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出版情報：Proceedings of the Japan Academy Series A : Mathematical Sciences. 86 (2), pp.33-37, 2010-02. 日本学士院
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A remark on monotonicity for the Glauber dynamics on finite graphs

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(Communicated by Shigefumi Mori, M.J.A., Jan. 12, 2010)

Abstract: We show that under the heat-bath Glauber dynamics for the ferromagnetic Ising model on a finite graph, the single spin expectation at a fixed time starting at the all-up configuration is not necessarily an increasing function of coupling constants.

Key words: Glauber dynamics; spectral gap; spin expectation; monotonicity conjecture.

1. Introduction. The Glauber dynamics for the ferromagnetic Ising model on a finite graph has been widely studied. One of the most interesting open problems is whether the spectral gap, the difference between the first and second largest eigenvalues of the transition matrix of the Glauber dynamics is monotone decreasing in each coupling constant in the Hamiltonian, which is conjectured by Yuval Peres (cf. [6, 7]). For this conjecture, there has been a result in [7] which shows that the monotonicity holds for cycles of any length. The proof is based on two facts that the linear subspace spanned by single spins is invariant under the Glauber dynamics and the expectation of a spin is equal to the survival probability of a certain random walk with killing. Several correlation inequalities for spin systems such as GKS and GHS had been intensively investigated from the late 1960s to early 1980s (cf. [1–5]). They have many important implications among which is that the expectation of the product of spins in the equilibrium is monotone increasing in each coupling constant for a wide class of ferromagnetic Ising models (cf. [8]). Taking this result into account, it is also natural to ask whether or not the single site spin expectation for a fixed time in the relaxation process starting from the all-up configuration is monotone increasing in each coupling constant. This is a stronger conjecture in the sense that if it is verified the monotonicity of the spectral gap follows, as is remarked by Yuval Peres. Since known correlation inequalities are devised mainly for the equilibrium states, it does not seem that we can apply them directly to the fixed time cases; indeed, we will see that the stronger conjecture does not hold in general.

2000 Mathematics Subject Classification. Primary 60K35, 82C20.

2. Result. Let $G = (V, E)$ be a finite connected graph. We define a probability measure π on $S = \{-1, 1\}^V$ by

$$\pi(\sigma) = Z^{-1} \exp\left(\sum_{xy \in E} J_{xy}\sigma_x\sigma_y\right),$$

where $\sigma_x \in \{-1, 1\}$ is the spin value at x, Z is the normalization constant and each coupling constant J_{xy} is non-negative. Since the involution $\sigma \mapsto -\sigma$ leaves π invariant, it follows that $\mathbf{E}_\pi[\sigma_x] = 0$ for any $x \in V$. The transition matrix of the Glauber dynamics on S is then defined by

$$A(\sigma, \eta) = \begin{cases} \frac{1}{|V|}\frac{\pi(\sigma^x)}{\pi(\sigma)+\pi(\sigma^x)}, & \eta = \sigma^x, x \in V \\ 1 - \sum_{x \in V} A(\sigma, \sigma^x), & \eta = \sigma \\ 0, & \text{otherwise}, \end{cases}$$

where $\sigma^x \in S$ is the spin configuration obtained from $\sigma \in S$ by flipping the spin at x and leaving all other spins unchanged. The probability measure π is reversible under this dynamics in which a vertex is chosen from V uniformly at random and then the spin on it is flipped with probability $\frac{\pi(\sigma^x)}{\pi(\sigma)+\pi(\sigma^x)}$. The transition matrix A acts on $\ell^2(S)$ as a bounded self-adjoint operator in a natural manner. Indeed, it is easy to see that $O \le A \le I$ since

$$\langle (I - A)f, f\rangle = \frac{1}{2|V|}\sum_{\sigma \in S}\sum_{x \in V}\frac{|f(\sigma^x) - f(\sigma)|^2}{\pi(\sigma)^{-1} + \pi(\sigma^x)^{-1}} \ge 0$$

and

$$\langle Af, f\rangle = \frac{1}{2|V|}\sum_{\sigma \in S}\sum_{x \in V}\frac{|\pi(\sigma)f(\sigma) + \pi(\sigma^x)f(\sigma^x)|^2}{\pi(\sigma) + \pi(\sigma^x)} \ge 0,$$

doi: 10.3792/pjaa.86.33

where $\langle f, g\rangle = \sum_{\sigma\in S} f(\sigma)g(\sigma)\pi(\sigma)$. Hence we can enumerate the eigenvalues of A as

$$1 = \lambda_1 > \lambda_2 \geq \cdots \geq \lambda_{M-1} > \lambda_M = 0,$$

where $M = 2^{|V|}$. Note that the eigenfunction corresponding to 0 is given by $\phi_M(\sigma) = (-1)^{n(\sigma)}\pi(\sigma)^{-1}$ where $n(\sigma)$ is the number of 1's in σ. The original conjecture on the spectral gap mentioned in the introduction is then phrased as "the second largest eigenvalue λ_2 of the Glauber dynamics for the ferromagnetic Ising model on any finite graph is monotone increasing in each coupling constant J_{xy}."

Now let us consider the case where G is the cycle C_n of length n, that is, $V = \{1, 2, \ldots, n\}$ and $E = \{12, 23, \ldots, n1\}$. In this case, it is easy to see that for $x \in V$ (V being considered in modulo n as $\mathbf{Z}_n$)

$$(2.1)\qquad Ae_x = \left(1 - \frac{1}{n}\right)e_x + \frac{1}{n}(\alpha_x e_{x-1} + \beta_x e_{x+1}),$$

where $e_x(\sigma) = \sigma_x$ for $\sigma \in S$ and

$$\alpha_x = \frac{s_{x-1}}{c_{x-1} + c_x}, \quad \beta_x = \frac{s_x}{c_{x-1} + c_x}$$

with $s_x = \sinh(2J_{x,x+1})$ and $c_x = \cosh(2J_{x,x+1})$ (cf. [7]). We remark that the operator A in (2.1) leaves the subspace H_1 of $\ell^2(S)$ spanned by $\{e_x, x \in V\}$ invariant. We define Q^{lazy} and Q as follows:

$$(2.2)\qquad Q^{lazy} = \left(1 - \frac{1}{n}\right)I + \frac{1}{n}Q$$

with

$$(2.3)\qquad Q(x, y) = \begin{cases} \alpha_x, & y = x - 1, \\ \beta_x, & y = x + 1, \\ 0, & \text{otherwise}. \end{cases}$$

The operator Q^{lazy} and Q are sub-stochastic and Q^{lazy} is nothing but the restriction of A on the invariant subspace H_1. Denote by $\{X_t, Q_x, \zeta\}$ and $\{X_t, Q_x^{lazy}, \zeta\}$ the discrete-time Markov chains on V with life time ζ associated with Q and Q^{lazy}, respectively. Let $\mathbf{1} \in S$ be the all-up spin configuration, i.e., $\mathbf{1}_x = 1$ for any $x \in V$, and $\sigma_x(t)$ the spin at $x \in V$ and at time $t \in \mathbf{Z}_{\geq 0} = \{0, 1, 2, \ldots\}$. Our main concern of this paper is the monotonicity of the spin expectation $\mathbf{E_1}[\sigma_x(t)]$ as a function of coupling constants $\mathbf{J} = (J_{xy}, xy \in E)$. Here $\mathbf{E_1}$ stands for the expectation with respect to the Glauber dynamics starting at the all-up configuration $\mathbf{1}$. It is easy to see that the quantity $\mathbf{E_1}[\sigma_x(t)]$ is equal to the survival probability $Q_x^{lazy}(\zeta > t)$ up to time t of the lazy Q-Markov chain starting at x since both functions of $x \in V$ and t satisfy the same linear equation with the same boundary condition:

$$(2.4)\qquad \begin{cases} \phi(x, t+1) = Q^{lazy}\phi(x, t), & t \in \mathbf{Z}_{\geq 0} \\ \phi(x, 0) \equiv 1 \end{cases}$$

where Q^{lazy} acts on the x-variable as $A\big|_{H_1}$ in (2.1). More directly,

$$(2.5)\qquad \mathbf{E_1}[\sigma_x(t)] = Q_x^{lazy}(\zeta > t) = \sum_{y\in V}(Q^{lazy})^t(x, y).$$

The monotonicity problem is then reduced to the problem of whether $Q_x^{lazy}(\zeta > t)$ is increasing in each coupling constant $J_{x,x+1}$.

The main result of this paper is the following theorem. See also Figures 1 and 2.

Theorem. Suppose a finite graph $G = (V, E)$ has a path of length 3 as a subgraph. Then there exist $a \in V$, $pq \in E$, $t \in \mathbf{Z}_{\geq 0}$ and positive coupling constants $\mathbf{j} = \{j_{xy}, xy \in E\}$ so that $\mathbf{E_1}[\sigma_a(t)]$ is decreasing near at $\mathbf{J} = \mathbf{j}$ in the coupling constant J_{pq}.

In order to prove this theorem, it suffices to consider the case of $G = P_3$, the path of length 3, and find $a \in V$, $pq \in E$, $t \in \mathbf{Z}_{\geq 0}$ and coupling constants $\mathbf{j}$ at which the derivative of $Q_a^{lazy}(\zeta > t)$ with respect to the coupling constant J_{pq} is negative because of the following observations: (i) if G has a path of length 3, say $V = \{1, 2, 3, 4\}$ and $E = \{12, 23, 34\}$, as a subgraph, we can compute the quantities on P_3 from those on G by setting $J_{xy} = 0$ except J_{12}, J_{23} and J_{34}, (ii) the derivative of $Q_a^{lazy}(\zeta > t)$ with respect to a coupling constant is jointly continuous in the coupling constants $\mathbf{J}$.

Before showing the theorem, as a warm-up, we discuss the monotonicity for a smaller graph P_2, for which the conjecture is true.

3. The case of P_2. We first consider the case where $G = (V, E)$ is the path P_2 of length 2, that is, $V = \{1, 2, 3\}$ and $E = \{12, 23\}$. We claim the following

Proposition 1. Let $G = P_2$. Then, for every $x \in V$ and $t \in \mathbf{Z}_{\geq 0}$, the expectation $\mathbf{E_1}[\sigma_x(t)]$ is increasing in both of coupling constants J_{12} and J_{23}.

Proof. Since we can regard this example as the case where $G = C_3$ and the coupling constant $J_{31} = 0$, by putting $x_1 = 2J_{12}$ and $x_2 = 2J_{23}$, it follows from (2.3) that

$$q_{12} = \frac{\sinh x_1}{1+\cosh x_1}, \qquad q_{21} = \frac{\sinh x_1}{\cosh x_1 + \cosh x_2},$$

$$q_{23} = \frac{\sinh x_2}{\cosh x_1 + \cosh x_2}, \quad q_{32} = \frac{\sinh x_2}{1+\cosh x_2},$$

where $q_{xy} = Q(x,y)$. Set $\phi_x(t) = Q_x(\zeta > t)$, the survival probability up to time t of the Q-Markov chain starting at x. We observe that

$$\begin{aligned}
\phi_2(0) &\equiv 1, \\
\phi_2(1) &= q_{21} + q_{23} = \tanh\Big(\frac{x_1+x_2}{2}\Big), \\
\phi_2(2) &= q_{21}q_{12} + q_{23}q_{32} \\
&= 1 - \frac{2}{\cosh x_1 + \cosh x_2},
\end{aligned}$$

and these are obviously increasing functions of x_1 and x_2. It follows from the Q-version of (2.4) for $n=3$ and $J_{31}=0$ that

$$\text{(3.1)} \qquad \begin{cases} \phi_1(t+1) = q_{12}\phi_2(t) \\ \phi_2(t+1) = q_{21}\phi_1(t) + q_{23}\phi_3(t) \\ \phi_3(t+1) = q_{32}\phi_2(t) \end{cases}$$

and

$$\text{(3.2)} \qquad \phi_2(t+2) = \phi_2(2)\phi_2(t), \ t \in \mathbf{Z}_{\geq 0},$$

from which together with the observation above, we conclude that $\phi_2(t)$ is non-decreasing both in x_1 and x_2 for any $t \in \mathbf{Z}_{\geq 0}$, and hence so are $\phi_1(t)$ and $\phi_3(t)$ because of (3.1) and the fact that q_{12} and q_{32} are increasing functions of x_1 and x_2, respectively. From (2.2) and (2.5), we see that

$$Q_x^{lazy}(\zeta > t) = \sum_{k=0}^{t} \binom{t}{k} \Big(\frac{2}{3}\Big)^{t-k} \Big(\frac{1}{3}\Big)^{k} Q_x(\zeta > k),$$

and hence $Q_x^{lazy}(\zeta > t)$ is a positive linear combination of increasing functions. □

Remark 2. We do not know whether the same claim holds for the case of C_3 instead of P_2.

4. Counter example: the case of P_3. Now we consider the case where $G = (V,E)$ is the path P_3 of length 3, that is, $V = \{1,2,3,4\}$ and $E = \{12, 23, 34\}$. In the same way as before, by regarding this example as the case where $G = C_4$ and the coupling constant $J_{41} = 0$, it follows from (2.3) that

$$q_{12} = \frac{\sinh x_1}{1+\cosh x_1}, \quad q_{21} = \frac{\sinh x_1}{\cosh x_1 + \cosh x_2},$$

$$q_{23} = \frac{\sinh x_2}{\cosh x_1 + \cosh x_2}, \quad q_{32} = \frac{\sinh x_2}{\cosh x_2 + \cosh x_3},$$

$$q_{34} = \frac{\sinh x_3}{\cosh x_2 + \cosh x_3}, \quad q_{43} = \frac{\sinh x_3}{1+\cosh x_3},$$

where $q_{xy} = Q(x,y)$. Set $\phi_2(t) = Q_2(\zeta > t)$. Then we see that

$$\begin{aligned}
\phi_2(1) &= q_{21} + q_{23} \\
\phi_2(2) &= q_{21}q_{12} + q_{23}q_{32} + q_{23}q_{34} \\
\phi_2(3) &= (q_{21}q_{12} + q_{23}q_{32})(q_{21}+q_{23}) + q_{23}q_{34}q_{43}
\end{aligned}$$

for the Q-Markov chain starting at the vertex 2. We can show the following

Proposition 3. As $s \to \infty$,

$$\frac{\partial Q_2(\zeta > k)}{\partial x_2}\Big|_{(x_1,x_2,x_3)=(2s,s,s)} = O(e^{-3s}) \quad (k=1,2)$$

$$\frac{\partial Q_2(\zeta > 3)}{\partial x_2}\Big|_{(x_1,x_2,x_3)=(2s,s,s)} = -\frac{e^{-2s}}{2} + O(e^{-3s})$$

Proof. In this proof, f' means $\frac{\partial f}{\partial x_2}$. We easily see that

$$q'_{21} = -q_{21}q_{23}, \quad q'_{23} = \frac{1}{2}(1 - q_{21}^2 - q_{23}^2),$$

$$q'_{32} = \frac{1}{2}(1 - q_{32}^2 - q_{34}^2), \quad q'_{34} = -q_{32}q_{34},$$

and so

$$\text{(4.1)} \qquad \phi'_2(1) = q'_{21} + q'_{23} = \frac{1}{2}\{1 - \phi_2(1)^2\}$$

$$\text{(4.2)} \quad (q_{23}q_{34})' = \{\phi'_2(1) + q_{23}(q_{21} - q_{32})\}q_{34}.$$

We also rewrite

$$\text{(4.3)} \quad \phi_2(2) = \phi_2(1)q_{12} + q_{23}(q_{32} + q_{34} - q_{12}),$$

$$\text{(4.4)} \quad \phi_2(3) = (\phi_2(2) - q_{23}q_{34})(\phi_2(1) - q_{43}) + \phi_2(2)q_{43}.$$

Now we set $(x_1,x_2,x_3) = (2s,s,s)$ and regard functions like $f(2s,s,s)$ and $f'(2s,s,s)$ as those of the variable $u = e^{-s}$. Since

$$q_{21} = 1 - u + u^2 + O(u^3), \tag{4.5}$$

$$q_{23} = u - u^2 + O(u^4), \tag{4.6}$$

we have

$$\phi_2(1) = q_{21} + q_{23} = 1 + O(u^3), \tag{4.7}$$

and then it follows from (4.1) that

$$\phi_2'(1) = \frac{1}{2}\{1 - \phi_2(1)^2\} = O(u^3). \tag{4.8}$$

Next we note that

$$q_{32} = q_{34} = \frac{1}{2} q_{12} = \frac{1}{2} - u^2 + O(u^4), \tag{4.9}$$

$$q_{12}' \equiv 0, \ q_{32}' + q_{34}' = 2u^2 + O(u^4). \tag{4.10}$$

Then, from (4.3), and (4.6) through (4.10), we obtain

$$\phi_2'(2) = q_{23}(q_{32}' + q_{34}') + O(u^3) = O(u^3). \tag{4.11}$$

From (4.4), (4.7), (4.8), (4.11), and

$$q_{43} = 1 - 2u(1-u) + O(u^3), \ q_{43}' \equiv 0,$$

we have

$$\phi_2'(3) = -2u(1-u)(q_{23}q_{34})' + O(u^3).$$

On the other hand, from (4.2), (4.5), (4.6), (4.8) and (4.9), we see that

$$(q_{23}q_{34})' = \{\phi_2'(1) + q_{23}(q_{21} - q_{32})\}q_{34} = \frac{u}{4} + O(u^2).$$

Consequently, we obtain

$$\phi_2'(3) = -\frac{u^2}{2} + O(u^3). \qquad \square$$

Remark 4. By similar computation, we can also show that for $a > 1$ and $b \in \mathbf{R}$

$$\frac{\partial Q_2(\zeta > 3)}{\partial x_2}\Big|_{(x_1,x_2,x_3)=(as,s+b,s)} = -\frac{e^{-as}}{1+\cosh(b)} + O(e^{-s\min(a+1,2a-1)})$$

as $s \to \infty$.

Corollary 5. There exists $s_0 > 0$ such that for any $s \ge s_0$, $Q_2^{lazy}(\zeta > 3)\Big|_{(x_1,x_2,x_3)=(2s,x_2,s)}$ is decreasing in x_2 near at $x_2 = s$.

Proof. We have already shown the same assertion for $Q_2(\zeta > 3)$. For a lazy version of the Q-Markov chain, $Q_2^{lazy}(\zeta > 3)$ is a positive linear combination of $Q_2(\zeta > k), k = 0, 1, 2, 3$. Indeed, from (2.2) and (2.5), it is easy to see that

$$Q_2^{lazy}(\zeta > 3) = \sum_{k=0}^{3} \binom{3}{k} \left(\frac{3}{4}\right)^{3-k} \left(\frac{1}{4}\right)^k Q_2(\zeta > k).$$

Therefore, from Proposition 3, we obtain

$$\frac{\partial Q_2^{lazy}(\zeta > 3)}{\partial x_2}\Big|_{(x_1,x_2,x_3)=(2s,s,s)} = -\frac{1}{128}e^{-2s} + O(e^{-3s})$$

as s tends to ∞. This implies the assertion. $\square$

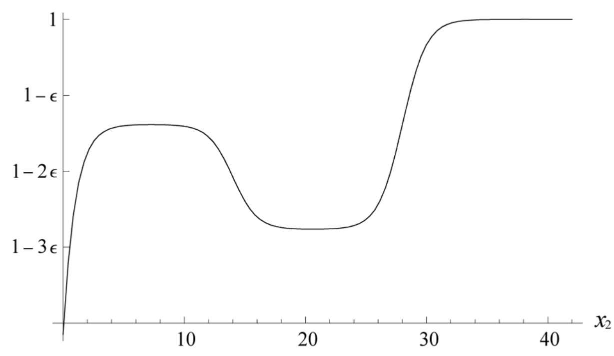

Fig. 1. The case of $G = P_3$: the graph of $Q_2(\zeta > 3)$ as a function of x_2 with coupling constants $(28, x_2, 14)$. The constant $\epsilon = 1.0 \times 10^{-12}$.

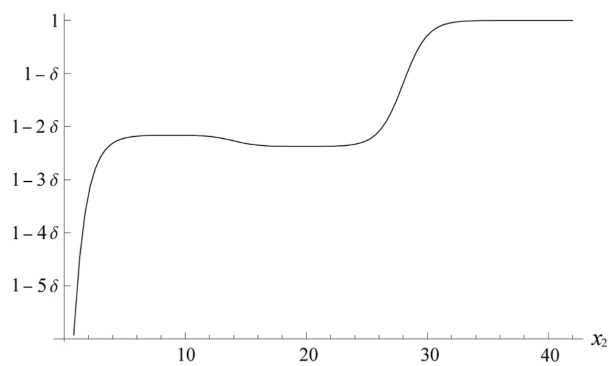

Fig. 2. The case of $G = P_3$: the graph of $\mathbf{E_1}[\sigma_2(3)]$ as a function of x_2 with coupling constants $(28, x_2, 14)$. The constant $\delta = 1.0 \times 10^{-13}$.

In Figs. 1, 2 one can see that $Q_2(\zeta > 3)$ and $\mathbf{E_1}[\sigma_2(3)]$ is decreasing in x_2 near at $(x_1, x_2, x_3) = (28, 14, 14)$.

Acknowledgments. The author would like to thank Yuval Peres and Jian Ding for fruitful discussions. This work is partially supported by Grant-in-Aid for Scientific Research (C)(18540130), Japan Society for the Promotion of Science.

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