Bounded and inhomogeneous Ising models. IV. Specific-heat amplitude for regular defects

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The amplitude, $\dot{A}(x,\tau)$, of the logarithmic specific-heat singularity of a square Ising lattice with bond defects regularly spaced on an $m\times n$ grid (with $x=1/mn$ and $\tau=n/m$) is calculated asymptotically with the result $\dot{A}(x,\tau)=A_0-A_1x\ln x^{-1}-|A_2(\tau)x-A_3x^2\ln^2x+O(x^2\ln x)$, as $x\to 0$. The coefficient A_1 verifies the scaling prediction $A_1=C_1$, where C_1 is the amplitude of the $(\ln|t|)^2$ term in the incremental specific heat due to a single, isolated defect.

I. INTRODUCTION

In the accompanying paper (part III of this series)[1] we have shown that the specific heat $C(T,x,\tau)$ of a plane square Ising lattice with various point defects regularly distributed on an $m\times n$ grid is logarithmically divergent, namely,

$$C(T,x;\tau)/k_B\approx -\dot{A}(x)\ln|T_c(x,\tau)-T| \quad \text{as } T\to T_c(x,\tau), \quad (1.1)$$

where $x=1/nm$ is the impurity concentration and $\tau=n/m$ specifies the "shape" of the defect distribution. The shifted critical temperature $T_c(x,\tau)$ was investigated in III and its behavior as $x\to 0$ related to a scaling theory. In this paper, we calculate the amplitude $\dot{A}(x,\tau)$ of the logarithmic singularity for the cases of modified single-bond defects and bent-missing-double-bond defects. [The nature of these defects is illustrated in Figs. 2(b) and 2(c) of III.] We find that the amplitude has the form

$$\dot{A}(x,\tau)=A_0-A_1x\ln x^{-1}-A_2(\tau)x - A_3x^2\ln^2x+O(x^2\ln x), \quad (1.2)$$

in which A_0 is the amplitude of the logarithmic specific-heat singularity for the pure Ising lattice while A_1 satisfies the scaling relation[2]

$$A_1=C_1, \quad (1.3)$$

where C_1 is the amplitude of the $(\ln|t|)^2$ term in the incremental specific heat due to an isolated defect. [As usual $t\sim T-T_c^0$ measures the deviation from $T_c^0=T_c(0,\tau)$.] Note that the coefficients A_1 and A_3 are independent of the distribution ratio τ.

II. AMPLITUDE FOR SINGLE-BOND DEFECTS (*b*)

It is shown in Sec. IV of III that the free energy of a system with a regular array of modified single-bond defects (*b*) is

$$f^b(T)=f_0(T)+(nm)^{-1}\left[\ln\left(\frac{\cosh K_1'}{\cosh K_1}\right)-\ln|z_1'-z_1|\right] +\frac{1}{2mn}\int_0^{2\pi}\frac{d\theta_1}{2\pi}\int_0^{2\pi}\frac{d\theta_2}{2\pi}\ln D_b(\theta_1,\theta_2), \quad (2.1)$$

where $f_0(T)$ is the free energy of the perfect Ising lattice while $D_b(\theta_1,\theta_2)$ is the 2×2 determinant

$$D_b(\theta_1,\theta_2)=|\mathrm{y}_b+\mathrm{G}_b| =\begin{vmatrix}[0,0]_{RR} & [0,1]_{RL}-(z_1'-z_1)^{-1}\\ [0,-1]_{LR}+(z_1'-z_1)^{-1} & [0,0]_{LL}\end{vmatrix}, \quad (2.2)$$

whose elements $[l,k]_{\lambda\mu}$ are double sums depending on θ_1 and θ_2 which are defined in Eq. (2.23) of III. It is convenient to define the prototype sums

$$R_{p,q}(\theta_1,\theta_2)=\frac{1}{nm}\sum_{\phi_1}\sum_{\phi_2}\frac{e^{-ip\phi_1-iq\phi_2}}{\Delta(\phi_1,\phi_2)}, \quad (2.3)$$

in which, retaining the notation defined in detail in III,

$$\Delta(\phi_1,\phi_2)=a-2b\cos\phi_1-2c\cos\phi_2, \quad (2.4)$$

$$a=(1+z_1^2)(1+z_2^2),\quad b=z_1(1-z_2^2),\quad c=z_2(1-z_1^2) \quad (2.5)$$

while the sums run over the mn distinct values

$$\phi_1=(\theta_1+2\pi l)/m,\quad l=1,\ldots,m;$$
$$\phi_2=(\theta_2+2\pi k)/n,\quad k=1,\ldots,n. \quad (2.6)$$

The matrix elements $[l,k]_{\lambda\mu}$ can then be expressed in terms of the $R_{p,q}$; in particular, we find

$$[0,0]_{RR}=-[0,0]_{LL}=z_2(R_{0,-1}-R_{0,1}), \quad (2.7)$$

$$[0,1]_{RL}=W(\theta_1,\theta_2)-\tfrac{1}{2}(1-z_2^2)(R_{-1,0}-R_{1,0}), \quad (2.8)$$

and

$$[0,-1]_{LR}=-W(\theta_1,\theta_2)-\tfrac{1}{2}(1-z_2^2)(R_{-1,0}-R_{1,0}), \quad (2.9)$$

where

$$W(\theta_1,\theta_2)=\tfrac{1}{2}(1-z_2^2)(R_{1,0}+R_{-1,0})-z_1(1+z_2^2)R_{0,0}-z_1z_2(R_{0,1}+R_{0,-1}). \tag{2.10}$$

From the definition (2.3) of $R_{p,q}$, we find that $R_{\pm p,\pm q}(0,0)=S_{pq}$, where S_{pq} was analyzed in detail in III. Thus on using III(4.4), we obtain the relation

$$W(0,0)=[0,1]^0_{RL}. \tag{2.11}$$

To extract the leading logarithmic singularity from (2.1) it is essential to evaluate the determinant $D_b(\theta_1,\theta_2)$ correct to quadratic orders in θ_1 and θ_2 before integrating. It is now clear from (2.3) that $W(\theta_1,\theta_2)$ is an even function of θ_1 and θ_2, and so we have

$$\Delta W(\theta_1,\theta_2)\equiv W(\theta_1,\theta_2)-W(0,0)\propto\theta_1^2,\ \theta_2^2. \tag{2.12}$$

Likewise, $R_{-1,0}-R_{1,0}$ is even in θ_2 but odd in θ_1, and so we may write

$$(R_{-1,0}-R_{1,0})/2i=\theta_1U_{10}+O(\theta_1^2,\theta_2^2), \tag{2.13}$$

in which U_{10} is the first derivative of $R_{-1,0}-R_{1,0}$ with respect to θ_1. Similarly we may write

$$(R_{0,-1}-R_{0,1})/2i=\theta_2U_{01}+O(\theta_1^2,\theta_2^2). \tag{2.14}$$

The derivatives U_{10} and U_{01} will be evaluated below.

Now we can write the 2×2 determinant of (2.2) as

$$\begin{aligned}D_b(\theta_1,\theta_2)&=\{[0,1]^0_{RL}-(z_1'-z_1)^{-1}\}^2+2\Delta W\{[0,1]^0_{RL}-(z_1'-z_1)^{-1}\}+\Delta W^2-z_2^2(R_{0,-1}-R_{0,1})^2-\tfrac{1}{4}(1-z_2^2)^2(R_{-1,0}-R_{1,0})^2\\&=(T-T_0^b)^2+4z_2^2U_{01}^2\theta_2^2+(1-z_2^2)^2U_{10}^2\theta_1^2+O[\theta_1^4,(T-T_0^b)\theta_1^2],\end{aligned} \tag{2.15}$$

where we have put

$$[0,1]^0_{RL}-(z_1'-z_1)^{-1}=T-T_0^b, \tag{2.16}$$

which will be seen to measure the deviation from the shifted critical point. On substituting this expression into (2.1), we find the leading singular term of the free energy to be given by

$$\begin{aligned}f_{\rm sing}(T)&\approx\frac{1}{2mn}\int_0^\pi\frac{d\theta_1}{\pi}\int_0^\pi\frac{d\theta_2}{\pi}\ln|(T-T_0^b)^2+(1-z_2^2)^2U_{10}^2\theta_1^2+4z_2^2U_{01}^2\theta_2^2|\\&\approx-[8\pi z_2(1-z_2^2)U_{01}U_{10}mn]^{-1}(T-T_0^b)^2\ln|T-T_0^b|+\dots.\end{aligned} \tag{2.17}$$

This completes the first step of the argument since the specific heat of the system with single-bond defects can now be seen to diverge as

$$C(T,x,\tau)/k_B\approx-\dot{A}^b(x,\tau)\ln|T-T_0^b|,\quad \text{as } T-T_0^b\to0, \tag{2.18}$$

where the amplitude is given explicitly by

$$\dot{A}^b(x,\tau)=\beta_c^2\left(\frac{\partial t}{\partial\beta}\right)_c^2\left\{\left(\frac{\partial(T-T_0^b)}{\partial t}\right)^2\Big/4\pi z_2(1-z_2^2)U_{10}U_{01}mn\right\}_{T=T_0^b}, \tag{2.19}$$

in which $\beta=1/k_BT$.

The derivative U_{01} of $R_{0,-1}-R_{0,1}$ with respect to θ_2, evaluated at the origin, is easily found to be

$$U_{01}=n^{-1}(nm)^{-1}\sum_{l=1}^{m}\sum_{k=1}^{n}\left[\cos\left(\frac{2\pi k}{n}\right)\Delta^{-1}\left(\frac{2\pi l}{m},\frac{2\pi k}{n}\right)-2c\sin^2\left(\frac{2\pi k}{n}\right)\Delta^{-2}\left(\frac{2\pi l}{m},\frac{2\pi k}{n}\right)\right]. \tag{2.20}$$

It is shown in Appendix A that in the limit $t=(T-T_c^0)/T_c^0$ approaches zero while $n,m\to\infty$ with n/m fixed, this double sum reduces to

$$nU_{01}=\left[\frac{1}{mnt^2}-\frac{1}{\pi(bc)^{1/2}}\frac{\overline{n}}{\overline{m}}G\left(\frac{\overline{n}}{\overline{m}}\right)+O(t^2m^2)\right], \tag{2.21}$$

where $\overline{n}$ and $\overline{m}$ are defined in (3.43) of III, while

$$G(\tau)=\frac{\pi}{12}-\sum_{l=1}^{\infty}\frac{2\pi l}{e^{2\pi l\tau}-1}. \tag{2.22}$$

Likewise we find

$$mU_{10}\approx\left[\frac{1}{mnt^2}-\frac{1}{\pi(bc)^{1/2}}\frac{\overline{m}}{\overline{n}}G\left(\frac{\overline{m}}{\overline{n}}\right)+O(t^2m^2)\right]. \tag{2.23}$$

The result (2.16) together with (4.10) of III yields

$$T-T_0^b=\frac{1+z_{2c}}{tmn}+B_c+\frac{1}{nm}\left[E_3+\left(\frac{dz_2}{dt}\right)_c\right]+t(1+z_{2c})\tilde{A}_c[\tfrac{1}{2}\ln(mn)+P_0(\tau)]+tB_c'+O(t^2\ln m). \tag{2.24}$$

Now the reduced shift in critical temperature t_c

is evidently determined by the equation $T - T_0^b = 0$ and it has the form[1]

$$t_c = -u_b(nm)^{-1} \times\{1 + v_b \ln(nm)/nm + w_b/nm + O(n^{-2}m^{-2}\ln^2 n)\}, \quad (2.25)$$

in which the amplitudes were found in III to be

$$u_b = \frac{1+z_{2c}}{B_c} = \frac{r_1 C_0^b}{A_0}, \quad v_b = \tfrac{1}{2}u_b^2 \tilde{A}_c = \frac{\tfrac{1}{2}(C_0^b)^2}{A_0}, \quad (2.26)$$

$$w_b(\tau) = -\left[\left(\frac{dz_2}{dt}\right)_c + E_3\right]\Big/ B_c + [\tilde{A}_c(1+z_{2c})^2 P_0(\tau) + B_c'(1+z_{2c})]/B_c^2, \quad (2.27)$$

where $r_1 = -\beta_c(\partial t/\partial\beta)_c$ and $A_0 = r_1^2\tilde{A}_c$ is the bulk specific-heat amplitude for the pure Ising lattice, while C_0^b is the amplitude of the incremental specific heat due to an isolated single-bond defect. On differentiating $T - T_0^b$ of (2.24) with respect to t, we find

$$\left(\frac{d}{dt}(T - T_0^b)\right)^2_{T=T_0^b} = \frac{(1+z_{2c})^2}{t_c^4 m^2 n^2} \times\left(1 - 2(t_c^2 mn)\left[\tfrac{1}{2}\tilde{A}_c \ln(nm) + \tilde{A}_c P_0(\tau) + \frac{B_c'}{1+z_{2c}}\right] + \tfrac{1}{4}\tilde{A}_c^2 (t^2 mn)^2 \ln^2(nm) + O(t^2 \ln m)\right). \quad (2.28)$$

From (2.21) and (2.23), one gets

$$nmU_{10}U_{01} = \frac{1}{t_c^4 m^2 n^2}\left\{1 - 2t_c^2 mn\tilde{A}_c\left[\frac{\overline{n}}{\overline{m}}G\left(\frac{\overline{n}}{\overline{m}}\right) + \frac{\overline{m}}{\overline{n}}G\left(\frac{\overline{m}}{\overline{n}}\right)\right] + O(m^{-2}n^{-2})\right\}, \quad (2.29)$$

where we have used the relation $\tilde{A}(t) = 1/2\pi(bc)^{1/2}$. The identity for $G(\tau)$ presented in III(3.51) then yields

$$nmU_{10}U_{01} = \frac{1}{t_c^4 m^2 n^2}\{1 - t_c^2 mn\tilde{A}_c + O(m^{-2}n^{-2})\}. \quad (2.30)$$

Next we make the expansion

$$z_2^{-1}(1 - z_2^2)^{-1} = z_{2c}^{-1}(1 - z_{2c}^2)^{-1} - t_c\left(\frac{dz_2}{dt}\right)_c (1 - 3z_{2c}^2)z_{2c}^{-2}(1 - z_{2c}^2)^{-2} + O(t_c^2). \quad (2.31)$$

On substituting (2.28), (2.30), and (2.31) into (2.19), and then using (2.25) for t_c, we finally see that the specific-heat amplitude is

$$\mathring{A}^b(x,\tau) = A_0 - A_1^b x \ln x^{-1} - A_2^b(\tau)x - A_3^b x^2 \ln^2 x + O(x^2 \ln x), \quad (2.32)$$

with $x = 1/nm$, where

$$A_0 = r_1^2/2\pi(bc)_c^{1/2} = r_1^2(1+z_{2c})/4\pi(1-z_{2c})z_{2c} \quad (2.33)$$

is the amplitude of the logarithmic specific-heat singularity of the pure Ising lattice, while

$$A_1^b = 2A_0 v_b, \quad A_3^b = 3A_0 v_b^2,$$
$$A_2^b(\tau) = 2C_1^b P_0(\tau) - 2C_1^b + 2u_b^2 A_0 B_c'(1+z_{2c})^{-1} - u_b A_0(1 - 3z_{3c}^2)z_{2c}^{-1}(1 - z_{2c}^2)^{-1}\left(\frac{dz_2}{dt}\right)_c. \quad (2.34)$$

On using III(4.8) and III(3.68) we find that

$$A_1^b = (C_0^b)^2 = C_1^b \quad \text{and} \quad A_3^b = \tfrac{3}{4}(C_1^b)^2/A_0. \quad (2.35)$$

The first of these relations checks the general scaling relation $A_1 = C_1$ derived earlier.[2]

III. AMPLITUDE FOR BENT-BOND DEFECTS (c)

The free energy of a system with missing, bent-bond defects has the singular term

$$f^c(T) \approx \frac{1}{2mn}\int_0^\pi \frac{d\theta_1}{\pi}\int_0^\pi \frac{d\theta_2}{\pi}\ln D_c(\theta_1,\theta_2), \quad (3.1)$$

where $D_c(\theta_1,\theta_2)$ is the 2×2 determinant

$$D_c(\theta_1,\theta_2) = |\mathrm{y}_c + \mathrm{G}_c| = [0,0]_{UU}[0,0]_{LL} - [0,0]_{UL}[0,0]_{LU}. \quad (3.2)$$

The elements $[0,0]_{\lambda\mu}$ can again be expressed in terms of the double sums $R_{p,q}$ of (2.3) as

$$[0,0]_{UU} = -z_1(R_{-1,0} - R_{1,0}), \quad (3.3)$$

$$[0,0]_{UL} = \overline{W}(\theta_1,\theta_2) - \tfrac{1}{2}z_1(R_{-1,0} - R_{1,0}) - \tfrac{1}{2}z_2(R_{0,-1} - R_{0,1}) - \tfrac{1}{2}z_1 z_2(R_{-1,-1} - R_{1,1}), \quad (3.4)$$

$$[0,0]_{LU} = -\overline{W}(\theta_1,\theta_2) - \tfrac{1}{2}z_1(R_{-1,0} - R_{1,0}) - \tfrac{1}{2}z_2(R_{0,-1} - R_{0,1}) - \tfrac{1}{2}z_1 z_2(R_{-1,-1} - R_{1,1}), \quad (3.5)$$

where

$$\overline{W}(\theta_1, \theta_2) = R_{0,0} - \tfrac{1}{2}z_1(R_{-1,0} + R_{1,0}) - \tfrac{1}{2}z_2(R_{0,-1} + R_{0,1}) - \tfrac{1}{2}z_1z_2(R_{-1,-1} + R_{1,1}), \tag{3.6}$$

while $[0, 0]_{LL}$ is given by (2.7). It is easy to verify the relations

$$\frac{\partial}{\partial \theta_1}\overline{W}(\theta_1, \theta_2)\bigg|_{\theta_1=\theta_2=0} = \frac{\partial}{\partial \theta_2}\overline{W}(\theta_1, \theta_2)\bigg|_{\theta_1=\theta_2=0} = 0, \tag{3.7}$$

$$\overline{W}(0, 0) = [0, 0]^0_{UL} = (T - T^c_0). \tag{3.8}$$

Hence we may write

$$\overline{W}(\theta_1, \theta_2) = (T - T^c_0) + O(\theta_1^2, \theta_2^2, \theta_1\theta_2). \tag{3.9}$$

In Appendix A we show that

$$(R_{-1,-1} - R_{1,1})/2i = \theta_1 U_{10} + \theta_2 U_{01} + O(\theta_1^2, \theta_2^2), \tag{3.10}$$

with U_{10} and U_{01} given by (2.23) and (2.21). Consequently, we may write

$$\begin{aligned} D_c(\theta_1, \theta_2) &= +z_1z_2(R_{0,-1} - R_{0,1})(R_{-1,0} - R_{1,0}) + \overline{W}(\theta_1, \theta_2)^2 \\ &\quad - [\tfrac{1}{2}z_1(R_{-1,0} - R_{1,0}) + \tfrac{1}{2}z_2(R_{0,-1} - R_{0,1}) + \tfrac{1}{2}z_1z_2(R_{-1,-1} - R_{1,1})]^2 \\ &= (T - T^c_0)^2 - 4z_1z_2U_{01}U_{10}\theta_1\theta_2 + [z_1(1+z_2)U_{10}\theta_1 + z_2(1+z_1)U_{01}\theta_2]^2 + O[(T - T^c_0)\theta_1^2, \theta_1^4]. \end{aligned} \tag{3.11}$$

On diagonalizing the quadratic terms in θ_1 and θ_2 and integrating, the singular term of the free energy (3.1) becomes

$$f^c_{\text{sing}}(T) \approx -[8\pi z_1z_2(z_1 + z_2 + z_1z_2)^{1/2}U_{01}U_{10}mn]^{-1}(T - T^c_0)^2 \ln|T - T^c_0|, \tag{3.12}$$

and so the specific heat diverges logarithmically as

$$C^c(T, x, \tau) = -\dot{A}^c(x, \tau) \ln|T - T^c_0|, \tag{3.13}$$

with the amplitude

$$\dot{A}^c(x, \tau) = r_1^2 \left\{ \left(\frac{d(T - T^c_0)}{dt}\right)^2 \Big/ 4\pi z_1z_2(z_1 + z_2 + z_1z_2)^{1/2}U_{01}U_{10}mn \right\}_{T=T^c_0}. \tag{3.14}$$

From (3.9), III(4.34), and III(4.35), we deduce

$$\left(\frac{d(T - T^c_0)}{dt}\right)^2_{T=T^c_0} = \frac{1}{t^4m^2n^2}\{1 - 2(t_c^2mn)[\tfrac{1}{2}\tilde{A}_c \ln(nm) + \tilde{A}_cP_0(\tau) + \overline{B}'_c] + \tfrac{1}{4}(t_c^2mn)^2\tilde{A}_c^2 \ln^2(mn)\}, \tag{3.15}$$

where t_c is determined by the equation $T - T^c_0 = 0$. This yields the form

$$t_c = -u_c(nm)[1 + v_c \ln(nm)/nm + w_c/nm + O(n^{-2}m^{-2}\ln nm)], \tag{3.16}$$

with the amplitudes given by

$$u_c = 1/\overline{B}_c, \quad v_c = \tfrac{1}{2}u_c^2\tilde{A}_c, \tag{3.17}$$

$$w_c(\tau) = \frac{-E_4(\tau)}{\overline{B}_c} + \frac{\overline{B}'_c}{\overline{B}_c^2} + \frac{\tilde{A}_cP_0(\tau)}{\overline{B}_c^2}. \tag{3.18}$$

Finally, we make the expansion

$$z_1^{-1}z_2^{-1}(z_1 + z_2 + z_1z_2)^{-1/2} \approx z_{1c}^{-1}z_{2c}^{-1}\left\{1 - \tfrac{1}{2}t\left[\left(\frac{dz_1}{dt}\right)_c(3 - z_{2c})z_{1c}^{-1} + \left(\frac{dz_2}{dt}\right)_c(3 - z_{1c})z_{2c}^{-1}\right]\right\}. \tag{3.19}$$

These relations together with (2.30) imply the final result

$$\dot{A}^c(x, \tau) = A_0 - A^c_1x \ln x^{-1} - A^c_2(\tau)x - A^c_3x^2 \ln^2 x + O(x^2 \ln x), \tag{3.20}$$

where

$$A_0 = r_1^2\tilde{A}_c = r_1^2/4\pi z_{1c}z_{2c}, \tag{3.21}$$

$$A^c_1 = 2A_0v_c, \quad A^c_3 = 3A_0v_c^2, \tag{3.22}$$

$$\begin{aligned} A^c_2(\tau) &= 2C^c_1P_0(\tau) - 2C^c_1 + 2u_c^2A_0\overline{B}'_c \\ &\quad - \tfrac{1}{2}u_cA_0\left[\left(\frac{dz_1}{dt}\right)_c(3 - z_{2c})z_{1c}^{-1} + \left(\frac{dz_2}{dt}\right)_c(3 - z_{1c})z_{2c}^{-1}\right]. \end{aligned} \tag{3.23}$$

Again, it is trivial to check the scaling relation $A^c_1 = C^c_1$ by utilizing (4.33) of III. We may note that the simple form of the coefficient $A_3 = \frac{3}{4}(C_1)^2/A_0$, found also for single-bond defects, has not been interpreted.

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APPENDIX A: DOUBLE SUMS

We shall first calculate exactly the sum

$$I=n^{-1}\sum_{l=1}^{n} r\left(\frac{2\pi l}{n}\right), \tag{A1}$$

whose summand is

$$r(\theta)=\cos\theta(x-y\cos\theta)^{-1} - y\sin^2\theta(x-y\cos\theta)^{-2}. \tag{A2}$$

In Appendix B of III we found

$$n^{-1}\sum_{l=1}^{n}\left[x-y\cos\left(\frac{2\pi l}{n}\right)\right]^{-1}=X^{-1}\left(1+\frac{2}{Y}\right), \tag{A3}$$

where

$$X=x^2-y^2,$$
$$Y=\left[\frac{x}{y}+\left(\frac{x^2}{y^2}-1\right)^{1/2}\right]^n-1. \tag{A4}$$

By differentiating both sides of equation (A3) with respect to x, we find

$$n^{-1}\sum_{l=1}^{n}\left[x-y\cos\left(\frac{2\pi l}{n}\right)\right]^{-2} = xX^{-3}\left(1+\frac{2}{Y}\right)+2nX^{-2}(Y^{-1}+Y^{-2}). \tag{A5}$$

It is easy to verify the relation

$$r\left(\frac{2\pi l}{n}\right)=\frac{-x}{y}\left[x-y\cos\left(\frac{2\pi l}{n}\right)\right]^{-1} +\frac{X^2}{y}\left[x-y\cos\left(\frac{2\pi l}{n}\right)\right]^{-2}. \tag{A6}$$

Now, on using (A3) and (A5), the sum is found to be

$$I=\frac{(2n/y)(Y+1)}{Y^2}. \tag{A7}$$

Hence the double sum U_{01} of (2.20) becomes

$$nU_{01}=\left(\frac{n}{c}\right)m^{-1}\sum_{l=1}^{m}\frac{Y(2\pi l/m)+1}{Y^2(2\pi l/m)}, \tag{A8}$$

where $Y(\theta)$ is defined by III(B8). The approximations III(B45) and III(B47) for the function $Y(\theta)$ when $2\pi l_c/m \leq \theta \leq \pi$ and $0 \leq \theta \leq 2\pi l_c/m$ (with $l_c \ll m$), respectively, yield the result

$$nU_{01}=\frac{n}{mc}\left(\tfrac{1}{4}\operatorname{csch}^2(\tfrac{1}{2}\bar{n}\,|t|)+\frac{1}{2}\sum_{l=1}^{\infty}\operatorname{csch}^2\left[\frac{\bar{n}(t^2\bar{m}^2+4\pi^2l^2)^{1/2}}{2\bar{m}}\right]+O(m^{-4}, e^{-\theta l_c})\right) \tag{A9}$$

where

$$\bar{n}=n/c^{1/2}, \quad \bar{m}=m/b^{1/2}. \tag{A10}$$

On expanding the first term in powers of $\bar{n}|t|$ and the second term in powers of $\bar{m}|t|$, we find

$$nU_{01}\approx\frac{n}{mc}\left((\bar{n}\,|t|)^{-2}-\tfrac{1}{12}+\frac{1}{2}\sum_{l=1}^{\infty}\operatorname{csch}^2\left[\frac{\bar{n}\pi l}{\bar{m}}\right]+O(\bar{n}^2t^2,\bar{m}^2t^2)\right). \tag{A11}$$

Since[3]

$$\tfrac{1}{4}\operatorname{csch}^2(\pi l\tau)=\frac{\partial}{\partial\tau}\left[\frac{1}{2\pi l(e^{2\pi l\tau}-1)}\right], \tag{A12}$$

the results (B62) and (B74) of III give

$$\frac{1}{4}\sum_{l=1}^{\infty}\operatorname{csch}^2\left(\frac{\pi l}{\tau}\right)=\frac{-G(\tau)}{2\pi}+\frac{1}{24}. \tag{A13}$$

Therefore (A11) becomes

$$nU_{01}\approx(nmt^2)^{-1}-\frac{(\bar{n}/\bar{m})G(\bar{n}/\bar{m})}{\pi(bc)^{1/2}}+O(m^2t^2). \tag{A14}$$

By interchanging m and n, b and c, we obtain

$$mU_{10}\approx(nmt^2)^{-1}-\frac{(\bar{m}/\bar{n})G(\bar{m}/\bar{n})}{\pi(bc)^{1/2}}+O(t^2m^2). \tag{A15}$$

Finally, from (2.3) we find

$$\frac{(R_{-1,-1}-R_{1,1})}{2i}=(nm)^{-1}\sum_{\phi 1}\sum_{\phi 2}(\sin\phi_1\cos\phi_2+\cos\phi_1\sin\phi_2)\,\Delta^{-1}(\phi_1,\phi_2)=V_{10}\theta_1+V_{01}\theta_2+O(\theta_1^2,\theta_2^2)\,, \tag{A16}$$

where the derivatives V_{10} and V_{01} can be easily found; in particular,

$$-V_{01}+U_{01}=n^{-1}(nm)^{-1}\sum_{l=1}^{m}\sum_{k=1}^{n}2\sin^2\left(\frac{\pi l}{m}\right)\left\{\cos\left(\frac{2\pi k}{n}\right)-2c\sin^2\left(\frac{2\pi k}{n}\right)\right\}\times\Delta^{-1}\left(\frac{2\pi l}{m},\frac{2\pi k}{n}\right). \tag{A17}$$

On using (A4), we have

$$-(V_{01}-U_{01})=(cm)^{-1}\sum_{l=1}^{m}2\frac{\sin^2(\pi l/m)[1+Y(2\pi l/m)]}{Y^2(2\pi l/m)}\,. \tag{A18}$$

This term can be seen from (B45) and (B47) of III to be of the order m^{-3}. Similarly we find

$$V_{10}=U_{10}+O(m^{-3})\,. \tag{A19}$$

This leads to the result

$$(R_{-1,-1}-R_{1,1})/2i=\theta_1U_{10}+\theta_2U_{01}+O(\theta^2,m^{-3})\,. \tag{A20}$$

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[1]H. Au-Yang, M. E. Fisher, and A. E. Ferdinand, preceding paper, Phys. Rev. B 13, 1238 (1975), referred to as III.

[2]M. E. Fisher and H. Au-Yang, J. Phys. C 8, L418 (1975).

[3]I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products* (Academic, New York, 1965), Eq. 1.411.