PHYSICAL REVIEW B VOLUME 43, NUMBER 7 1 MARCH 1991

Surface thermodynamic properties of a semi-infinite Ising ferromagnet in the presence of a surface transverse field

Qing Jiang and Zhen-ya Li
*China Center of Advanced Science and Technology (World Laboratory), P.O. Box 8730, Beijing, 100080, China and Department of Physics, Suzhou University, Suzhou 215006 China**
(Received 18 January 1990; revised manuscript received 16 July 1990)

By use of a combination of the two-spin cluster approximation with the discretized path-integral representation, the surface phase diagrams and surface thermodynamic quantities, such as free energy, specific heat, and susceptibility, of a semi-infinite Ising ferromagnet in the presence of a surface transverse field are investigated.

I. INTRODUCTION

In earlier work,[1] we have proposed a method that combines the two-spin cluster expansion[2] with the discretized path-integral representations[3,4] (DPIR's) to study the transverse Ising model (TIM) in a quantum spin system. The coordinate dependencies of the critical transverse field for spin $\frac{1}{2}$ and spin 1, as well as mixed spin system, are obtained analytically.[1,5]

On the other hand, surface magnetism has been a subject of increasing interest, both theoretical and experimental. The surface critical behaviors of semi-infinite magnetic solids have been extensively studied by using a variety of techniques.[6,7] As for the semi-infinite Ising ferromagnet with a surface transverse field, the surface thermodynamic properties have not been studied, although the surface critical properties have been examined.

The purpose of this Brief Report is to investigate the thermodynamic properties of surface in the spin-$\frac{1}{2}$ semi-infinite Ising ferromagnet with a surface transverse field by means of the same framework as that of our earlier paper.[1]

II. FORMALISM

For a semi-infinite Ising ferromagnet with surface transverse field Ω and bulk transverse field Γ, the surface Hamiltonian of this system can be written as

$$H_s=-\sum_{i,j} J_s u_i^z u_j^z - B\sum_i u_i^z - \Omega\sum_i u_i^x - \sum_i J u_i^z s_i^z \ , \tag{1}$$

where u_i^z and s_i^z are z components of Pauli matrices, corresponding to the surface and bulk spin, respectively. J_s is the nearest-neighbor exchange interactions of surface spins, and J is the exchange interactions between other spins. The sum ($\sum_{i,j}$) is performed over a pair of nearest-neighbor spins on the surface. B is the external longitudinal field acting on the whole system and is assumed to be in the negative direction.

We introduce the surface and bulk spin deviation operators δ_i and σ_i, respectively, as follows:

$$\delta_i=\bar{t}-u_i^z, \quad \sigma_i=\bar{s}-s_i^z \ , \tag{2}$$

where $\bar{t}$ and $\bar{s}$ are the parameters whose best values will be determined by minimizing the surface and bulk free energy, respectively.

From our earlier paper,[1] we know that the parameter $\bar{s}$ expresses a long-range order parameter of infinite system, and it satisfies the relation $g(\beta=1/k_B T,\bar{s},B,\Gamma)=0$ [Eq. (25) in our earlier paper[1]]; thus the parameter $\bar{s}$ is a function of bulk transverse field Γ and temperature T. When $\bar{s}$ tends to zero as the external field $B=0$, the bulk critical temperature approaches the critical value T_c, the critical coupling $K_c=J/k_B T_c$ decrease as the bulk transverse field increases.

In terms of δ_i and σ_i, the surface Hamiltonian can be broken into two parts, an unperturbed part,

$$H_{0s}=E_{0s}+\sum_i L_1\delta_i+\sum_i L_2\sigma_i-\Omega\sum_i u_i^x \ , \tag{3}$$

and a perturbed part,

$$V_s=-J_s\sum_{i,j}\delta_i\delta_j - J\sum_i \delta_i\sigma_i \ , \tag{4}$$

with

$$\begin{aligned} E_{0s}&=-\tfrac{1}{2}N'Z'J_s\bar{t}^2-BN'\bar{t}-N'J\bar{t}\bar{s} \ , \\ L_1&=B+Z'J_s\bar{t}+J\bar{s} \ , \\ L_2&=J\bar{t} \ , \end{aligned} \tag{5}$$

where N' and Z' are the total numbers of lattice sites and the coordinates on the surface. This choice of the perturbation is reasonable as the spin deviations are presumably small.

Correspondingly, the unperturbed part F_{0s} and the perturbed part F_s' of the surface free energy are defined by

$$\begin{aligned} -\beta F_{0s}&=\ln \mathrm{Tr} e^{-\beta H_{0s}} \ , \\ -\beta F_s'&=\ln\langle e^{-\beta V_s}\rangle \ . \end{aligned} \tag{6}$$

By use of the two-spin cluster approximation, the contribution to the surface free energy from all spin pairs is given by

$$-\beta F'_{s(2)}=\tfrac{1}{2}N'Z'\ln\langle e^{\beta J_s\delta_i\delta_j}\rangle_2+N'\ln\langle e^{\beta J\delta_i\sigma_i}\rangle \ . \qquad (7)$$

The final form for the surface free energy is obtained as

$$-\beta F_s=\tfrac{1}{2}N'Z'\ln \mathrm{Tr}e^{-\beta H_{\mathrm{II}s}}+N'\ln \mathrm{Tr}e^{-\beta H'_{\mathrm{II}s}}-N'Z'\ln \mathrm{Tr}e^{-\beta H_{\mathrm{I}s}} \ , \qquad (8)$$

with

$$\begin{aligned} H_{\mathrm{II}s}&=-J_s u_i^z u_j^z-[B+(Z'-1)J_s\bar{t}+J\bar{s}](u_i^z+u_j^z)-\Omega(u_i^x+u_j^x) \ ,\\ H'_{\mathrm{II}s}&=-Ju_i^z s_i^z-(B+Z'J_s\bar{t})u_i^z-\Omega u_i^x \ ,\\ H_{\mathrm{I}s}&=-(B+Z'J_s\bar{t}+J\bar{s})u_i^z-\Omega u_i^x \ . \end{aligned} \qquad (9)$$

In the calculation of surface free energy F_s, the diagonalizations of $H_{\mathrm{I}s}$ and $H'_{\mathrm{II}s}$ are simple and one can directly calculate their partition function. For $H_{\mathrm{II}s}$, we will use the DPIR's to calculate its contribution to F_s.

The average surface free energy per spin is obtained by

$$\begin{aligned} -\beta F_s=&\ Z'\ln(2\cosh\beta\{[B+(Z'-1)J_s\bar{t}+J\bar{s}]^2+\Omega^2\}^{1/2})-Z'\ln\{2\cosh\beta[(B+Z'J_s\bar{t}+J\bar{s})^2+\Omega^2]^{1/2}\}\\ &+\ln\{2\cosh\beta[(B+Z'J_s\bar{t}+J)^2+\Omega^2]^{1/2}+2\cosh\beta[(B+Z'J_s\bar{t}-J)^2+\Omega^2]^{1/2}\}\\ &+\frac{Z'\beta J_s}{2}\frac{[B+(Z'-1)J_s\bar{t}+J\bar{s}]^2\tanh^2\beta\{[B+(Z'-1)J_s\bar{t}+J\bar{s}]^2+\Omega^2\}^{1/2}}{[B+(Z'-1)J_s\bar{t}+J\bar{s}]^2+\Omega^2} \ . \end{aligned} \qquad (10)$$

III. RESULTS AND DISCUSSION

From $\partial F_s/\partial\bar{t}=r(\beta,B,\bar{s},\bar{t})=0$, the self-consistency equation for $\bar{t}$ is derived as

$$\begin{aligned} &-\frac{Z'(B+Z'J_s\bar{t}+J\bar{s})}{[(B+Z'J_s\bar{t}+J\bar{s})^2+\Omega^2]^{1/2}}\tanh\beta[(B+Z'J_s\bar{t}+J\bar{s})^2+\Omega^2]^{1/2}\\ &+\frac{(Z'-1)[B+(Z'-1)J_s\bar{t}+J\bar{s}]}{\{[B+(Z'-1)J_s\bar{t}+J\bar{s}]^2+\Omega^2\}^{1/2}}\tanh\beta\{[B+(Z'-1)J_s\bar{t}+J\bar{s}]^2+\Omega^2\}^{1/2}\\ &+\{\cosh\beta[(B+Z'J_s\bar{t}+J)^2+\Omega^2]^{1/2}+\cosh\beta[(B+Z'J_s\bar{t}-J)^2+\Omega^2]^{1/2}\}^{-1}\\ &\times\left\{\frac{(B+Z'J_s\bar{t}+J)\sinh\beta[(B+Z'J_s\bar{t}+J)^2+\Omega^2]^{1/2}}{[(B+Z'J_s\bar{t}+J)^2+\Omega^2]^{1/2}}+\frac{(B+Z'J_s\bar{t}-J)\sinh\beta[(B+Z'J_s\bar{t}-J)^2+\Omega^2]^{1/2}}{[(B+Z'J_s\bar{t}-J)^2+\Omega^2]^{1/2}}\right\}\\ &+\frac{(Z'-1)J_s\Omega^2[B+(Z'-1)J_s\bar{t}+J\bar{s}]}{\{[B+(Z'-1)J_s\bar{t}+J\bar{s}]^2+\Omega^2\}^2}\tanh^2\beta\{[B+(Z'-1)J_s\bar{t}+J\bar{s}]^2+\Omega^2\}^{1/2}\\ &+\frac{(Z'-1)\beta J_s[B+(Z'-1)J_s\bar{t}+J\bar{s}]^3}{\{[B+(Z'-1)J_s\bar{t}+J\bar{s}]^2+\Omega^2\}^{3/2}}\tanh^2\beta\{[B+(Z'-1)J_s\bar{t}+J\bar{s}]^2+\Omega^2\}^{1/2}\\ &\times\mathrm{sech}^2\beta\{[B+(Z'-1)J_s\bar{t}+J\bar{s}]^2+\Omega^2\}^{1/2}=0 \ . \end{aligned} \qquad (11)$$

Surface magnetization M_s can be obtained by $M_s=-\partial F_s/\partial B$. For sufficiently large surface coupling J_s, both the surface spontaneous magnetization M_s and $\bar{t}$ tend to zero near T_c^s (and thus $\bar{s}=0$), so that $\bar{t}$ expresses the long-range order on the surface. We can only take the linear terms of $\bar{t}$ in Eq. (11) as the external field $B=0$. The resulting equation yields the surface critical temperature

$$\frac{\tanh K_c^s\eta}{\eta}(2Z'-1)=\frac{Z'\eta^2\tanh K_c^s(1+\eta^2)^{1/2}}{(1+\eta^2)^{3/2}}+\frac{(z'-1)^2(1+\Delta)\tanh^2K_c^s\eta}{\eta^2}+\frac{z'K_c^s}{1+\eta^2} \ , \qquad (12)$$

where $K_c^s=J/k_BT_c^s$, $\eta=\Omega/J$, $J_s=(1+\Delta)J$. If the surface critical temperature K_c^s equals the bulk critical temperature K_c,[1] the surface coupling approaches a critical value $J_{sc}=(1+\Delta_c)J$. As mentioned above, the bulk critical K_c depends on the bulk transverse field Γ, so that the transverse field Γ also has an effect on the surface critical coupling Δ_c. Figure 1 shows the phase diagram for some selected surface and bulk transverse fields. We denote, respectively, paramagnetic, surface ferromagnetic, and bulk ferromagnetic phases by the use of P, SF, and BF. It can be seen from Fig. 1 that reduced surface critical temperature T_c^s/T_c decreases with the decrease of the bulk transverse field, but increasing surface transverse field reduces the T_c^s/T_c.

Figure 2 shows that critical coupling Δ_c changes with surface transverse field. The surface and bulk transverse

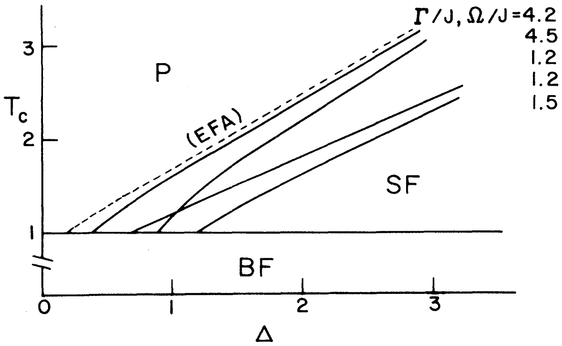

FIG. 1. Phase diagram for some selected bulk and surface transverse field. The dashed line indicates the result with $\Gamma=0$ of effective field approximation (EFA).

field has an opposite effect on Δ_c. The stronger the surface transverse field, the bigger the critical value Δ_c. Otherwise the bulk transverse field suffices.

The surface susceptibility and the specific heat are given by

$$\chi_s=\frac{\partial M_s}{\partial B}+\frac{\partial M_s}{\partial \bar{t}}\frac{\partial \bar{t}}{\partial B}+\frac{\partial M_s}{\partial \bar{s}}\frac{\partial \bar{s}}{\partial B} \tag{13}$$

and

$$C_s/k_B=-2\beta^2\frac{\partial F_s}{\partial \beta}-\beta^3\left[\frac{\partial^2 F_s}{\partial \beta^2}+\frac{\partial^2 F_s}{\partial \bar{t}\partial \beta}\frac{\partial \bar{t}}{\partial \beta}+\frac{\partial^2 F_s}{\partial \bar{s}\partial \beta}\frac{\partial \bar{s}}{\partial \beta}\right], \tag{14}$$

where the derivatives $\partial\bar{s}/\partial\beta$ and $\partial\bar{s}/\partial B$ can be determined as that in our earlier work[1] and

$$\frac{\partial \bar{t}}{\partial \beta}=-\left[\frac{\partial r}{\partial \beta}+\frac{\partial r}{\partial \bar{s}}\frac{\partial \bar{s}}{\partial \beta}\right]\Big/\frac{\partial r}{\partial \bar{t}},$$
$$\frac{\partial \bar{t}}{\partial B}=-\left[\frac{\partial r}{\partial B}+\frac{\partial r}{\partial \bar{s}}\frac{\partial \bar{s}}{\partial B}\right]\Big/\frac{\partial r}{\partial \bar{t}}. \tag{15}$$

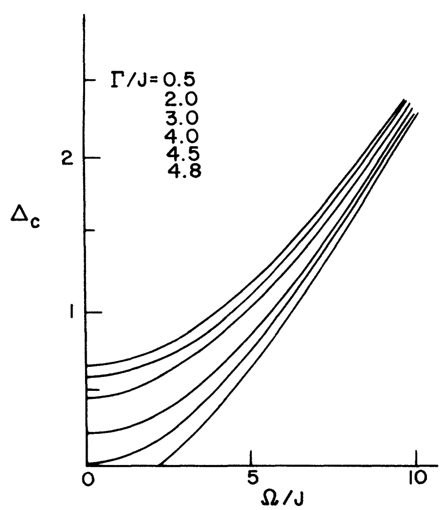

FIG. 2. Critical value Δ_c as a function of Ω/J for some selected Γ/J.

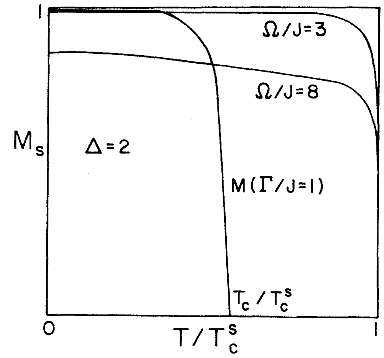

FIG. 3. Surface magnetization curves as a function of reduced temperature.

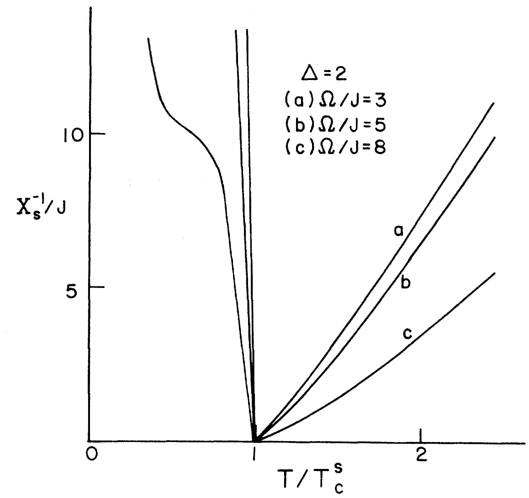

FIG. 4. Inverse surface susceptibility as a function of reduced temperature.

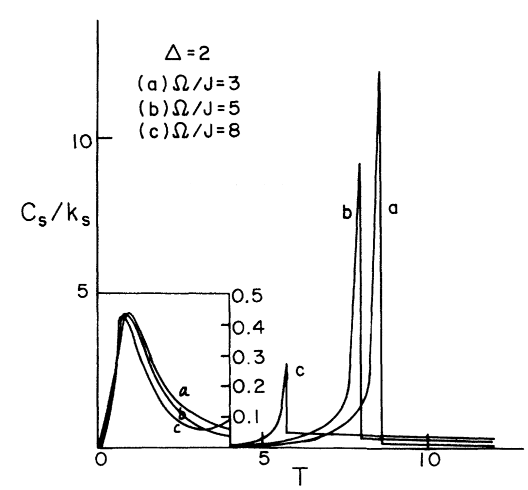

FIG. 5. Surface specific heat as a function of temperature.

The expression for all these thermodynamic properties are very tedious. Owing to the limitation of pages, we will not list them here. The temperature dependence of surface magnetization, susceptibility, and specific heat are shown in Figs. 3–5 respectively. It should be pointed out that the expression for the surface free energy F_s includes the bulk parameter $\bar{s}$, so the corresponding surface thermodynamic quantities are related to the bulk transverse field Γ. Our calculation shows that the influence of the bulk transverse field on the quantities is relatively small, and we only show the relation with the $\Gamma/J=1$ case. We find that the surface susceptibility diverges at the surface critical temperature T_c^s. For the large transverse field case ($\Omega/J=8$), the surface susceptibility exhibits anomaly at a temperature near the bulk critical point. The surface specific heat jumps at the surface critical temperature T_c^s. In the low-temperature range, due to the effect of bulk critical phenomena near T_c on the surface, the surface specific heat exhibits a weak peak, but an obvious jump does not exist.

Although TIM has been intensively studied by many authors, most work was limited to study the critical properties. Surface TIM is a quite complicated problem due to breaking of translational invariance. There are only few works related to the surface free energy, specific heat, and susceptibility near and above the critical temperature. In this paper, we use the DPIR's on the basis of two-spin cluster expansion; the surface thermodynamic quantities of a semi-infinite Ising ferromagnet with a surface transverse field are obtained in the whole temperature range.

ACKNOWLEDGMENTS

The project was supported by the National Natural Science Foundation of China.

---

*Corresponding address.

[1]Zhen-ya Li and Qing Jiang, Phys. Lett. A **138**, 247 (1989).
[2]V. K. Saxena, Phys. Rev. B **27**, 6884 (1983).
[3]R. M. Stratt, J. Chem. Phys. **80**, 5764 (1984); **84**, 2315 (1986).
[4]R. M. Stratt, Phys. Rev. B **33**, 1921 (1986).
[5]Song-tau Dai, Qing Jiang, and Zhen-ya Li, Phys. Rev. B **42**, 2597 (1990).
[6]T. Kaneyoshi, J. Phys. C **21**, 5259 (1988).
[7]E. F. Sarmento and T. Kaneyoshi, J. Phys. C **21**, 3993 (1988).