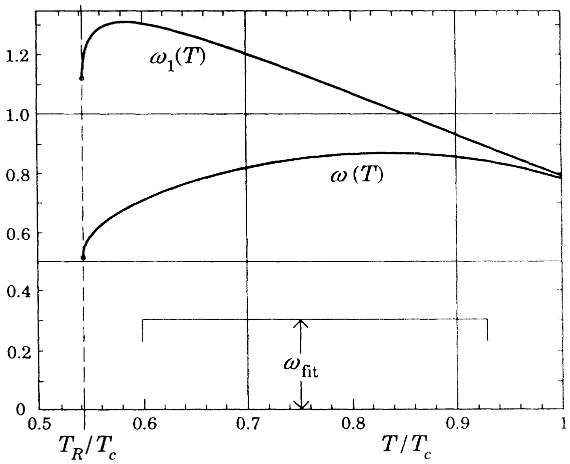

FIG. 1. Wetting parameters $\omega(T)$ with ξ_β and $\omega_1(T)$ with ξ_1.

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Michael E. Fisher and Han Wen
Institute for Physical Science and Technology
University of Maryland
College Park, Maryland 20742

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