Surface Tension and Phase Coexistence
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Using inequalities, we give a simple proof that the surface tension $\tau$ of an Ising model with interaction $\beta J = K$ on a $d$-dimensional lattice, $\sigma_i = \pm 1$, $i \in \mathbb{Z}^d$, a simple-cubic (sc) lattice in $d$ dimensions. In this note we extend these results. All our results hold when the $\sigma_i$ are distributed according to an even probability $\nu(\sigma_i)$, e.g., distributed uniformly in $[-1,1]$.

To define $\tau$ we start with our system confined in a parallelepiped $\Lambda \subset \mathbb{Z}^d$ of sides $L_d$, $d' = 1, \ldots, d$, centered on the origin; in particular, $L_1 = 2M$, $-M \leq i \leq M - 1$. We shall write $\Lambda = (M, L)$, $L$ being the infinite cylinder obtained by letting $M \to \infty$.

Let $\mu^A$ be the Gibbs measure (canonical ensemble) on the spins in $\Lambda$ with boundary conditions (b.c.) $\gamma$, with $\gamma = +$, $-$, or $\pm$.

For $A \subset \Lambda$, the averages $\langle \sigma_i \rangle_{\gamma, A}$ is $A$; $\langle \sigma_i \rangle_{\gamma, \Lambda}$ and $\langle \sigma_i \rangle_{\gamma}$, the averages, respectively, in the cylinder $L$ (infinite in the 1 direction) and in the infinite-volume limit $L_d \to \infty$, $d' = 1, \ldots, d$. This limit is known to exist and the approach has some monotonicity properties. We shall sometimes write $i = (i_1, x)$, $x \in \mathbb{Z}^{d'}$.

Let $Z_\Lambda(\gamma)$ be the partition function in $\Lambda$,

$$Z_\Lambda(\gamma) = \sum_{\sigma_i = \pm 1} \exp(\beta K \sum_{i \in \Lambda} \sigma_i \sigma_{i+j}),$$

where the sum in the exponent is over all nearest-neighbor pairs, such that $j \in \Lambda$; if $k \in \Lambda$, then $\sigma_k$ is determined by $\gamma$.

Define

$$\tau_\Lambda(\gamma) = |X|^{-1} \text{ln} Z_\Lambda(\gamma)/Z(\gamma),$$

where $|X| = L_2 \cdots L_d$ is the cross-sectional area.

Then the surface tension (times $\beta$) is given by Abraham, Gallavotti, and Martin,

$$\tau(\gamma) = \lim_{\beta \to 0} \tau_\Lambda(\gamma).$$

The limits (2) and (3) exist and $\tau(\gamma) = \tau(\gamma; d)$ is monotonically increasing in $K$ and (consequently) in $d$.

For $d = 1$, $\tau(\gamma) = 0$, while for $d = 2$ Onsager derived the formula $\tau(\gamma; 2) = 2K \ln(\tanh K)$ for $K > K_c$ and $\tau(\gamma; 2) = 0$ for $K < K_c$, where $K_c = d/T_c$ and $T_c$ is the $d = 2$ critical temperature. For $d > 2$, one still expects that $\tau(\gamma) = 0$ for $K < K_c$ and $\tau(\gamma) > 0$ for $K > K_c$, $K_c$ being defined by the nonvanishing of the spontaneous magnetization for $K > K_c$.

A proof that $\tau = 0$ for $K$ sufficiently small and $\tau > 0$ for $K$ sufficiently large was given by Fontaine and Gruber. In Ref. 1 we gave proof that $\tau(\gamma) = 0$ for $K < K_c$ by deriving the following inequalities:

$$\tau(\gamma) \leq 2M \langle m^*(\gamma) \rangle^2,$$

$$\tau(\gamma) \leq 2K \langle \sigma_i \rangle_{\gamma},$$

where $\langle \sigma_i \rangle_{\gamma}$ is the expectation value of the spin at the origin in the semi-infinite system with $+$ b.c., i.e., imagine all boundary conditions between the surface $i = 0$ and $i = -1$ to be cut. It is known that generally $\langle \sigma_i \rangle_{\gamma} < m^*(\gamma)$ and that for $d = 2$, $\langle \sigma_i \rangle_{\gamma} > 0$ for $T > T_c$ [near $T_c$, for $d = 2$, $\langle \sigma_i \rangle_{\gamma} > (T_c - T)^{1/2}$]. It was not known before, however, whether $\langle \sigma_i \rangle_{\gamma} > 0$ for all $T > T_c$ in $d > 2$ dimensions. It is a consequence of our result that this is the case.
We now state the main result of this note:
\[ d\tau_{\Lambda}(K)/dK \geq 2|m|^2 \left( \sum_{\Lambda} \langle \sigma_{i+1,1} \rangle_{\Lambda} \right)^2. \] (6)

Note that \( \langle \sigma_{i+1,1} \rangle_{\Lambda} \), independent of \( i \), since the system in \( \Lambda \) with + b.c. is translation invariant in the (vertical) direction. The inequality carries through in an obvious way in the limit \( \Lambda \to \infty \) to yield
\[ d\tau(K)/dK \geq 2|m|^2 \left( \langle \sigma \rangle \right)^2 = 2|m|^2 \langle \sigma \rangle^2. \] (7)

**Proof.** It follows from the definition that
\[ d\tau_{\Lambda}(K)/dK = \left| \sum_{j=0}^{M} \langle \sigma_{j+1,1} \sigma_{j+1,1} \rangle_{\Lambda} - \langle \sigma_{j,1} \sigma_{j+1,1} \rangle_{\Lambda} \right|, \] (8)

where \( \sum_{j} \) is the sum over all neighbors of the site \( i = (j, x) \). By known inequalities, each term in the sum is nonnegative. We now take the limit \( M \to \infty \). Using the fact that \( \Lambda \) is "one dimensional" so that the terms in the sum go to zero exponentially fast as \( |j| \to \infty \), we obtain
\[ d\tau_{\Lambda}/dK = \left| \sum_{j=0}^{M} \langle \sigma_{j+1,1} \sigma_{j+1,1} \rangle_{\Lambda} - \langle \sigma_{j,1} \sigma_{j+1,1} \rangle_{\Lambda} \right| + R, \] (9)

where \( R \) is the sum over horizontal neighbors of the site \( (j, x) \) which is nonnegative.

The next step is to use another simple inequality,
\[ \langle \sigma_{A} \sigma_{B} \rangle_{\Lambda} - \langle \sigma_{A} \sigma_{B} \rangle_{\Lambda} \geq \left| \langle \sigma_{A} \sigma_{B} \rangle_{\Lambda} - \langle \sigma_{A} \rangle_{\Lambda} \left( \langle \sigma_{B} \rangle_{\Lambda} \right) \right|. \] (10)

This yields, for (9),
\[ d\tau_{\Lambda}/dK \geq \left| \sum_{j} \langle \sigma_{j+1,1} \sigma_{j+1,1} \rangle_{\Lambda} - \langle \sigma_{j,1} \sigma_{j+1,1} \rangle_{\Lambda} \right|, \] (11)

where we have used the translation invariance of \( \langle \sigma_{i,1} \rangle_{\Lambda} \) in the 1 direction. Using now again the fact that
\[ \langle \sigma_{j,1} \rangle_{\Lambda} = \langle \sigma_{0,1} \rangle_{\Lambda}, \quad j \to \infty \] (12)

the sum in (11) telescopes to yield the desired result, Eq. (6) (the derivative existing almost everywhere).

It follows now from (4) and (7) that if near \( T_c \), \( m \sim (T - T_c)^{3/2} \) and \( \tau \sim (T - T_c)^{3/2} \), then
\[ 2\beta \leq \mu \leq 2\beta + 1. \] (13)

In mean field (presumably correct for \( d = 5 \)) \( \beta = \frac{1}{2} \) so that \( \mu \) must lie between 1 and 2 (cf. discussion by Oliveira, Furman, and Griffiths).

We make the following extensions and remarks:

1. It should be pointed out (cf. Ref. 1) that \( \tau(K) \) in three dimensions is equal to \( \alpha(K^*) \), the coefficient of the area decay of the Wilson loop in the dual gauge model with interactions \( K^* \). It follows then from (7) that \( \alpha(K^*) > 0 \) for \( K^* < K_c^* \), the dual critical point. Thus the fact that extrapolation of low-temperature series indicates a vanishing of \( \alpha(K^*) \) at some \( K_r^* < K_c^* \) may indeed is an indication\(^8\) of a breakdown of analyticity of \( \tau(K) \) at the "roughening temperature" \( T_r < T_c \).

2. At low temperatures \( \tau \sim K^{-2} \) is analytic in \( \exp(-K)^{1/2} \).

3. Equation (7) remains valid for a two-component rotator with an anisotropic interaction \( \beta J = K \). This follows from (10), which holds when \( \sigma_A \) is replaced by \( \cos \varphi_1 \) and \( \sigma_B \) by \( \cos \varphi_2 \). The b.c. now refer to the values taken by \( \cos \varphi_j \) for \( j \in L \).

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New Models for Metal-Induced Reconstructions on Si(111)

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Angle-resolved photoelectron spectroscopy and surface-core-level chemical shifts have been used to study electronic structure and derive structural models of the Al, Ag, and Ni metal-induced reconstructions on Si(111). We show, for the first time, the connection between the Ni-stabilized \(\sqrt{19}\times\sqrt{19}\) and clean \(7\times7\) surfaces, and report a new Si(111)-(\(\sqrt{7}\times\sqrt{7}\))Al structure at \(<0.5\) monolayer coverage of Al.

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The origin of the surface reconstructions on the Si(111) surface have been of active interest for some time.\(^1\)\(^2\) The interaction between silicon and initial metal overlayers has also been the subject of many studies with low-energy electron-diffraction (LEED), electron energy-loss, Auger, and photoelectron spectroscopies,\(^3\)\(^4\) but a full understanding of the reconstructions and surface electronic states has not been obtained.\(^5\)

New results are presented in this paper which provide insight into metal-silicon surface structures from angle-resolved valence-band photoemission and surface-core-level chemical-shift measurements carried out on ordered metal-silicon systems where the number of metal atoms ranges from \(<0.1\) monolayer Ni to 0.5 monolayer Al to 1.0 monolayer Ag. We show the similarity of the electronic states for the \(\sqrt{19}\times\sqrt{19}\)Ni and \(7\times7\) reconstructions and present for the first time a model which relates the two. By using the angular dependence of the emission as well as the energy dispersion of the metal-silicon bands we derive structural models for the \(\sqrt{3}\times\sqrt{3}\)Al and \(\sqrt{3}\times\sqrt{3}\)Ag and the new \(\sqrt{7}\times\sqrt{7}\)Al surface structures on Si(111).

The metal-silicon structures have been prepared by evaporating controlled amounts of metal onto clean room-temperature Si(111) \(7\times7\) surfaces. This generally results in a metal-covered surface that shows a \(7\times7\) reconstruction, but does not necessarily correspond to an ordered metal overlayer. To obtain the ordered metal-silicon reconstructions, the surfaces have to be annealed. Typically the change to an ordered phase is accompanied by a change in surface chemical shifts. For example, for the Al \(2p\) at submonolayer coverages on Si(111), a binding energy 0.15 eV higher than the metallic core line is obtained. When the surface reconstructs to either the \(\sqrt{3}\times\sqrt{3}\) or the \(\sqrt{7}\times\sqrt{7}\), the shift to higher binding energy further increases to 0.35 eV. The line shape broadens by 15% with respect to the metallic core line because of the Si-Al bond. We have also studied the characteristic surface-core-level line shapes and shifts of the Si(111) \(2p\) for the \(2\times1\) and \(7\times7\) surfaces\(^6\)\(^7\) in the course of this work and this will be reported elsewhere.

We discuss first the Si(111) \(\sqrt{19}\times\sqrt{19}\), which is often obtained as an unintentional impurity-stabilized surface\(^6\) after long annealings at quite high temperatures (1000–1200 °C). The Auger spectra always show some amount of impurity Ni. We also have found, under some circumstances, such high-temperature annealing can produce cop-