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Solutions in Advanced Statistical Physics

Solution 16: Correlations and boundary effects for the Ising chain

a.) effect of boundary condition

For all cases, the partition function takes the form

$$Z = {\sum_{\sigma_1,\sigma_L}}' \left\{ \sum_{\sigma_2,\ldots,\sigma_{L-1}} \exp\left(K \sum_{i=1}^{L-1} \sigma_i \sigma_{i+1} \right) \right\} \equiv {\sum_{\sigma_1,\sigma_L}}' \zeta(\sigma_1,\sigma_L), \tag{1}$$

where $K = \beta J$ and the meaning of $\sum'$ varies according to the boundary conditions. As was done in the lecture, let's introduce the transfer matrix $\hat{T}$ such that

$$\langle \sigma | \hat{T} | \sigma' \rangle = e^K \delta_{\sigma,\sigma'} + e^{-K}(1 - \delta_{\sigma,\sigma'}) \Rightarrow \hat{T} = e^K \mathbb{1} + e^{-K} \hat{\sigma}_x, \tag{2}$$

where $\mathbb{1}$ is the identity operator and $\hat{\sigma}_x$ is a Pauli matrix. Since

$$e^{K^* \hat{\sigma}_x} = e^{K^*} \frac{\mathbb{1} + \hat{\sigma}_x}{2} + e^{-K^*} \frac{\mathbb{1} - \hat{\sigma}_x}{2} = \mathbb{1} \cosh K^* + \hat{\sigma}_x \sinh K^*, \tag{3}$$

the transfer matrix can be written as $\hat{T} = A e^{K^* \hat{\sigma}_x}$, with $A = \sqrt{2 \sinh 2K}$ and $\tanh K^* = e^{-2K}$ or equivalently $e^{2K^*} = \coth K$. By the definition of the transfer matrix,

$$\begin{aligned} \zeta(\sigma_1,\sigma_L) &= \langle \sigma_1 | \hat{T}^{L-1} | \sigma_L \rangle = \langle \sigma_1 | A^{L-1} \exp\left[(L-1) K^* \hat{\sigma}_x \right] | \sigma_L \rangle \\ &= A^{L-1} \left\{ \cosh((L-1)K^*) \delta_{\sigma_1,\sigma_L} + \sinh((L-1)K^*)(1 - \delta_{\sigma_1,\sigma_L} \right\}) \\ &= \frac{1}{2} (A e^{K^*})^{L-1} (1 + O(e^{-K^* L})), \end{aligned} \tag{4}$$

which clearly does not depend on the details of the boundaries once L is very large. From the definition of K^* one can easily show that $A e^{K^*} = 2 \cosh K$ which is the largest eigenvalue of the transfer matrix. Hence for any boundary conditions, the free energy density per spin in the thermodynamic limit is $-k_B T \ln \lambda_1$.

b.) correlation length

$$\begin{aligned}
\langle\sigma_1\sigma_r\rangle &= \frac{1}{Z}\sum_{\{\sigma\}}\sigma_1\sigma_r\exp\left(\sum_{i=1}^{L}\left(K\sigma_i\sigma_{i+1}+h\frac{\sigma_i+\sigma_{i+1}}{2}\right)\right)\\
&= \frac{1}{Z}\mathrm{Tr}\left(\hat\sigma_z\hat T^{r-1}\hat\sigma_z\hat T^{L-r+1}\right),\quad (r>1) \qquad (5)\\
\langle\sigma_k\rangle &= \frac{1}{Z}\sum_{\{\sigma\}}\sigma_k\exp\left(\sum_{i=1}^{L}\left(K\sigma_i\sigma_{i+1}+h\frac{\sigma_i+\sigma_{i+1}}{2}\right)\right) = \frac{1}{Z}\mathrm{Tr}\left(\hat\sigma_z\hat T^{L}\right),
\end{aligned}$$

where $\hat T$ is the transfer matrix

$$\hat T = \begin{pmatrix} e^{K+h} & e^{-K}\\ e^{-K} & e^{K-h}\end{pmatrix} = \begin{pmatrix} A+B & C\\ C & A-B\end{pmatrix},$$

where $A=e^K\cosh h$, $B=e^K\sinh h$, $C=e^{-K}$, and $\hat\sigma_z$ is the Pauli matrix. One can easily see that the unitary matrix

$$U=\begin{pmatrix}\alpha & \gamma\\ \gamma & -\alpha\end{pmatrix}\ \text{with}\ \alpha=\frac{1}{\sqrt2}\left(1+\sqrt{\frac{B^2}{B^2+C^2}}\right)^{1/2},\gamma=\frac{1}{\sqrt2}\left(1-\sqrt{\frac{B^2}{B^2+C^2}}\right)^{1/2}$$

diagonalizes $\hat T$ such that

$$U^{-1}TU=\begin{pmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{pmatrix}=\begin{pmatrix}A+\sqrt{B^2+C^2} & 0\\ 0 & A-\sqrt{B^2+C^2}\end{pmatrix}.$$

Since

$$U^{-1}\hat\sigma_z U=\begin{pmatrix}\alpha^2-\gamma^2 & 2\alpha\gamma\\ 2\alpha\gamma & -\alpha^2+\gamma^2\end{pmatrix}\equiv\begin{pmatrix}D & E\\ E & -D\end{pmatrix},\ U^{-1}\hat\sigma_z\hat T^n U=\begin{pmatrix}D\lambda_1^n & E\lambda_2^n\\ E\lambda_1^n & -D\lambda_2^n\end{pmatrix},$$

one can find that

$$\begin{aligned}
\langle\sigma_k\rangle &= D\frac{\lambda_1^L-\lambda_2^L}{\lambda_1^L+\lambda_2^L}\to D,\\
\langle\sigma_1\sigma_r\rangle &= D^2+E^2\frac{\lambda_1^{L-r+1}\lambda_2^{r-1}+\lambda_1^{r-1}\lambda_2^{L-r+1}}{\lambda_1^L+\lambda_2^L}\to D^2+E^2\left(\frac{\lambda_2}{\lambda_1}\right)^{r-1}
\end{aligned}$$

Hence the (connected) correlation function becomes

$$\langle\sigma_1\sigma_r\rangle-\langle\sigma_1\rangle\langle\sigma_r\rangle=\frac{1}{e^{4K}\sinh^2h+1}\left(\frac{\lambda_2}{\lambda_1}\right)^{r-1}=\frac{1}{e^{4K}\sinh^2h+1}e^{-(r-1)/\xi}, \qquad (6)$$

with $\xi^{-1}=\ln(\lambda_1/\lambda_2)$.

Solution 17: Solid-on-solid approximation for the Ising domain wall

The 'grand' partition function with the chemical potential μ is

$$Y = e^{-2\beta JL}\left(\sum_u e^{-2\beta J|u|-\beta\mu u}\right)^L = e^{-2\beta JL}\left(1+\frac{\zeta}{e^{2\beta J}-\zeta}+\frac{e^{-2\beta J}}{\zeta-e^{-2\beta J}}\right)^L, \tag{7}$$

where $\zeta = \exp(-\beta\mu)$ which will be determined by the global constraint. From $\zeta\dfrac{\partial \log Y}{\partial\zeta} = \sum_x \langle u(x)\rangle = L\tan\theta$, we get

$$\tan\theta = 1+\zeta\left(\frac{1}{e^{2\beta J}-\zeta}-\frac{1}{\zeta-e^{-2\beta J}}\right) \to \zeta(\theta,T) = \frac{\tan\theta\cosh 2\beta J+\sqrt{1+\tan^2\theta\sinh^2 2\beta J}}{1+\tan\theta}. \tag{8}$$

Finally, the free energy per unit length is obtained from the Legendre transformation

$$\begin{aligned} F(\theta,T) &= -L\mu(\theta,T)\tan\theta - k_BT\ln Y(\mu(\theta,T),T),\\ \Rightarrow \gamma_{\mathrm{SOS}}(\theta,T) = \frac{F(\theta,T)}{L/\cos\theta} &= -\mu\sin\theta+\left[2J+k_BT\ln\left(\frac{\cosh 2\beta J-\cosh\beta\mu}{\sinh 2\beta J}\right)\right]\cos\theta, \end{aligned} \tag{9}$$

where $-\mu = k_BT\ln\zeta(\theta,T)$. For $\theta = 0$ ($\pi/4$), we found $\zeta = 1$ ($\cosh 2\beta J$). Hence

$$\gamma_{\mathrm{SOS}}(0,T) = 2J + k_BT\ln\tanh\beta J, \tag{10}$$

which happens to be the same as the exact result and

$$\gamma_{\mathrm{SOS}}(\pi/4,T) = \frac{1}{\sqrt{2}}\left(2J+k_BT\ln\frac{\sinh 2\beta J}{2}\right) = \gamma(\pi/4,T)-\frac{1}{\sqrt{2}}k_BT\ln(1-e^{-4\beta J}), \tag{11}$$

which is larger than the exact result. Since the entropy of the SOS model is smaller than the true domain wall entropy, the critical temperature of the SOS model should be larger than that of the Ising model, which is clear in Eq. (11).

For $\theta = \pi/2$, γ_{SOS} becomes $2J$, which is due to the prohibition of overhangs. Unlike the SOS model, the Ising model has a (discrete) rotational symmetry, that is, invariance under the transformation $\theta \to \theta+\pi/2$, In general, the SOS model has no symmetry under the transformation $\theta\to\theta+\pi/2$; see Eq. (9).

Solution 18: Toom's CA

First observe that when $p = q$, Toom's CA has up-down symmetry, that is, there is a one-to-one correspondence from the configuration $\{\sigma\}$ to the configuration $\{-\sigma\}$ with exactly the same probability weight. So it is enough to show the behavior of a droplet of (+)-spins inside a sea of (−)-spins. By the dynamic rule, spins in the bulk of either sea or droplet do not change. The configuration change only occurs around the boundary (recall that $p = q = 0$).

Boundary of the droplet is defined by the set of sites with (+) spin at least one of whose neighbors is occupied by (−) spin.

For simplicity, let us assume that the initial droplet takes the form of square. Remember that a spin flip occurs when both spins at north-east neighbor sites have different sign from the spin in question. So initially there is one site which satisfies this criterion at the north-east corner of the droplet. Then the (+) spin neighbors of the flipped spin are in peril; they have to flip at the next time step. This continues until the whole square has flipped to (−). As this investigation reveals, the time for flipping the whole square is same as the "chemical" distance (number of connecting bonds) from the north-east corner to the south-west corner of the droplet. This is depicted in the figure below.

$$
\begin{array}{ccccc} - & - & - & - & - \\ + & + & + & + & - \\ + & + & + & + & - \\ + & + & + & + & - \\ + & + & + & + & - \end{array}
\Rightarrow
\begin{array}{ccccc} - & - & - & - & - \\ + & + & + & - & - \\ + & + & + & + & - \\ + & + & + & + & - \\ + & + & + & + & - \end{array}
\Rightarrow
\begin{array}{ccccc} - & - & - & - & - \\ + & + & - & - & - \\ + & + & + & - & - \\ + & + & + & + & - \\ + & + & + & + & - \end{array}
\Rightarrow
\begin{array}{ccccc} - & - & - & - & - \\ + & - & - & - & - \\ + & + & - & - & - \\ + & + & + & - & - \\ + & + & + & + & - \end{array}
$$

What happens if the shape of a droplet is not square? In this case, the (−) spins neighboring the droplet's boundary at the south-west corner can be flipped. Actually, there is an avalanche of flips of (−) spins but this avalanche ends when the south-west boundary forms the shape of a corner of a square. Then the avalanche of $(+) \rightarrow (-)$ flips originating from the north-east corner eventually covers the whole droplet. So in any case, the time of removing the droplet is the order of the linear extent of the initial droplet. The situation is depicted in the figure below.

$$
\begin{array}{ccccc} - & + & + & + & + \\ - & - & + & + & + \\ - & - & - & + & + \\ - & - & - & - & + \\ - & - & - & - & - \end{array}
\Rightarrow
\begin{array}{ccccc} - & + & + & + & + \\ - & + & + & + & + \\ - & - & + & + & + \\ - & - & - & + & + \\ - & - & - & - & - \end{array}
\Rightarrow
\begin{array}{ccccc} - & + & + & + & + \\ - & + & + & + & + \\ - & + & + & + & + \\ - & - & + & + & + \\ - & - & - & - & - \end{array}
\Rightarrow
\begin{array}{ccccc} - & + & + & + & + \\ - & + & + & + & + \\ - & + & + & + & + \\ - & + & + & + & + \\ - & - & - & - & - \end{array}
$$