ЖУРНАЛ ФІЗИЧНИХ ДОСЛІДЖЕНЬ
т. 13, № 4 (2009) 4006(3 с.)

JOURNAL OF PHYSICAL STUDIES
v. 13, No. 4 (2009) 4006(3 p.)

SPECIFIC HEAT OF THE SQUARE-LATTICE ISING ANTIFERROMAGNET IN A MAGNETIC FIELD

Seung-Yeon Kim
School of Liberal Arts and Sciences, Chungju National University, Chungju 380–702, South Korea
(Received October 16, 2009)

The specific heat for the square-lattice Ising antiferromagnet in a uniform magnetic field B is obtained from its exact grand partition functions on $L \times L$ lattices ($L = 4 \sim 16$), in an arbitrary nonzero external field at arbitrary temperature. In the limit $L \to \infty$, the antiferromagnetic (Néel) critical points for $B \neq 0$ are estimated from the locations of the specific-heat peaks. For the first time, the thermal scaling exponents y_t of the square-lattice Ising antiferromagnet in a magnetic field are obtained to be $y_t(B \neq 0) = 1.0$ directly from its specific heat, at the Néel critical points even in a uniform magnetic field.

Key words: Ising antiferromagnet, uniform magnetic field, exact grand partition function, specific heat.

PACS number(s): 05.50.+q, 05.70.Jk, 64.60.Cn, 75.50.Ee

The Ising model with only the nearest-neighbor interaction J in a uniform external magnetic field B on a lattice with N_s spins and N_b bonds is defined by the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} (\sigma_i \sigma_j + 1) + B \sum_i (1 - \sigma_i), \qquad (1)$$

where the magnetic spin σ_i at the lattice site i takes $\sigma_i = \pm 1$ and $\langle i, j \rangle$ indicates the sum over all nearest-neighbor pairs of lattice sites. The two-dimensional Ising model is the simplest model showing phase transitions at finite temperatures.

Since the Onsager solution [1] of the square-lattice Ising model in the absence of an external magnetic field, the Ising model has played a central role in our understanding of phase transitions and critical phenomena. The square-lattice Ising model for $B = 0$ has the paramagnetic-ferromagnetic phase transition at the critical temperature (the so-called Curie temperature) $T_{\rm C} = 2J/k_{\rm B} \ln(\sqrt{2} + 1) = 2.26919(J/k_{\rm B})$ for the ferromagnetic interaction ($J > 0$) and the paramagnetic–antiferromagnetic transition at $T_{\rm N}$ (Néel temperature) $T_{\rm N} = 2J/k_{\rm B} \ln(\sqrt{2} - 1) = 2.26919(-J/k_{\rm B})$ for the antiferromagnetic interaction ($J < 0$). In the case of the square-lattice Ising model for $B = 0$, the logarithmic singularity of the specific heat $C(T)$ near the transition temperature T_t (Curie or Néel temperature) is expressed as

$$C(T) \sim -\ln|T - T_t| = \lim_{\alpha \to 0} \frac{|T - T_t|^{-\alpha} - 1}{\alpha} \qquad (2)$$

with the critical exponent $\alpha = 0$. Consequently, we have the thermal scaling exponent $y_t = 1/\nu = d/(2 - \alpha) = 1$ in two dimensions ($d = 2$).

However, the exact solution of the Ising model in an arbitrary nonzero external field at arbitrary temperature is not known even in two dimensions [2]. The introduction of a nonzero magnetic field ($B \neq 0$) destroys the phase transition of the ferromagnetic Ising model [3], whereas the nonzero uniform field does not destroy the transition of the antiferromagnetic Ising model [4–10]. Due to this fact, the properties of the antiferromagnetic Ising model in a uniform external magnetic field are much less well understood than those of the ferromagnetic model. For example, we do not know even the exact locations of Néel temperature $T_{\rm N}(B \neq 0)$, the most fundamental information on phase transition, of the the square-lattice Ising antiferromagnet in an external magnetic field. Instead, we have only the different *approximations* [11, 12] to the critical line (Néel temperature $T_{\rm N}(B)$ as a function of B) for the square-lattice Ising antiferromagnet in an external magnetic field.

We define the number of states, $\Omega(E, M)$, with a given exchange energy

$$E = \frac{1}{2} \sum_{\langle i,j \rangle} (\sigma_i \sigma_j + 1) \qquad (3)$$

and a given magnetization

$$M = \frac{1}{2} \sum_i (1 - \sigma_i), \qquad (4)$$

where E and M are non-negative integers $0 \leq E \leq N_b$ and $0 \leq M \leq N_s$. Introducing the number of states, the grand partition function of the Ising model

$$Z = \sum_{\{\sigma_n\}} e^{-\beta H} = \sum_{\{\sigma_n\}} e^{2\beta(JE - BM)}, \qquad (5)$$

the sum over 2^{N_s} possible spin configurations, can be written as the simple sum over E and M,

$$Z(a, x) = \sum_{E=0}^{N_b} \sum_{M=0}^{N_s} \Omega(E, M) a^E x^M, \qquad (6)$$

where $\beta = (k_{\rm B}T)^{-1}$, $a = e^{2\beta J}$, and $x = e^{-2\beta B}$. For antiferromagnetic interaction the physical interval is $0 \leq a \leq 1$ ($0 \leq T \leq \infty$), while for ferromagnetic interaction it is $1 \leq a \leq \infty$ ($\infty \geq T \geq 0$). The interval $0 < B < \infty$ ($-\infty < B < 0$) corresponds to $1 > x > 0$ ($\infty > x > 1$).

Because the Ising model has the symmetry $x \leftrightarrow 1/x$, we can consider only the interval $0 \le x \le 1$.

Given the number of states $\Omega(E, M)$, the grand partition function is a polynomial in a and x. The states with $E = 0$ (or $E = N_b$) correspond to the antiferromagnetic (or ferromagnetic) ground states. The value of magnetization $M = 0$ (or N_s) means that all spins have $\sigma = 1$ (or -1), corresponding to the ferromagnetic ground states.

From the *exact* integer values for the number of states $\Omega(E, M)$ of the Ising model on $L \times L$ square lattices (up to $L = 16$) [13], we construct the exact grand partition functions $Z(a, x)$ in an arbitrary nonzero uniform magnetic field at arbitrary temperature. For $L = 16$, the total number of states (i.e., the number of all possible spin configurations) is equal to $2^{16\times16} = 2^{256} \approx 1.158 \times 10^{77}$. Given the grand partition function, we obtain the exact specific heat

$$\begin{aligned} C(a, x) &= (N_s k_\mathrm{B} T^2)^{-1} \frac{\partial^2}{\partial \beta^2} \ln Z(a, x) \\ &= \frac{k_\mathrm{B}}{N_s} (\ln a)^2 (\langle E^2 \rangle - \langle E \rangle^2) \end{aligned} \quad (7)$$

as a function of a for a fixed value of x. In this paper, we estimate the critical points and the thermal scaling exponents for the square-lattice Ising antiferromagnet in nonzero uniform magnetic fields using its specific heat.

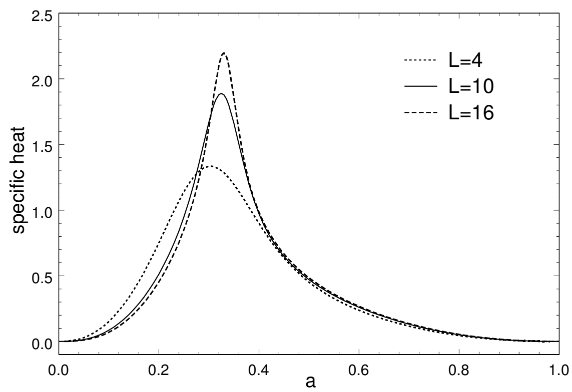

Fig. 1. The specific heat (in unit of k_B) of the Ising antiferromagnet on $L \times L$ square lattices, as a function of $a = e^{2\beta J}$, for $x = e^{-2\beta B} = 1/10$.

Figure 1 shows the exact specific heat of the Ising antiferromagnet on $L \times L$ square lattices ($L = 4$, 10, and 16) for $x = 1/10$, as a function of a. Here, the dimensionless variable a is used instead of real temperature T because the short finite interval $a = [0, 1]$ covers the whole temperature range $T = 2J/(k_\mathrm{B} \ln a) = [0, \infty]$ (in unit of $-J/k_\mathrm{B}$). As L increases, the specific heat becomes sharper and the height of the specific-heat peak increases. Also, the second column of Table 1 shows the locations $a(L)$ of the specific-heat peaks of the Ising antiferromagnet on $L \times L$ square lattices ($L = 4 \sim 16$) for $x = 1/10$. As the system size L increases, the values of the specific-heat peak locations $a(L)$ increase slowly. By using the Bulirsch–Stoer (BST) algorithm [14], we extrapolated our results for finite lattices to infinite size, and we obtained the extrapolated value of the Néel critical point, $a_\mathrm{N}(x = 1/10) = 0.33771(3)$, corresponding to the Néel temperature $T_\mathrm{N} = 1.8424(1)(-J/k_\mathrm{B})$ in a uniform magnetic field $B = 2.121(-J)$.

L	$a(L)$	$y_t(L)$
4	0.303071	1.074031
6	0.315300	1.077952
8	0.321275	1.067096
10	0.324758	1.056631
12	0.327027	1.048369
14	0.328621	1.041984
16	0.329802	

Table 1. The locations $a(L)$ of the specific-heat peaks of the Ising antiferromagnet on $L \times L$ square lattices for $x = 1/10$. Here, $y_t(L)$ denotes the thermal scaling exponents for finite lattices.

Assuming that the locations $a(x, L)$ of the specific-heat peaks scale like [15]

$$a(x, L) - a_\mathrm{N}(x) = \Delta a(x, L) \sim L^{-y_t(x)}, \quad (8)$$

we can define the thermal scaling exponent

$$y_t(L) = -\frac{\ln[\Delta a(L+2)/\Delta a(L)]}{\ln[(L+2)/L]} \quad (9)$$

for finite lattices [9]. The third column of Table 1 shows the values of $y_t(L)$ for $x = 1/10$. Here, as the value of $a_\mathrm{N}(x)$, our estimated value 0.33771(3) is used because the exact location of $a_\mathrm{N}(x)$ is not known for $x \neq 1$. The extrapolated value by BST algorithm is $y_t(x = 1/10) = 1.000(1)$. To test the validity of our approach, we evaluated the Néel critical point and the thermal scaling exponent for $B = 0$ ($x = 1$) where the exact values are known [1]. The estimated values are $a_\mathrm{N} = 0.41423(6)$ and $y_t = 1.01(1)$ in excellent agreement with the exact values $a_\mathrm{N} = \sqrt{2} - 1 = 0.414214$ and $y_t = 1$, clearly validating the approach.

x	$a_\mathrm{N}(x)$	$T_\mathrm{N}(x)$	$y_t(x)$
1	0.41423(6)	2.269(6)	1.01(1)
1/2	0.40584(2)	2.218(6)	1.00(2)
1/5	0.37286(8)	2.0273(2)	1.00(1)
1/10	0.33771(3)	1.8424(1)	1.000(1)
10^{-2}	0.21449(3)	1.2991(2)	1.00(5)
10^{-3}	0.12525(6)	0.9627(3)	1.00(3)
10^{-4}	0.07124(10)	0.7571(4)	1.00(13)
10^{-5}	0.04021(4)	0.6224(2)	1.010(6)

Table 2. The Néel critical points $a_\mathrm{N}(x)$, the Néel temperatures $T_\mathrm{N}(x)$ (in unit of $-J/k_\mathrm{B}$), and the thermal scaling exponents $y_t(x)$, in the limit $L \to \infty$, for the square-lattice Ising antiferromagnet, estimated from the specific-heat data on finite lattices $L = 4 \sim 16$ (even sizes only).

x	Wu-Wu	Wang-Kim
1/2	0.40581	0.40578
1/5	0.37283	0.37280
1/10	0.33768	0.33802
10^{-2}	0.21440	0.21625
10^{-3}	0.12516	0.12677
10^{-4}	0.07125	0.07215
10^{-5}	0.04022	0.04068

Table 3. The results of the closed-form approximations, Wu–Wu approximation [11] and Wang–Kim approximation [12], for the antiferromagnetic critical line $a_{\mathrm{N}}(x)$.

Table 2 shows the Néel critical points $a_{\mathrm{N}}(x)$ (equivalently, the Néel temperatures $T_{\mathrm{N}}(x)$) and the thermal scaling exponents $y_t(x)$, in the limit $L \to \infty$, of the square-lattice Ising antiferromagnet for various values of x, estimated from the specific-heat data. The estimated values for $y_t(x)$ imply that the exact value of the thermal scaling exponent is $y_t(x) = 1$ (equivalently, $\alpha(x) = 0$) for the square-lattice Ising antiferromagnet in a nonzero uniform magnetic field ($B \neq 0$). Therefore, we may assume that its specific heat retains the logarithmic singularity at the Néel critical points, based on the fact that the specific heat for the two-dimensional super-exchange Ising antiferromagnet diverges logarithmically in a magnetic field [4,5]. Also, we compare our results for the Néel critical points with the closed-form approximations [11,12], as shown in Table 3. Our results agree well with those of the closed-form approximations. Especially, the results of Wu–Wu approximation [11] are closer to ours.

In conclusion, the specific heat for the Ising antiferromagnet in a uniform external magnetic field hase been investigated using its exact grand partition functions on $L \times L$ square lattices ($L = 4 \sim 16$). The Néel critical points for $B \neq 0$ have been estimated from the locations of the specific-heat peaks and compared with the closed-form approximations, preferring Wu–Wu approximation. The thermal scaling exponents $y_t(x \neq 1) = 1.0$ of the square-lattice Ising antiferromagnet in a magnetic field have been obtained directly from its specific heat for the first time. It is also possible to calculate the magnetic scaling exponent (y_h) using the specific heat. For example, for $a = 1/5$, the estimated value of the magnetic exponent is $y_h = 1.04(9)$, in excellent agreement with the result obtained from Yang–Lee zeros [7].

[1] L. Onsager, Phys. Rev. **65**, 117 (1944).
[2] F. Mancini, Phase transitions in Ising chains, Plenary lecture at *The Third Conference of Statistical Physics*, Lviv, Ukraine, June 23, 2009.
[3] T. D. Lee and C. N. Yang, Phys. Rev. **87**, 410 (1952).
[4] M. E. Fisher, Proc. R. Soc. London A **254**, 66 (1960); *ibid.* **256**, 502 (1960).
[5] W. T. Lu, F. Y. Wu, Phys. Rev. E **71**, 046120 (2005).
[6] M. Kaufman, Phys. Rev. B **36**, 3697 (1987).
[7] S.-Y. Kim, Phys. Rev. Lett. **93**, 130604 (2004).
[8] S.-Y. Kim, Phys. Rev. E **71**, 017102 (2005).
[9] S.-Y. Kim, Phys. Lett. A **358**, 245 (2006).
[10] S.-Y. Kim, C.-O. Hwang, J. M. Kim, Nucl. Phys. B **805**, 441 (2008).
[11] X. N. Wu, F. Y. Wu, Phys. Lett. A **144**, 123 (1990).
[12] X.-Z. Wang, J. S. Kim, Phys. Rev. Lett. **78**, 413 (1997); J. L. Monroe, Phys. Rev. E **64**, 016126 (2001).
[13] S.-Y. Kim, Phys. Rev. E **74**, 011119 (2006).
[14] W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery, *Numerical Recipes in Fortran 77*, 2nd edition (Cambridge University Press, Cambridge, 1992), p. 104.
[15] J. L. Cardy, *Finite-Size Scaling* (Elsevier Science Publishers, Amsterdam, 1988).

ПИТОМА ТЕПЛОЄМНІСТЬ ІЗИНҐІВСЬКОГО АНТИФЕРОМАГНЕТИКА НА КВАДРАТНІЙ ҐРАТЦІ В МАГНІТНОМУ ПОЛІ

Сьонґ-Йон Кім
Школа вільних мистецтв та наук, Національний університет Чунгджу,
Чунгджу, 380–702, Південна Корея

Розраховано питому теплоємність ізинґівського антиферомагнетика на квадратній ґратці в однорідному магнітному полі B з використанням точної великої канонічної суми для гратки $L \times L$ ($L = 4 \sim 16$) у довільному ненульовому зовнішньому полі при довільній температурі. У границі $L \to \infty$ зроблено оцінку антиферомагнітних (Нееля) критичних точок для $B \neq 0$, виходячи з розташування піків питомої теплоємності. Уперше безпосередньо з питомої теплоємності отримано, що тепловий масштабний показник ізинґівського антиферомагнетика на квадратній ґратці в магнітному полі $y_t(B \neq 0) = -1.0$ в критичних точках Нееля в однорідному магнітному полі.