at higher angles indicate about 10% expansion of the calculated values compared with the observed one. Further, about 4% expansion may be expected[13] from the orbital moment since $g = 2.30$. We believe the above-mentioned expansion of the calculated form factor would be attributed to the approximate nature of the Hartree-Fock atomic wave functions. It should be noted that even in an ionic crystal such as K_2CuF_4, covalency effect on the form factor is quite large and one tends to overlook such an effect with the use of conventional Bragg scattering technique.

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Phase Separation in the Two-Dimensional Ising Ferromagnet

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The interface density profile of the two-dimensional Ising ferromagnet is investigated for all temperatures below the critical point. The width of the interface diverges in the thermodynamic limit.

The phase-separation phenomenon in the Ising model of ferromagnetism with dimensionality $d = 2, 3$ has recently been investigated. It has been shown[1,2] that symmetry-breaking boundary conditions can induce *phase separation* with an associated *surface tension.* Gallavotti[3] then demonstrated that the interface for $d = 2$ is *very diffuse*, unlike the situation for $d = 3$, where the interface was shown by Dobrushin[4] to be localized. These results were obtained for $0 \leq T < T_0(d)$ with $T_0(d) \ll T_c(d)$, where $T_c(d)$ is the critical temperature for dimension d. This shows, contrary to folklore, that the existence of surface tension is not necessarily concomitant with the existence of a sharp interface. Subsequently Weeks, Gilman, and Leamy[5] investigated the interface profile for the three-dimensional system at higher temperatures $[0 \leq T < T_c(d)]$ than Dobrushin considered using a series-expansion procedure. They found the interface to be *well defined* for $0 \leq T < T'$ but *diffuse* for $T' < T \leq T_c(d)$, where $T' \sim T_c(2)$. These results motivated a more detailed investigation of the $d = 2$ separation phenomenon, valid for $0 \leq T < T_c(2)$, the results of which are reported here.

We consider a vertical-right-cylindrical lattice with M columns and $2N+1$ rows. There is a spin $\sigma_i = \pm 1$ at each vertex, labeled $i = (m, n)$ in Cartesian coordinates, where $n = -N, -N+1, \ldots, N$ and $m = 1, \ldots, M$. The energy of a spin configuration is

$$E_\Lambda(\{\sigma_i\}) = -J\sum \sigma_i \sigma_j - \sum h_j \sigma_j , \qquad (1)$$

where the first sum is over nearest-neighbor pairs of spins on Λ and the second sum is over spins in the top and bottom rows; $J > 0$ is a ferromagnetic coupling. The second term represents fields h_j acting on the top and bottom boundary rows of Λ, denoted $\partial\Lambda_+$ and $\partial\Lambda_-$. Two different boundary conditions are considered: On both $\partial\Lambda_+$ and $\partial\Lambda_-$ we have either (i) $h_j = +\infty$ for $j = 1, \ldots, s$ and $h_j = -\infty$ for $j = s+1, \ldots, M$, denoted $+-$, or

(ii) $h_j = +\infty$ for all j, denoted $++$. In the thermodynamic limit, the $++$ boundary conditions should lead to a pure state with magnetization $+m^*$,[6] whereas in the $+-$ case as $s\to\infty$ we should have a macroscopic region with magnetization $+m^*$ lying between regions with magnetization $-m^*$ to the left and right. There will be two interface regions; with each of these we may associate a long contour on the dual lattice separating opposite spins on Λ, in the sense of Ref. 2. The contours, whose ends are pinned, cluster (become independent) as $s\to\infty$.

The canonical partition for a lattice at temperature β^{-1} is denoted $Z_{NM}{}^b(\beta)$ where $b=+-$ or $b=++$. The surface tension τ is defined by[1,2]

$$\tau = \lim_{N\to\infty}\frac{1}{4N}\lim_{s\to\infty}\lim_{M\to\infty}\ln\left(\frac{Z_{NM}{}^{+-}(\beta)}{Z_{NM}{}^{++}(\beta)}\right), \tag{2}$$

and the interface profile is described by the magnetization

$$\langle\sigma_{0p}\rangle = \lim_{s\to\infty}\lim_{M\to\infty}[Z_{NM}{}^{+-}(\beta)]^{-1}\,\mathrm{Tr}[\exp(-\beta E_\Lambda)\sigma_{0p}]. \tag{3}$$

These quantities have been obtained rigorously using the transfer matrix V along the cylinder axis and the matrix element techniques of Abraham.[7] Our results are

$$\tau = \lim_{N\to\infty}\frac{1}{2N}\ln\left(\frac{1}{2\pi i}\oint\frac{dt}{t}g(t)^{2N}f(t)\right), \tag{4}$$

and

$$\langle\sigma_{0p}\rangle_N = -\frac{m^*}{2}\left(\frac{1}{\pi i}\oint\frac{dt}{t}g(t)^{2N}f(t)\right)^{-1}\frac{1}{\pi i}\oint dt\,t^{p-2}g(t)^N\frac{1}{\pi i}\oint\left(\frac{dz}{z-t}z^{3-p}-dz\,z^{2-p}\right)\times g(z)^N[U(z)T(t)+U(t)T(z)], \tag{5}$$

with

$$f(t) = -t\,\Phi(t)/[1-t\Phi(t)]^2,$$

$$g(t) = e^{-\gamma(t)},$$

where $\gamma(t)\geq 0$ for $|t|=1$,

$$\cosh\gamma(t) = \cosh 2K^*\cosh 2K - (t+t^{-1})/2,$$

and

$$\Phi(t) = -\frac{A^{1/2}}{B}\frac{1}{t}\left(\frac{(t-A^{-1})(t-B)}{(t-A)(t-B^{-1})}\right)^{1/2},$$

with $K=\beta J$, $\exp(-2K^*)=\tanh K$, $A=\exp[2(K+K^*)]$, and $B=\exp[2(K-K^*)]$. Therefore, $A>B>1$ for $T<T_c$.

Finally,

$$T(z) = \frac{\Phi(z)}{1-z\Phi(z)}\left(\frac{z-B^{-1}}{z-A^{-1}}\right)^{1/2},$$

and

$$z^2U(z)T(z) = f(z).$$

All the contours are the positive unit circle, and principal parts are to be taken where appropriate. In (4) and (5) there are corrections due to additional bands in the spectrum of V but these are $O(\exp[-4N\gamma(0)])$ and may be neglected as $N\to\infty$ compared with the given terms.

Asymptotic analysis gives the result

$$\tau = -\gamma(0), \tag{6}$$

in agreement with results based on different definitions.[8] With the scaling $p=\alpha N^\delta$, $\delta\geq 0$, (5) gives

$$\lim_{N\to\infty}\langle\sigma_{0p}\rangle_N = 0 \text{ if } \delta<\tfrac{1}{2},$$
$$\lim_{N\to\infty}\langle\sigma_{0p}\rangle_N = m^*\,\mathrm{sgn}\,p \text{ if } \delta>\tfrac{1}{2} \tag{7}$$

for $T_c(2)>T>0$. When $T=0$, we have

$$\langle\sigma_{0p}\rangle_N = m^*\,\mathrm{sgn}\,p \text{ for all } \delta, N. \tag{8}$$

Thus for $d=2$ we obtain a rigid interface only when $T=0$. For $T_c(2)>T>0$ the interface has width $\sim N^{1/2}$ in agreement (in an appropriate domain of T) with the analysis of Gallavotti.[3] One cannot induce a translationally noninvariant equilibrium state for $T>0$ with the type of symmetry-breaking boundary conditions considered. Nevertheless, we suspect, but cannot prove, that suppression (in a suitable sense) of the long-wave-length Fourier components of the "long contour" would make the interface sharp, possibly without affecting the surface tension appreciably.[9]

Identical results may be obtained using a rectangular lattice with + (−) boundary in the upper (lower) half.[10]

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