Existence of de Almeida-Thouless-type instability in the transverse field Sherrington-Kirkpatrick model

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March 14, 2024

Abstract

The interpolation method for mean field spin glass models developed by Guerra and Talagrand is extended to a quantum mean field spin glass model. This extension enables us to obtain both replica-symmetric (RS) and one step replica-symmetry breaking (1RSB) solutions of the free energy density in the transverse field Sherrington-Kirkpatrick model. It is shown that the RS solution is exact in the paramagnetic phase. We provide a sufficient condition on coupling constants where the 1RSB solution gives better bound than the RS one. This condition reduced to physical quantities in disordered single spin systems allows a simple computer-assisted proof for the existence of the de Almeida-Thouless-type instability.

Contents

1 Introduction

The transverse field Sherrington-Kirkpatrick (SK) model is well-known as one of the simplest quantum spin glass models, and has been studied extensively. Several studies have been conducted in mathematically rigorous methods [1, 5, 11, 13, 15, 16]. Recently, Leschke, Manai, Ruder and Warzel have proven that the variance of the overlap operator does not vanish in the transverse SK model [15] using the Falk-Bruch inequality [7, 18] and the $\mathbb{Z}_2$-symmetry of the model. Their rigorous and striking result has been appreciated by many researchers studying spin glasses and quantum complex systems, since the finite variance of the overlap operator is recognized as a necessary condition for the existence of replica-symmetry breaking (RSB) [12]. This has brought further attention to the interesting question of whether the distribution of the overlap operator is broadened around the one of two peaks of the $\mathbb{Z}_2$-symmetric pair, since their argument relies on the fact that the expectation of the overlap operator vanishes due to the $\mathbb{Z}_2$-symmetry.

It is well-known that the square root interpolation method developed by Guerra and Talagrand is useful to obtain rigorous bounds on many physical quantities in the spin glass models [8, 22]. This method gives the replica-symmetric (RS) and the RSB bounds on the free energy density in SK model, rigorously. In particular, one step RSB (1RSB) solution gives the de Almeida-Thouless (AT) line which is a phase boundary of the unstable region of the RS solution [2, 22]. To extend this method to quantum systems is interesting to study.

In the present paper, we obtain variational solutions of the free energy density in the transverse field SK model. We extend the square root interpolation method for RS and 1RSB variational solutions of the free energy density given by Guerra and Talagrand [8, 22] to quantum mechanically perturbed models. First, we prove that the obtained RS solution becomes exact in the paramagnetic phase assuming the unbroken replica- and $\mathbb{Z}_2$-symmetries. For sufficiently low temperature and sufficiently weak transverse field, however, the finite variance of the overlap operator [15] enables us to prove that this paramagnetic RS solution cannot be exact. In this case, our interest is possibility that another spin glass RS solution becomes exact. Next, we construct a 1RSB solution, and find a condition on the unstable region of the RS solution, where the 1RSB solution gives better bound on the free energy density than RS solutions. If the condition is satisfied, the AT-type instability exists in the transverse field SK model. We represent a sufficient condition for AT-type instability in terms of disordered single spin systems, using the Falk-Bruch inequality [7, 18]. Then, a computer-assisted proof by simple numerical calculations becomes possible to confirm this condition. This unstable region specified in the coupling constant space must be contained in the RSB phase.

The present paper is organized as follows. In section 2, we define the Hamiltonian and other physical quantities in the transverse field SK model. In section 3, the RS solution of the free energy density in the transverse field SK model is obtained by the square root interpolation method extended to quantum spin glass systems. The exactness and inexactness of the paramagnetic RS solution are shown even in this quantum model in the paramagnetic phase, as in the classical SK model. In section 4, the 1RSB solution of the free energy density in the transverse field SK model is obtained. In section 5, we obtain a sufficient condition that the 1RSB solution gives better bound on the free energy density than the RS solution. This condition is confirmed numerically at several points in the coupling constant space.

2 Definitions of the model

Here, we study quantum spin systems with random interactions. Let N be a positive integer and a site index i $(\leq N)$ is also a positive integer. A sequence of spin operators $(\sigma_i^w)_{w=x,y,z,1\leq i\leq N}$ on a Hilbert space $\mathcal{H} := \bigotimes_{i=1}^N \mathcal{H}_i$ is defined by a tensor product of the Pauli matrix σ^w acting on $\mathcal{H}_i \cong \mathbb{C}^2$ and unities. These operators are self-adjoint and satisfy the commutation relation

$$[\sigma_k^y, \sigma_j^z] = 2i\delta_{k,j}\sigma_j^x, \qquad [\sigma_k^z, \sigma_j^x] = 2i\delta_{k,j}\sigma_j^y, \qquad [\sigma_k^x, \sigma_j^y] = 2i\delta_{k,j}\sigma_j^z,$$

and each spin operator satisfies

$$(\sigma_j^w)^2 = \mathbf{1}.$$

The Sherrington-Kirkpatrick (SK) model is well-known as a disordered classical spin system [21]. The transverse field SK model is a simple quantum extension. Here, we study a magnetization process for a local field in these models. Consider the following Hamiltonian with coupling constants $b, c \in \mathbb{R}$, $c \geq 0$

$$H(\sigma, b, g) := -\frac{1}{\sqrt{N}} \sum_{1\leq i<j\leq N} g_{i,j}\sigma_i^z\sigma_j^z - \sum_{j=1}^N b\sigma_j^x, \tag{1}$$

where $g = (g_{i,j})_{1\leq i<j\leq N}$ are independent identically distributed (i.i.d) standard Gaussian random variables obeying a probability density function

$$p(g) := \prod_{1\leq i<j\leq N} \frac{1}{\sqrt{2\pi}} e^{-\frac{g_{i,j}^2}{2}} \tag{2}$$

The Hamiltonian is invariant under $\mathbb{Z}_2$-symmetry $U\sigma_i^zU^\dagger = -\sigma_i^z$ for the discrete unitary transformation $U := \prod_{1\leq i\leq N} \sigma_i^x$. For a positive β, the partition function is defined by

$$Z_N(\beta, b, g) := \mathrm{Tr} e^{-\beta H(\sigma, b, g)}, \tag{3}$$

where the trace is taken over the Hilbert space $\mathcal{H}$.

3 RS bound on the free energy density

Guerra and Talagrand have provided the well-known square root interpolation method, which represents a variational solution of the free energy density in the classical mean field model in terms of that in the single spin model with suitable corrections [8, 22]. Here, we apply this method to the transverse field SK model, as for the SK model. Let $(z_j)_{1\le j\le N}$ be a sequence of i.i.d standard Gaussian random variables. Consider the following interpolated Hamiltonian with parameters $s\in[0,1]$ for $q\in[0,1]$

$$H(s,\sigma):=-\sqrt{\frac{s}{N}}\sum_{1\le i<j\le N} g_{i,j}\sigma_i^z\sigma_j^z-\sum_{j=1}^N[\sqrt{q(1-s)}z_j\sigma_j^z+b\sigma_j^x]. \tag{4}$$

This interpolated Hamiltonian for $b=0$ is identical to that in the SK model obtained by Guerra and Talagrand [8, 22]. Define an interpolated function $\varphi_N(s)$

$$\varphi_N(s):=\frac{1}{N}\mathbb{E}\log \mathrm{Tr}e^{-\beta H(s,\sigma)} \tag{5}$$

where $\mathbb{E}$ denotes the expectation over all Gaussian random variables $(g_{i,j})_{1\le i<j\le N}$ and $(z_i)_{1\le i\le N}$. Since the function $\varphi_N(1)$ is given by

$$\varphi_N(1)=\frac{1}{N}\mathbb{E}\log Z_N(\beta,b,g), \tag{6}$$

the free energy density of the transverse field SK model is $-\varphi_N(1)/\beta$. Let f be an arbitrary function of a sequence of spin operators $\sigma=(\sigma_i^w)_{w=x,y,z,1\le i\le N}$. The expectation of f in the Gibbs state is given by

$$\langle f(\sigma)\rangle_s=\frac{\mathrm{Tr}f(\sigma)e^{-\beta H(s,\sigma)}}{\mathrm{Tr}e^{-\beta H(s,\sigma)}}. \tag{7}$$

The derivative of $\varphi_N(s)$ with respect to s is given by

$$\varphi_N'(s)=\frac{\beta}{2N^{\frac{3}{2}}\sqrt{s}}\sum_{1\le<j\le N}\mathbb{E}g_{i,j}\langle\sigma_i^z\sigma_j^z\rangle_s-\frac{\beta\sqrt{q}}{2N\sqrt{1-s}}\sum_{i=1}^N\mathbb{E}z_i\langle\sigma_i^z\rangle_s. \tag{8}$$

Identities for the Gaussian random variables $g_{i,j}$ and z_i and their probability distribution function

$$g_{i,j}p(g,z)=-\frac{\partial p}{\partial g_{i,j}},\quad z_ip(g,z)=-\frac{\partial p}{\partial z_i}$$

and the integration by parts imply

$$\begin{aligned}\varphi_N'(s)&=\frac{\beta^2}{2N^2}\sum_{1<i\le<j\le N}\mathbb{E}[(\sigma_i^z\sigma_j^z,\sigma_i^z\sigma_j^z)_s-\langle\sigma_i^z\sigma_j^z\rangle_s^2]-\frac{\beta^2 q}{2N}\sum_{i=1}^N\mathbb{E}[(\sigma_i^z,\sigma_i^z)_s-\langle\sigma_i^z\rangle_s^2]\\&=\frac{\beta^2(N-1)}{4N}\mathbb{E}(\sigma_i^z\sigma_j^z,\sigma_i^z\sigma_j^z)_s-\frac{\beta^2 q}{2}\mathbb{E}(\sigma_i^z,\sigma_i^z)_s-\frac{\beta^2}{4}\mathbb{E}\langle(R_{1,2}-q)^2\rangle_s+\frac{\beta^2}{4}\Big(q^2+\frac{1}{N}\Big),\end{aligned} \tag{9}$$

where The Duhamel function for bounded linear operators A,B is defined by

$$(A,B)=\int_0^1 dt\langle e^{\beta tH}Ae^{-\beta tH}B\rangle, \tag{10}$$

and the overlap operator $R_{a,b}$ is defined by

$$R_{a,b}:=\frac{1}{N}\sum_{i=1}^N\sigma_i^{z,a}\sigma_i^{z,b}, \tag{11}$$

for independent replicated Pauli operators $\sigma_i^{z,a}$ $(a=1,2,\cdots,n)$ obeying the same Gibbs state with the replica Hamiltonian

$$H(s,\sigma^1,\cdots,\sigma^n):=\sum_{a=1}^n H(s,\sigma^a).$$

This Hamiltonian is invariant under permutation of replica spins. This permutation symmetry is known to be the replica symmetry. The order operator $R_{a,b}$ measures the replica symmetry breaking as an order operator. Define a function

$$\rho(s,q):=\frac{(N-1)}{N}[1-\mathbb{E}(\sigma_i^z\sigma_j^z,\sigma_i^z\sigma_j^z)_s]+2q[\mathbb{E}(\sigma_i^z,\sigma_i^z)_s-1], \tag{12}$$

which is non-negative valued. The identity (9) imply

$$\varphi_N'(s)=\frac{\beta^2}{4}(1-q)^2-\frac{\beta^2}{4}\mathbb{E}\langle(R_{1,2}-q)^2\rangle_s-\frac{\beta^2}{4}\rho(s,q) \tag{13}$$

Integration of this identity over $s\in[0,1]$ gives the following lemma.

Lemma 3.1 *(Extended Guerra's identity for RS bound)*
Define a function by

$$\Phi(\beta, b, q) := \mathbb{E} \log 2 \cosh X(z, q) + \frac{\beta^2}{4}(1-q)^2 - \frac{\beta^2}{4} \int_0^1 ds \rho(s, q), \tag{14}$$

where the above random variable is defined by

$$X(z, q) := \beta \sqrt{q z^2 + b^2}. \tag{15}$$

For arbitrary $(\beta, b, q) \in [0, \infty)^2 \times [0, 1]$, the following identity is valid

$$\varphi_N(1) = \Phi(\beta, b, q) - \frac{\beta^2}{4} \int_0^1 ds \mathbb{E} \langle (R_{1,2} - q)^2 \rangle_s, \tag{16}$$

Proof. Integration of the identity (13) over $s \in [0, 1]$ gives

$$\varphi_N(1) = \varphi_N(0) + \frac{\beta^2}{4} \int_0^1 ds [(1-q)^2 - \rho(s, q) - \mathbb{E} \langle (R_{1,2} - q)^2 \rangle_s].$$

The model at $s = 0$ becomes independent spin model, and therefore $\varphi_N(0)$ is represented in terms of the partition function of a disordered single spin system

$$\varphi_N(0) = \mathbb{E} \log \mathrm{Tr} \exp \beta [\sqrt{q} z \sigma^z + b \sigma^x] = \mathbb{E} \log 2 \cosh X(z, q). \tag{17}$$

This completes the proof. $\square$

Note that $\Phi(\beta, b, q)$ gives the following bound

$$\varphi_N(1) \leq \Phi(\beta, b, q), \tag{18}$$

where the right hand side is called the RS bound.

To obtain lower and upper bounds on $\Phi(\beta, b, q)$, let us evaluate $\rho(s, q)$. The Falk-Bruch inequality [7, 18] and a well-known inequality [3, 19] for the Duhamel function of an arbitrary bounded linear operator A give

$$F\Big(\frac{\langle [A^\dagger, [\beta H, A]] \rangle_s}{2 \langle \{A^\dagger, A\} \rangle_s} \Big) \leq \frac{2 (A^\dagger, A)_s}{\langle \{A^\dagger, A\} \rangle_s} \leq 1, \tag{19}$$

where the function $F : [0, \infty) \to (0, 1]$ is defined by

$$F(x \tanh x) = \frac{\tanh x}{x}, \tag{20}$$

and $F(0) = 1$. This function is monotonically decreasing and convex. Therefore

$$F(2\beta b \tanh \beta b) \leq F(\beta b (\langle \sigma_i^x \rangle_s + \langle \sigma_j^x \rangle_s)) = F\Big(\frac{\beta}{4} \langle [\sigma_i^z \sigma_j^z, [H, \sigma_i^z \sigma_j^z]] \rangle_s \Big) \leq (\sigma_i^z \sigma_j^z, \sigma_i^z \sigma_j^z)_s \leq 1, \tag{21}$$

$$\frac{\tanh \beta b}{\beta b} = F(\beta b \tanh \beta b) \leq F(\beta b \langle \sigma_i^x \rangle_s) = F\Big(\frac{\beta}{4} \langle [\sigma_i^z, [H, \sigma_i^z]] \rangle_s \Big) \leq (\sigma_i^z, \sigma_i^z)_s \leq 1, \tag{22}$$

where an upper bound $\tanh \beta b \geq \langle \sigma_i^x \rangle_s$ has been used as shown by Leschke, Manai, Ruder and Warzel [15]. These inequalities (21), (22) and a well-known inequality given by Dyson, Lieb and Simon [6]

$$F(t) \geq t^{-1}(1 - e^{-t}), \tag{23}$$

yield the following lower and upper bounds on the function $\rho(s, q)$

$$2q \Big(\frac{\tanh \beta b}{\beta b} - 1 \Big) \leq \rho(s, q) \leq \frac{N-1}{N} \Big(1 - \frac{1 - e^{-2\beta b \tanh \beta b}}{2 \beta b \tanh \beta b} \Big). \tag{24}$$

Lower and upper bounds (24) on $\rho(s, q)$ give the following lemma for the RS bound.

Lemma 3.2 *The RS bound $\Phi(\beta, b, q)$ satisfies*

$$\Phi_L(\beta, b, q) \leq \Phi(\beta, b, q) \leq \Phi_U(\beta, b, q), \tag{25}$$

where lower and upper bounds are defined by

$$\Phi_L(\beta, b, q) := \mathbb{E} \log 2 \cosh X(z, q) + \frac{\beta^2}{4} \Big[(1-q)^2 - \Big(1 - \frac{1 - e^{-2\beta b \tanh \beta b}}{2 \beta b \tanh \beta b} \Big) \Big] \tag{26}$$

$$\Phi_U(\beta, b, q) := \mathbb{E} \log 2 \cosh X(z, q) + \frac{\beta^2}{4} \Big[(1-q)^2 + 2q \Big(1 - \frac{\tanh \beta b}{\beta b} \Big) \Big]. \tag{27}$$

A variational solution with the best bound is obtained by minimizing the right hand side of (14). The minimizer q should satisfy

$$0 = \frac{\partial}{\partial q}\Phi(\beta, b, q) = \frac{\beta^2}{4}\Big[2\mathbb{E}\frac{z^2 \tanh X(z,q)}{X(z,q)} + 2q - 2 - \frac{\partial}{\partial q}\int_0^1 ds\rho(s,q)\Big]. \tag{28}$$

This minimizer q gives the best bound on $\varphi_N(1)$ as a variational solution

$$\begin{aligned}\varphi_N(1) &\leq \min_{q\in[0,1]} \Phi(\beta, b, q)\\ &= \min_{q\in[0,1]}\Big[\mathbb{E}\log 2\cosh X(z,q) + \frac{\beta^2}{4}(1-q)^2 - \frac{\beta^2}{4}\int_0^1 ds\rho(s,q)\Big], \end{aligned}\tag{29}$$

$\min_{q\in[0,1]}\Phi(\beta, b, q)$ is called RS solution.

Here, we discuss the exactness of the RS solution. Assume that the replica-symmetry is unbroken and there exists $q \in [0,1]$ such that

$$\lim_{N\to\infty}\int_0^1 ds\mathbb{E}\langle(R_{1,2}-q)^2\rangle_s = 0. \tag{30}$$

The bound $\Phi(\beta, b, q)$ with the above q gives the exact solution of $\varphi_\infty(1)$, as in the classical SK model. Only the minimizer q of $\Phi(\beta, b, q)$ can give the equality, since the inequality (18) is valid for any q. In fact, this exactness can be shown in the case for $q = 0$. Consider the model for $q = 0$ in the paramagnetic phase where the replica-symmetry and $\mathbb{Z}_2$-symmetry are unbroken. Substitute $q = 0$ into the equation (16) in Lemma 3.1, and the extended Guerra's identity becomes

$$\varphi_N(1) = \Phi(\beta, b, 0) - \int_0^1 ds\mathbb{E}\langle R_{1,2}^2\rangle_s \tag{31}$$

$$\leq \Phi(\beta, b, 0) = \log 2\cosh\beta b + \frac{\beta^2}{4} - \frac{\beta^2}{4}\int_0^1 ds\rho(s,0). \tag{32}$$

Then, the following theorem is obtained.

Theorem 3.3 *(Exactness of the paramagnetic RS solution)*
In the paramagnetic phase, $\Phi(\beta, b, 0)$ gives the exact solution

$$\lim_{N\to\infty}\Phi(\beta, b, 0) = \lim_{N\to\infty}\varphi_N(1). \tag{33}$$

Proof. The existence of the right hand side in the infinite-volume limit is proven by [1, 5]. The $\mathbb{Z}_2$-symmetry and the replica-symmetry imply

$$\langle R_{1,2}\rangle_s = 0, \quad \lim_{N\to\infty}\mathbb{E}\langle(R_{1,2}-\mathbb{E}\langle R_{1,2}\rangle_s)^2\rangle_s = 0.$$

These and the above identity (31) conclude that the paramagnetic RS solution is exact

$$\lim_{N\to\infty}\Phi(\beta, b, 0) = \varphi_\infty(1).$$

This completes the proof. □

Theorem 3.3 is consistent with the result in [16]. On the other hand, using the Falk-Bruch inequality (19), and assuming the ground state energy density $-\kappa \simeq -0.763$ of the classical SK model and the $\mathbb{Z}_2$-symmetry $\langle R_{1,2}\rangle_s = 0$, Leschke, Manai Ruder and Warzel have proven

$$\liminf_{N\to\infty}\mathbb{E}\langle R_{1,2}^2\rangle_s \geq F(2\beta b\tanh\beta b) - \frac{2\kappa}{\beta\sqrt{s}}, \tag{34}$$

in the model defined by the Hamiltonian (4) for $q = 0$ [15], where the function F is defined by (20). This inequality and the identity (31) imply the following theorem.

Theorem 3.4 *(Non-exactness of the paramagnetic RS solution)*
If β and b satisfy $\beta F(2\beta b\tanh\beta b) > 2\kappa$, then the inequality (32) becomes strict

$$\varphi_\infty(1) < \liminf_{N\to\infty}\Phi(\beta, b, 0).$$

Proof. Define $\sqrt{s_0} := \dfrac{2\kappa}{\beta F(2\beta b \tanh \beta b)}$. Then, the assumption $s_0 < 1$ and inequality (34) enables us to evaluate the deviation

$$\begin{aligned}
&\liminf_{N\to\infty}[\Phi(\beta, b, 0) - \varphi_N(1)] \geq \liminf_{N\to\infty} \int_{s_0}^1 ds \mathbb{E}\langle R_{1,2}^2\rangle_s \\
&\geq \int_{s_0}^1 ds \Big[F(2\beta b \tanh \beta b) - \frac{2\kappa}{\beta\sqrt{s}}\Big] = F(2\beta b \tanh \beta b)(1-\sqrt{s_0})^2 > 0.
\end{aligned}$$

This completes the proof. □

In this case, the bound $\Phi(\beta, b, 0)$ becomes an approximate solution of $\varphi_\infty(1)$, and a better one may be given by a spin glass RS solution $\Phi(\beta, b, q)$ with the minimizer $q > 0$. Either spin glass RS or RSB phase is possible in this region of coupling constants, since there is no ferromagnetic long-range order in this model [11]. After next section, we show in a different way that the spin glass RS solution is not exact

$$\varphi_\infty(1) < \lim_{N\to\infty} \min_{q\in[0,1]} \Phi(\beta, b, q),$$

like the paramagnetic RS one, and therefore the identity (30) does not hold either.

In the classical limit $b \to 0$, the bound (14) becomes

$$\varphi_N(1) \leq \mathbb{E} \log 2\cosh \beta\sqrt{q}z + \frac{\beta^2}{4}(1-q)^2, \tag{35}$$

which is identical to the RS solution in the SK model. The equation (28) becomes

$$q = \mathbb{E} \tanh^2 \beta\sqrt{q}z. \tag{36}$$

This has a solution $q = 0$. In the classical case $b = 0$, it was conjectured that the replica symmetry is preserved with

$$\lim_{N\to\infty} \mathbb{E}\langle (R_{1,2} - q)^2\rangle_1 = 0,$$

and the SK solution of the free energy density is exact for

$$\mathbb{E}\frac{\beta^2}{\cosh^4 \beta\sqrt{q}z} \leq 1,$$

whose boundary is called the AT line [2, 23]. This condition becomes $\beta \leq 1$ for $q = 0$. Recently, Chen has proven rigorously that the SK solution is exact in the classical model [4].

4 1RSB bound on the free energy density

Guerra obtained the RSB bound in the SK model in the square root interpolation [9]. This bound can find the AT line [2, 22, 23]. Here, we extend this method to the transverse field SK model and demonstrate that a 1RSB solution gives better bound on the free energy density than the RS one (29). Assume the following square root interpolation of Hamiltonian with a parameter $s \in [0,1]$ between the transverse field Sherrington-Kirkpatrick model and an independent spin model

$$H(s, \sigma, g, z, z^1) := -\sqrt{\frac{s}{N}} \sum_{1\leq i<j\leq N} g_{i,j}\sigma_i^z\sigma_j^z - \sqrt{1-s}\sum_{j=1}^N (\sqrt{q_1}z_j + \sqrt{q_2-q_1}z_j^1)\sigma_j^z - \sum_{j=1}^N b\sigma_j^x, \tag{37}$$

where variational parameters q_1, q_2 satisfy $0 \leq q_1 \leq q_2 \leq 1$ and z_j, z_j^1 are i.i.d standard Gaussian random variables. This interpolated Hamiltonian for $b = 0$ is identical to that in the SK model given in [22]. Define a partition function

$$Z(s) := \mathrm{Tr} e^{-\beta H(s,\sigma,g,z,z^1)}. \tag{38}$$

Define an interpolation for a free energy density with another variational parameter $m \in [0,1]$

$$\psi_N(s) := \frac{1}{Nm}\mathbb{E} \log \mathbb{E}_1 Z(s)^m, \tag{39}$$

where $\mathbb{E}_1$ denotes the expectation only over $(z_i^1)_{1\leq i\leq N}$ and $\mathbb{E}$ denotes the expectation over all random variables. Note that this function for $s = 1$ is identical to the function (6)

$$\psi_N(1) = \varphi_N(1), \tag{40}$$

and $-\psi_N(1)/\beta$ is the free energy density of the transverse field SK model. The derivative of $\psi_N(s)$ is

$$\psi'_N(s) = -\frac{\beta}{N}\mathbb{E}\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m\langle\frac{\partial}{\partial s}H(s,\sigma,g,z,z^1)\rangle_s = \mathrm{I}+\mathrm{II}+\mathrm{III}, \tag{41}$$

where three terms are defined by

$$\begin{aligned}
\mathrm{I} &:= \frac{\beta}{N}\mathbb{E}\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m\frac{1}{2\sqrt{sN}}\sum_{1\leq i<j\leq N} g_{i,j}\langle\sigma_i^z\sigma_j^z\rangle_s, &(42)\\
\mathrm{II} &:= -\frac{\beta}{N}\mathbb{E}\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m\frac{1}{2\sqrt{1-s}}\sum_{j=1}^N\sqrt{q_1}z_j\langle\sigma_j^z\rangle_s, &(43)\\
\mathrm{III} &:= -\frac{\beta}{N}\mathbb{E}\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m\frac{1}{2\sqrt{1-s}}\sum_{j=1}^N\sqrt{q_2-q_1}z_j^1\langle\sigma_j^z\rangle_s. &(44)
\end{aligned}$$

Integration by parts and $(\sigma_i^z\sigma_j^z,\sigma_i^z\sigma_j^z)_s\leq 1$ for the first term (42) imply

$$\begin{aligned}
\mathrm{I} &= \frac{\beta}{2N^{\frac{3}{2}}\sqrt{s}}\sum_{1\leq i<j\leq N}\mathbb{E}\frac{\partial}{\partial g_{i,j}}\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m\langle\sigma_i^z\sigma_j^z\rangle_s\\
&= \frac{\beta^2}{2N^2}\sum_{1\leq i<j\leq N}\mathbb{E}\Big[-m\Big(\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m\langle\sigma_i^z\sigma_j^z\rangle_s\Big)^2\\
&+ \frac{m-1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m\langle\sigma_i^z\sigma_j^z\rangle_s^2+\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m(\sigma_i^z\sigma_j^z,\sigma_i^z\sigma_j^z)_s\Big]\\
&= \frac{\beta^2(1-N)}{4N}\mathbb{E}\Big[m\Big(\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m\langle\sigma_i^z\sigma_j^z\rangle_s\Big)^2\\
&+ \frac{1-m}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m\langle\sigma_i^z\sigma_j^z\rangle_s^2-\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m(\sigma_i^z\sigma_j^z,\sigma_i^z\sigma_j^z)_s\Big].
\end{aligned}\tag{45}$$

Integration by parts and $(\sigma_j^z,\sigma_j^z)_s\geq\tanh\beta b/(\beta b)$ by the Falk-Bruch inequality (19) for the second term (43) imply

$$\begin{aligned}
\mathrm{II} &= -\frac{\beta}{2N\sqrt{1-s}}\sum_{j=1}^N\mathbb{E}\frac{\partial}{\partial z_j}\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m\sqrt{q_1}\langle\sigma_j^z\rangle_s\\
&= \frac{\beta^2 q_1}{2}\mathbb{E}\Big[m\Big(\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m\langle\sigma_j^z\rangle_s\Big)^2+\frac{1-m}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m\langle\sigma_j^z\rangle_s^2\\
&- \frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m(\sigma_j^z,\sigma_j^z)_s\Big].
\end{aligned}\tag{46}$$

The third term (44) can be evaluated in the same way

$$\begin{aligned}
\mathrm{III} &= -\frac{\beta}{2N\sqrt{1-s}}\sum_{j=1}^N\mathbb{E}\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1\frac{\partial}{\partial z_j^1}Z(s)^m\sqrt{q_2-q_1}\langle\sigma_j^z\rangle_s\\
&= \frac{\beta^2(q_2-q_1)}{2}\mathbb{E}\Big[\frac{1-m}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m\langle\sigma_j^z\rangle_s^2-\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m(\sigma_j^z,\sigma_j^z)_s\Big].
\end{aligned}\tag{47}$$

Therefore, $\psi'_N(s)$ is represented as

$$\begin{aligned}
\psi'_N(s) &= \mathrm{I}+\mathrm{II}+\mathrm{III}\\
&= -\frac{\beta^2}{4}\Big[m\mathbb{E}\Big(\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m\langle\sigma_i^z\sigma_j^z\rangle_s\Big)^2+(1-m)\mathbb{E}\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m\langle\sigma_i^z\sigma_j^z\rangle_s^2\\
&- 2mq\mathbb{E}\Big(\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m\langle\sigma_j^z\rangle_s\Big)^2-2(1-m)q_2\mathbb{E}\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m\langle\sigma_j^z\rangle_s^2\\
&- 1+2q_2+\rho_1(s,m,q_1,q_2)\Big],
\end{aligned}\tag{48}$$

where a non-negative valued function $\rho_1(s,m,q_1,q_2)$ is defined by

$$\rho_1(s,m,q_1,q_2) := \mathbb{E}\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m[2q_2(\sigma_j^z,\sigma_j^z)_s-2q_2+\frac{N-1}{N}[1-(\sigma_i^z\sigma_j^z,\sigma_i^z\sigma_j^z)_s]]. \tag{49}$$

Inequalities (21), (22)and (23) give the following uniform lower and upper bounds independent of (s, m, q)

$$2q_2\Big(\frac{\tanh\beta b}{\beta b} - 1\Big) \leq \rho_1(s, m, q_1, q_2) \leq \frac{N-1}{N}\Big(1 - \frac{1 - e^{-2\beta b \tanh \beta b}}{2\beta b \tanh \beta b}\Big). \quad (50)$$

Next, we represent the above bound on $\psi_N'(s)$ in a replicated model. Define a two replicated Hamiltonian by

$$H_2(s, \sigma^1, \sigma^2) := H(s, \sigma^1, g, z^1) + H(s, \sigma^2, g, z^2), \quad (51)$$

where the right hand side consists of the interpolated one step RSB Hamiltonian defined by (37) with i.i.d. standard Gaussian random variables $(z_i^a)_{1\leq i\leq N, a=1,2}$. Note that the partition function of this replicated model is factorized into the original partition functions

$$Z_2(s) := \mathrm{Tr} e^{-\beta H(s,\sigma^1,\sigma^2)} = \mathrm{Tr} e^{-\beta H(s,\sigma,g,z^1)} \mathrm{Tr} e^{-\beta H(s,\sigma,g,z^2)}. \quad (52)$$

The following expectation of the overlap operator defined by (11) is represented in terms of expectation values of the original model

$$\mathbb{E}\frac{1}{\mathbb{E}_1\mathbb{E}_2 Z_2(s)^m}\mathbb{E}_1\mathbb{E}_2 Z_2(s)^m \langle R_{1,2}\rangle_{s,2} = \mathbb{E}\Big(\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m \langle \sigma_i^z\rangle_s\Big)^2, \quad (53)$$

where $\mathbb{E}_a$ denotes the expectation value only over $(z_i^a)_{1\leq i\leq N, a=1,2}$ and the Gibbs expectation value of $f(\sigma^1, \sigma^2)$ is defined by

$$\langle f(\sigma^1,\sigma^2)\rangle_{s,2} := \frac{1}{Z_2(s)}\mathrm{Tr} f(\sigma^1,\sigma^2) e^{-\beta H(s,\sigma^1,\sigma^2)}.$$

Note also

$$\mathbb{E}\frac{1}{\mathbb{E}_1\mathbb{E}_2 Z_2(s)^m}\mathbb{E}_1\mathbb{E}_2 Z_2(s)^m \langle R_{1,2}^2\rangle_{s,2} = \frac{N-1}{N}\mathbb{E}\Big(\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m \langle \sigma_i^z\sigma_j^z\rangle_s\Big)^2 + \frac{1}{N}. \quad (54)$$

These identities give

$$\begin{aligned}&\mathbb{E}\frac{1}{\mathbb{E}_1\mathbb{E}_2 Z_2(s)^m}\mathbb{E}_1\mathbb{E}_2 Z_2(s)^m \langle (R_{1,2}-q_1)^2\rangle_{s,2} \\ &= \frac{N-1}{N}\mathbb{E}\Big(\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m \langle \sigma_i^z\sigma_j^z\rangle_s\Big)^2 - 2q_1\mathbb{E}\Big(\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m \langle \sigma_i^z\rangle_s\Big)^2 + q_1^2 + \frac{1}{N}. \quad (55)\end{aligned}$$

If the delta function is defined by

$$\delta(z^1, z^2) := \prod_{i=1}^N \sqrt{2\pi} e^{\frac{(z_i^1)^2}{2}}\delta(z_i^1 - z_i^2), \quad (56)$$

then

$$\begin{aligned}&\mathbb{E}\frac{1}{\mathbb{E}_1\mathbb{E}_2 Z_2(s)^{\frac{m}{2}}\delta(z^1,z^2)}\mathbb{E}_1\mathbb{E}_2 Z_2(s)^{\frac{m}{2}} \langle R_{1,2}\rangle_{s,2}\delta(z^1,z^2) = \mathbb{E}\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m \langle \sigma_i^z\rangle_s^2, \\ &\mathbb{E}\frac{1}{\mathbb{E}_1\mathbb{E}_2 Z_2(s)^{\frac{m}{2}}\delta(z^1,z^2)}\mathbb{E}_1\mathbb{E}_2 Z_2(s)^{\frac{m}{2}} \langle R_{1,2}^2\rangle_{s,2}\delta(z^1,z^2) = \frac{N-1}{N}\mathbb{E}\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m \langle \sigma_i^z\sigma_j^z\rangle_s^2 + \frac{1}{N}.\end{aligned}$$

These identities give

$$\begin{aligned}&\mathbb{E}\frac{1}{\mathbb{E}_1\mathbb{E}_2 Z_2(s)^{\frac{m}{2}}\delta(z^1,z^2)}\mathbb{E}_1\mathbb{E}_2 Z_2(s)^{\frac{m}{2}} \langle (R_{1,2}-q_2)^2\rangle_{s,2}\delta(z^1,z^2) \\ &= \frac{N-1}{N}\mathbb{E}\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m \langle \sigma_i^z\sigma_j^z\rangle_s^2 - 2q_2\mathbb{E}\frac{1}{\mathbb{E}_1 Z(s)^m}\mathbb{E}_1 Z(s)^m \langle \sigma_i^z\rangle_s^2 + {q_2}^2 + \frac{1}{N}. \quad (57)\end{aligned}$$

Identities (48), (55) and (57) enable us to represent the upper bound on $\psi_N'(s)$

$$\begin{aligned}\psi_N'(s) = \; & - \frac{\beta^2}{4}\Big[m\mathbb{E}\frac{1}{\mathbb{E}_1\mathbb{E}_2 Z_2(s)^m}\mathbb{E}_1\mathbb{E}_2 Z_2(s)^m \langle (R_{1,2}-q_1)^2\rangle_{s,2} \\ & + (1-m)\mathbb{E}\frac{1}{\mathbb{E}_1\mathbb{E}_2 Z_2(s)^{\frac{m}{2}}\delta(z^1,z^2)}\mathbb{E}_1\mathbb{E}_2 Z_2(s)^{\frac{m}{2}} \langle (R_{1,2}-q_2)^2\rangle_{s,2}\delta(z^1,z^2)\Big] \\ & + \frac{\beta^2}{4}[m(q_1^2 - {q_2}^2) + (1-q_2)^2 - \rho_1(s,m,q_1,q_2)]. \quad (58)\end{aligned}$$

Since the first and second terms in (58) are non-positive, the $\psi_N(1)$ is bounded by

$$\psi_N(1) \leq \psi_N(0) + \frac{\beta^2}{4}\Big[m(q_1^2 - {q_2}^2) + (1-q_2)^2 - \int_0^1 \rho_1(s,m,q_1,q_2)ds\Big]. \tag{59}$$

The partition function for $s = 0$ can be calculated easily

$$Z(0) = \mathrm{Tr} \exp \beta \sum_{i=1}^N [\sqrt{q_1} z_i \sigma_i^z + \sqrt{q_2 - q_1} z_i^1 \sigma_i^z + b\sigma_i^x] = [2\cosh Y(z, z^1, q_1, q_2)]^N, \tag{60}$$

where the above random variable is defined by

$$Y(z, z^1, q_1, q_2) := \beta\sqrt{(\sqrt{q_1}z + \sqrt{q_2 - q_1}z^1)^2 + b^2}. \tag{61}$$

Note that $q_1 = q_2 = q$ implies the following relation to the random variable defined by (15)

$$Y(z, z^1, q, q) = X(z, q). \tag{62}$$

Define 1RSB bound by the following function

$$\begin{aligned}
&\Psi(\beta, b, m, q_1, q_2) := \\
&\frac{1}{m}\mathbb{E}\log \mathbb{E}_1[2\cosh Y(z, z^1, q_1, q_2)]^m + \frac{\beta^2}{4}\Big[m(q_1^2 - {q_2}^2) + (1-q_2)^2 - \int_0^1 \rho_1(s,m,q_1,q_2)ds\Big].
\end{aligned} \tag{63}$$

The following lemma represents $\psi_N(1)$ in terms of 1RSB bound.

Lemma 4.1 *(Extended Guerra's identity for 1RSB bound)*
For any $(\beta, b, m, q_1, q_2) \in [0,\infty)^2 \times [0,1]^3$ $\psi_N(1)$ has an upper bound

$$\begin{aligned}
\psi_N(1) &= \Psi(\beta, b, m, q_1, q_2) - \frac{\beta^2}{4}\int_0^1 ds\Big[m\mathbb{E}\frac{1}{\mathbb{E}_1\mathbb{E}_2 Z_2(s)^m}\mathbb{E}_1\mathbb{E}_2 Z_2(s)^m \langle (R_{1,2} - q_1)^2\rangle_{s,2} \\
&+ (1-m)\mathbb{E}\frac{1}{\mathbb{E}_1\mathbb{E}_2 Z_2(s)^{\frac{m}{2}}\delta(z^1, z^2)}\mathbb{E}_1\mathbb{E}_2 Z_2(s)^{\frac{m}{2}}\langle (R_{1,2} - q_2)^2\rangle_{s,2}\delta(z^1, z^2)\Big].
\end{aligned} \tag{64}$$

Obviously, $\Psi(\beta, b, m, q_1, q_2)$ for any (m, q_1, q_2) gives an upper bound on $\psi_N(1)$. The inequalities (50) give the following lemma.

Lemma 4.2 *Lower and upper bounds on $\Psi(\beta, b, m, q_1, q_2)$ are given by*

$$\Psi_L(\beta, b, m, q_1, q_2) \leq \Psi(\beta, b, m, q_1, q_2) \leq \Psi_U(\beta, b, m, q_1, q_2), \tag{65}$$

where above functions are defined by

$$\begin{aligned}
\Psi_L(\beta, b, m, q_1, q_2) &:= \frac{1}{m}\mathbb{E}\log \mathbb{E}_1 \cosh^m Y(z, z^1, q_1, q_2) \\
&+ \frac{\beta^2}{4}\Big[m(q_1^2 - {q_2}^2) + (1-q_2)^2 - \Big(1 - \frac{1 - e^{-2\beta b \tanh \beta b}}{2\beta b \tanh \beta b}\Big)\Big],
\end{aligned} \tag{66}$$

$$\begin{aligned}
\Psi_U(\beta, b, m, q_1, q_2) &:= \frac{1}{m}\mathbb{E}\log \mathbb{E}_1 \cosh^m Y(z, z^1, q_1, q_2) \\
&+ \frac{\beta^2}{4}\Big[m(q_1^2 - {q_2}^2) + (1-q_2)^2 + 2q_2\Big(1 - \frac{\tanh \beta b}{\beta b}\Big)\Big].
\end{aligned} \tag{67}$$

The identity (62) implies that the 1RSB bound is identical to the RS bound defined by (14) for $q_1 = q_2 = q \in [0,1]$ for any $m \in [0,1]$,

$$\Phi(\beta, b, q) = \Psi(\beta, b, m, q, q). \tag{68}$$

Define the 1RSB solution by

$$\min_{0 \leq m \leq 1, 0 \leq q_1 \leq q_2 \leq 1} \Psi(\beta, b, m, q_1, q_2). \tag{69}$$

5 AT-type instability

The lower bound (26) in Lemma 3.2 and the upper bound (67) in Lemma 4.2 enable us to obtain the following theorem.

Theorem 5.1 *For any $(\beta, b, q, m, q_1, q_2) \in [0, \infty)^2 \times [0, 1]^4$ with $q_1 \leq q_2$, the difference between the RS and the 1RSB variational solutions has a lower bound*

$$\min_{q\in[0,1]} \Phi(\beta, b, q) - \Psi(\beta, b, m, q_1, q_2) \geq \min_{q\in[0,1]} \Theta(\beta, b, q, m, q_1, q_2), \tag{70}$$

where the function in the right hand side is defined by

$$\Theta(\beta, b, q, m, q_1, q_2) \quad := \quad \Phi_L(\beta, b, q) - \Psi_U(\beta, b, m, q_1, q_2). \tag{71}$$

The RS solution cannot be the exact solution, if the 1RSB solution (69) gives better bound for $\psi_N(1) = \varphi_N(1)$ than the RS one (29). This corresponds to the AT-type instability. Let us show this instability in the RS solution on the basis of the bound given by Theorem 5.1. For some $(m, q_1, q_2) \in [0, 1]^3$ satisfying $q_1 \leq q_2$, the condition

$$\min_{q\in[0,1]} \Theta(\beta, b, q, m, q_1, q_2) > 0, \tag{72}$$

is sufficient for the AT-type instability in the RS solution (29). Since the function $\Theta(\beta, b, q, m, q_1, q_2)$ is represented in terms of physical quantities of disordered single spin systems, its numerical calculation can be done easily. Numerical calculations by Mathematica for $\Theta(\beta, b, q, m, q_1, q_2)$ with its minimizer $q \in [0, 1]$ at several points $(\beta, b) \in [0, \infty)^2$ are obtained as follows:

$$\Theta(1/0.10, 10^{-3}, 0.92, 0.70, 0.88, 0.99) = 3.60 \times 10^{-2}, \tag{73}$$
$$\Theta(1/0.30, 10^{-3}, 0.73, 0.76, 0.71, 0.91) = 4.64 \times 10^{-3}, \tag{74}$$
$$\Theta(1/0.50, 10^{-3}, 0.53, 0.78, 0.51, 0.64) = 4.81 \times 10^{-4}, \tag{75}$$
$$\Theta(1/0.70, 10^{-3}, 0.32, 0.90, 0.31, 0.38) = 1.44 \times 10^{-5}, \tag{76}$$
$$\Theta(1/0.90, 10^{-3}, 0.12, 0.99, 0.10, 0.22) = 1.50 \times 10^{-5}. \tag{77}$$

Therefore, a computer-assisted proof by simple calculations shows that the AT-type instability exists in the RS solution for the transverse field SK model.

6 Discussions

In the present paper, the square root interpolation method developed by Guerra and Talagrand has been extended to a mean field quantum spin glass model. We have studied the transverse field Sherrington-Kirkpatrick (SK) model with the $\mathbb{Z}_2$-symmetry. First, we obtain the replica-symmetric (RS) bound $\Phi(\beta, b, q)$ for the logarithm of partition function per spin, where $\beta > 0$, $b > 0$ and $q \in [0, 1]$ are inverse temperature, strength of the transverse field and a variational parameter, respectively. Theorem 3.3 shows that the RS bound $\Phi(\beta, b, 0)$ is the exact solution, if the replica-symmetry and the $\mathbb{Z}_2$-symmetry are unbroken in the paramagnetic phase. On the other hand, Theorem 3.4 indicates that this paramagnetic RS solution cannot be exact, if the variance of overlap $R_{1,2}$ does not vanish in sufficiently low temperature and sufficiently weak transverse field [15]. Next, we study whether the spin glass RS solution $\Phi(\beta, b, q)$ with a positive minimizer q can be exact in this low temperature region. We obtain also one step replica-symmetry breaking (1RSB) bound $\Psi(\beta, b, m, q_1, q_2)$ with variational parameters $(m, q_1, q_2) \in [0, 1]^3$ satisfying $q_1 \leq q_2$. Note that $\Psi(\beta, b, m, q, q) = \Phi(\beta, b, q)$ for any $m \in [0, 1]$. Using the Falk-Bruch inequality [7], we obtain Theorem 5.1, which gives a bound on the difference $\min_q \Phi(\beta, b, q) - \Psi(\beta, b, m, q_1, q_2)$ in terms of disordered single spin systems. On the basis of Theorem 5.1, simple numerical calculations for disordered single spin systems indicate that the 1RSB bound gives better bound than the RS bound at several points. These show the existence of the de Almeida-Thouless(AT)-type instability in the RS solution. Although surely confirmed unstable region is quite narrow in the coupling constant space, our result is consistent with recently obtained results including numerical simulations [14, 15, 17, 20, 24].

In the transverse field SK model under an applied $\mathbb{Z}_2$-symmetry breaking longitudinal field, there is no proof that the RS solution $\min_q \Phi(\beta, b, q)$ is exact even in the high temperature region, since $\mathbb{E}\langle R_{1,2}\rangle_s$ may depend on $s \in [0, 1]$. In the low temperature region of this model, however, it can be confirmed numerically also that the 1RSB solution gives better bound than the RS solution in sufficiently weak longitudinal and transverse fields, as in the classical SK model. Then, the RS solution cannot be exact either under the applied longitudinal field. It turns out that the existence of the AT-type instability is not sensitive against the application of any weak longitudinal field.

It should be studied still whether the infinite RSB (∞RSB) occurs in the transverse field SK model. Also 2RSB bound is confirmed numerically to be a better bound than 1RSB solution. Since a kRSB bound gives better bound than the $(k-1)$RSB solution in the classical SK model, there exists $b_0 > 0$, such that a kRSB bound gives a better bound than the $(k-1)$RSB solution for any $b \leq b_0$ also in the transverse field SK model [10]. Therefore, the ∞RSB solution is predicted to be exact in the transverse field SK model, as in the classical SK model.

Acknowledgments It is pleasure to thank K. Hukushima, H. Leschke and M. Yamaguchi for enlightening discussions. C.I. is supported by JSPS (21K03393).

Conflict of interest statement The authors declare no conflicts of interest.

Data availability statement The authors declare that the data (73)-(77) in this study are openly available. There are no other data.

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