Electron. Commun. Probab. **24** (2019), no. 16, 1–12.
https://doi.org/10.1214/19-ECP218
ISSN: 1083-589X

ELECTRONIC COMMUNICATIONS in PROBABILITY

Error bounds in normal approximation for the squared-length of total spin in the mean field classical N-vector models*

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Abstract

This paper gives the Kolmogorov and Wasserstein bounds in normal approximation for the squared-length of total spin in the mean field classical N-vector models. The Kolmogorov bound is new while the Wasserstein bound improves a result obtained recently by Kirkpatrick and Nawaz [Journal of Statistical Physics, **165** (2016), no. 6, 1114–1140]. The proof is based on Stein's method for exchangeable pairs.

Keywords: Stein's method; Kolmogorov distance; Wasserstein distance; mean-field model.
AMS MSC 2010: 60F05.
Submitted to ECP on July 5, 2018, final version accepted on February 16, 2019.

1 Introduction and main result

Let $N \geq 2$ be an integer, and let $\mathbb{S}^{N-1}$ denote the unit sphere in $\mathbb{R}^N$. In this paper, we consider the mean-field classical N-vector spin models, where each spin σ_i is in $\mathbb{S}^{N-1}$, at a complete graph vertex i among n vertices ([5, Chapter 9]). The state space is $\Omega_n = (\mathbb{S}^{N-1})^n$ with product measure $P_n = \mu \times \cdots \times \mu$, where μ is the uniform probability measure on $\mathbb{S}^{N-1}$. In the absence of an external field, each spin configuration $\sigma = (\sigma_1, \ldots, \sigma_n)$ in the state space Ω_n has a Hamiltonian defined by

$$H_n(\sigma) = -\frac{1}{2n} \sum_{i=1}^{n} \sum_{j=1}^{n} \langle \sigma_i, \sigma_j \rangle,$$

where $\langle \cdot, \cdot \rangle$ is the inner product in $\mathbb{R}^N$. Let $\beta > 0$ be the inverse temperature. The Gibbs measure with Hamiltonian H_n is the probability measure $P_{n,\beta}$ on Ω_n with density function:

$$dP_{n,\beta}(\sigma) = \frac{1}{Z_{n,\beta}} \exp\left(-\beta H_n(\sigma)\right) dP_n(\sigma),$$

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where $Z_{n,\beta}$ is the partition function: $Z_{n,\beta} = \int_{\Omega_n} \exp\left(-\beta H_n(\sigma)\right) dP_n(\sigma)$. This model is also called the mean field $O(N)$ model. It reduces to the XY model, the Heisenberg model and the Toy model when $N = 2, 3, 4$, respectively (see, e.g., [5, p. 412]).

Before proceeding, we introduce the following notations. Throughout this paper, Z is a standard normal random variable, and $\Phi(z)$ is the probability distribution function of Z. For a real-valued function f, we write $\|f\| = \sup_x |f(x)|$. The symbol C denotes a positive constant which depends only on the inverse temperature β, and its value may be different for each appearance. For two random variables X and Y, the Wasserstein distance d_{W} and the Kolmogorov distance d_{K} between $\mathcal{L}(X)$ and $\mathcal{L}(Y)$ are as follows:

$$d_{\mathrm{W}}(\mathcal{L}(X), \mathcal{L}(Y)) = \sup_{\|h'\| \leq 1} \left| Eh(X) - Eh(Y) \right|,$$

and

$$d_{\mathrm{K}}(\mathcal{L}(X), \mathcal{L}(Y)) = \sup_{z \in \mathbb{R}} \left| P\left(X \leq z\right) - P\left(Y \leq z\right) \right|.$$

In the Heisenberg model ($N = 3$), Kirkpatrick and Meckes [6] established large deviation, normal approximation results for total spin $S_n = \sum_{i=1}^n \sigma_i$ in the non-critical phase ($\beta \neq 3$), and a non-normal approximation result in the critical phase ($\beta = 3$). The results in [6] are generalized by Kirkpatrick and Nawaz [7] to the mean field N-vector models with $N \geq 2$.

Let I_ν denote the modified Bessel function of the first kind (see, e.g., [2, p. 713]) and

$$f(x) = \frac{I_{\frac{N}{2}}(x)}{I_{\frac{N}{2}-1}(x)}, \; x > 0. \tag{1.1}$$

By Lemma A.2 in the Appendix, we have

$$\left(\frac{f(x)}{x} \right)' < 0 \text{ for all } x > 0. \tag{1.2}$$

We also have

$$\lim_{x \to 0^+} \frac{f(x)}{x} = \frac{1}{N} \text{ and } \lim_{x \to \infty} \frac{f(x)}{x} = 0. \tag{1.3}$$

In the case $\beta > N$, from (1.2) and (1.3), there is a unique strictly positive solution b to the equation

$$x - \beta f(x) = 0. \tag{1.4}$$

Based on their large deviations, Kirkpatrick and Nawaz [7] argued that in the case $\beta > N$, there exists $\varepsilon > 0$ such that

$$P\left(\left| \frac{\beta |S_n|}{n} - b \right| \geq x \right) \leq e^{-Cnx^2}$$

for all $0 \leq x \leq \varepsilon$, where $S_n = \sum_{i=1}^n \sigma_i$ is total spin. It means that $|S_n|$ is close to bn/β with high probability. On the other hand, all points on the hypersphere of radius bn/β will have equal probability due to symmetry. Based on these facts, they considered the fluctuations of the squared-length of total spin:

$$W_n := \sqrt{n} \left(\frac{\beta^2}{n^2 b^2} \left| S_n \right|^2 - 1 \right), \tag{1.5}$$

where $S_n = \sum_{j=1}^n \sigma_j$. Let

$$B^2 = \frac{4\beta^2}{(1 - \beta f'(b)) b^2} \left[1 - \frac{(N-1) f(b)}{b} - \left(f(b) \right)^2 \right]. \tag{1.6}$$

Kirkpatrick and Nawaz [7] proved that when $\beta > N$, the bounded-Lipschitz distance between W_n/B and Z is bounded by $C(\log n/n)^{1/4}$. Their proof is based on Stein's method for exchangeable pairs (see Stein [10]). Recall that a random vector (W, W') is called an exchangeable pair if $(W, W^{'})$ and $(W^{'}, W)$ have the same distribution. Kirkpatrick and Nawaz [7] construct an exchangeable pair as follows. Let W_n be as in (1.5) and let $\sigma' = \{\sigma_1', \ldots, \sigma_n'\}$, where for each i fixed, σ_i' is an independent copy of σ_i given $\{\sigma_j, j \neq i\}$, i.e., given $\{\sigma_j, j \neq i\}$, σ_i' and σ_i have the same distribution and σ_i' is conditionally independent of σ_i (see, e.g., [4, p. 964]). Let I be a random index independent of all others and uniformly distributed over $\{1, \ldots, n\}$, and let

$$W_n^{'} = \sqrt{n}\left(\frac{\beta^2}{n^2 b^2}|S_n'|^2 - 1\right), \tag{1.7}$$

where $S_n' = \sum_{j=1}^{n} \sigma_j - \sigma_I + \sigma_I'$. Then $(W_n, W_n^{'})$ is an exchangeable pair (see Kirkpatrick and Nawaz [7, p. 1124], Kirkpatrick and Meckes [6, p. 66]).

The bound $C(\log n/n)^{1/4}$ obtained by Kirkpatrick and Nawaz [7] is not sharp. The aim of this paper is to give the Kolmogorov and Wasserstein distances between W_n/B and Z with optimal rate $Cn^{-1/2}$.

The main result is the following theorem. We recall that, throughout this paper, C is a positive constant which depends only on β, and its value may be different for each appearance.

Theorem 1.1. Let $\beta > N$ and f be as in (1.1). Let b be the unique strictly positive solution to the equation $x - \beta f(x) = 0$ and B^2 as in (1.6). For W_n as defined in (1.5), we have

$$\sup_{\|h'\| \leq 1} |Eh(W_n/B) - Eh(Z)| \leq Cn^{-1/2}, \tag{1.8}$$

and

$$\sup_{z \in \mathbb{R}} |P\left(W_n/B \leq z\right) - \Phi(z)| \leq Cn^{-1/2}. \tag{1.9}$$

The Wasserstein bound in Theorem 1.1 will be a consequence of the following proposition, a version of Stein's method for exchangeable pairs. It is a special case of Theorem 2.4 of Eichelsbacher and Löwe [4] or Theorem 13.1 in [3].

Proposition 1.2. Let $(W, W^{'})$ be an exchangeable pair and $\Delta = W - W'$. If $E(\Delta|W) = \lambda(W + R)$ for some random variable R and $0 < \lambda < 1$, then

$$\sup_{\|h'\| \leq 1} |Eh(W) - Eh(Z)| \leq \sqrt{2/\pi} E\left|1 - \frac{1}{2\lambda} E(\Delta^2|W)\right| + \frac{1}{2\lambda} E|\Delta|^3 + 2E|R|.$$

The Kolmogorov distance is more commonly used in probability and statistics, and is usually more difficult to handle than the Wasserstein distance. Recently, Shao and Zhang [9] proved a very general theorem. Their result is as follows.

Proposition 1.3. Let $(W, W^{'})$ be an exchangeable pair and $\Delta = W - W'$. Let $\Delta^* := \Delta^*(W, W')$ be any random variable satisfying $\Delta^*(W, W') = \Delta^*(W', W)$ and $\Delta^* \geq |\Delta|$. If $E(\Delta|W) = \lambda(W + R)$ for some random variable R and $0 < \lambda < 1$, then

$$\sup_{z \in \mathbb{R}} |P(W \leq z) - \Phi(z)| \leq E\left|1 - \frac{1}{2\lambda} E(\Delta^2|W)\right| + \frac{1}{\lambda} E\left|E(\Delta\Delta^*|W)\right| + E|R|.$$

Shao and Zhang [9] applied their bound in Proposition 1.3 to get optimal bound in many problems, including a bound of $O(n^{-1/2})$ for the Kolmogorov distance in normal approximation of total spin in the Heisenberg model. We note that if $|\Delta| \leq a$, then the following result is an immediate corollary of Proposition 1.3. In this case, the bound is much simpler than that of Proposition 1.3.

Corollary 1.4. If $|\Delta| \le a$, then

$$\sup_{z\in\mathbb{R}} |P(W \le z) - \Phi(z)| \le E\left|1 - \frac{1}{2\lambda}E(\Delta^2|W)\right| + (E|W|+1)a + E|R|. \tag{1.10}$$

Proof. In Proposition 1.3, let $\Delta^* = a$, then

$$E\,|E(\Delta\Delta^*|W)| = aE\,|E(\Delta|W)| \le a\lambda(E|W| + E|R|). \tag{1.11}$$

If $E|R| \ge 1$, then (1.10) is trivial. If $E|R| < 1$, then (1.10) follows immediately from (1.11) and Proposition 1.3. □

For $S_n = \sum_{i=1}^n \sigma_i$, and for W_n and $W_n^{'}$ respectively defined in (1.5) and (1.7), we have

$$|\Delta| = |W_n - W_n^{'}| = \frac{\beta^2}{n^{3/2}b^2}\left||S_n|^2 - |S_n^{'}|^2\right| \le \frac{4\beta^2}{n^{1/2}b^2},$$

since $|S_n| + |S_n^{'}| \le 2n$ and $|S_n| - |S_n^{'}| \le |\sigma_I - \sigma_I^{'}| \le 2$. Therefore, we will apply Corollary 1.4 to obtain the Kolmogorov bound in Theorem 1.1.

2 Proof of the main result

The proof of Theorem 1.1 depends on Kirkpatrick and Nawaz's finding [7]. Applying Proposition 1.2 and Corollary 1.4, Theorem 1.1 follows from the following proposition.

Proposition 2.1. Let $\beta > N$, and let f be as in (1.1), b the unique strictly positive solution to the equation $x - \beta f(x) = 0$. Let W_n and $W_n^{'}$ be as in (1.5) and (1.7), respectively. Then the following statements hold:

(i) $|W_n - W_n^{'}| \le 4\beta^2 b^{-2} n^{-1/2}$ and $EW_n^2 \le C$,

(ii) $E(W_n - W_n^{'}|W_n) = \lambda(W_n + R)$, where $\lambda = \dfrac{1-\beta f'(b)}{n}$ and R is a random variable satisfying $E|R| \le Cn^{-1/2}$,

(iii) $E\left|\dfrac{1}{2\lambda}E((W_n - W_n^{'})^2|W_n)) - B^2\right| \le Cn^{-1/2}$, where B^2 is defined in (1.6).

Remark 2.2. Kirkpatrick and Nawaz's [7] used their large deviation result for total spin S_n to prove that $EW_n^2 \le C\log n$. Intuitively, we see that this bound would be improved to $EW_n^2 \le C$ since W_n approximates a normal distribution. By a more careful estimate, we can prove that $E\left(\beta|S_n|/n - b\right)^2 \le C/n$ (see Lemma A.1). This will lead to desired bound $EW_n^2 \le C$. Kirkpatrick and Nawaz's [7] also proved that

$$E\left|\frac{1}{2\lambda}E((W_n - W_n^{'})^2|W_n)) - B^2\right| \le C\left(\frac{\log n}{n}\right)^{1/4}.$$

To get optimal bound of order $n^{-1/2}$ for this term, we use a fine estimate of function $f(x) = I_{\frac{N}{2}}(x)/I_{\frac{N}{2}-1}(x)$ (Lemma A.2) and a technique developed recently by Shao and Zhang [9, Proof of (5.51)].

Proof of Proposition 2.1. (i) We have

$$\begin{aligned}|W_n - W_n^{'}| &= \frac{\beta^2}{b^2n^{3/2}}\left||S_n|^2 - |S_n^{'}|^2\right| = \frac{\beta^2}{b^2n^{3/2}}\left|\langle S_n + S_n^{'}, S_n - S_n^{'}\rangle\right| \\ &\le \frac{2\beta^2 n|S_n - S_n^{'}|}{b^2n^{3/2}} = \frac{2\beta^2|\sigma_I - \sigma_I^{'}|}{b^2n^{1/2}} \le \frac{4\beta^2}{b^2n^{1/2}}.\end{aligned}$$

The proof of the first half of (i) is completed. Now, apply Lemma A.1 given in the Appendix, we have

$$EW_n^2 = nE\left(\left(\frac{\beta|S_n|}{nb}+1\right)\left(\frac{\beta|S_n|}{nb}-1\right)\right)^2 \le CnE\left(\frac{\beta|S_n|}{nb}-1\right)^2 \le C.$$

(ii) Kirkpatrick and Nawaz [7, equation (9)] showed that

$$E(W_n - W_n^{'}|W_n) = \frac{2}{n}W_n + \frac{2}{\sqrt{n}} - \frac{2\beta}{n^{1/2}b^2}\left(\frac{\beta|S_n|}{n}\right) f\left(\frac{\beta|S_n|}{n}\right) + R_1, \tag{2.1}$$

where R_1 is a random variable satisying $E|R_1| \le Cn^{-3/2}$. Set $g(x) = xf(x), x > 0$. By Taylor's expansion, we have for some positive random variable ξ:

$$g\left(\frac{\beta|S_n|}{n}\right) = g(b) + g'(b)\left(\frac{\beta|S_n|}{n}-b\right) + \frac{g''(\xi)}{2}\left(\frac{\beta|S_n|}{n}-b\right)^2. \tag{2.2}$$

Set $V = \dfrac{\beta|S_n|}{nb} + 1$, we have $1 \le V \le C$ and

$$\begin{aligned}\frac{\beta|S_n|}{n} - b &= b\left(\frac{\beta|S_n|}{nb}-1\right) = \frac{bW_n}{\sqrt{n}V} = \frac{bW_n}{2\sqrt{n}} - \frac{bW_n}{\sqrt{n}}\left(\frac{1}{2}-\frac{1}{V}\right)\\ &= \frac{bW_n}{2\sqrt{n}} - \frac{bW_n}{2\sqrt{n}V}\left(\frac{\beta|S_n|}{nb}-1\right) = \frac{bW_n}{2\sqrt{n}} - \frac{bW_n^2}{2nV^2}.\end{aligned} \tag{2.3}$$

Combining (2.1)-(2.3) and noting that $b = \beta f(b)$, we have

$$\begin{aligned}&E(W_n - W_n^{'}|W_n)\\ &= \frac{2W_n}{n} + \frac{2}{\sqrt{n}} + R_1 - \frac{2\beta}{n^{1/2}b^2}\left(g(b) + g'(b)\left(\frac{bW_n}{2\sqrt{n}} - \frac{bW_n^2}{2nV^2}\right) + \frac{g''(\xi)}{2}\left(\frac{\beta|S_n|}{n}-b\right)^2\right)\\ &= \frac{2W_n}{n} + \frac{2}{\sqrt{n}} + R_1 - \frac{2\beta}{n^{1/2}b^2}\left(\frac{b^2}{\beta} + \left(\frac{b}{\beta}+bf'(b)\right)\left(\frac{bW_n}{2\sqrt{n}} - \frac{bW_n^2}{2nV^2}\right) + \frac{g''(\xi)b^2W_n^2}{2nV^2}\right)\\ &= \frac{1-\beta f'(b)}{n}(W_n + R),\end{aligned}$$

where

$$R = \frac{n}{1-\beta f'(b)}\left(R_1 + \frac{\beta W_n^2}{n^{3/2}V^2}\left(\frac{1}{\beta} + f'(b) - g''(\xi)\right)\right).$$

By Lemma A.2 (ii), we have $|g''(\xi)| < 6$. Since $V \ge 1$, $EW_n^2 \le C$ and $E|R_1| \le Cn^{-3/2}$, we conclude that $E|R| \le Cn^{-1/2}$. The proof of (ii) is completed.

(iii) Denote Id is the $n \times n$ identity matrix and set $\sigma^{(i)} = S_n - \sigma_i,\ b_i = \beta|\sigma^{(i)}|/n,\ r_i = \dfrac{\sigma^{(i)}}{|\sigma^{(i)}|}$. From Kirkpatrick and Nawaz [7, Equations (11) and (12)], we have

$$\begin{aligned}E((W_n - W_n^{'})^2|\sigma) = 2\lambda B^2 &+ \frac{4\beta^4}{n^4b^4}\sum_{i=1}^n\left(1-\frac{N-1}{\beta}\right)\left(|\sigma^{(i)}|^2 - \frac{(n-1)^2b^2}{\beta^2}\right)\\ &- \frac{8\beta^3}{n^4b^3}\sum_{i=1}^n\left(|\sigma^{(i)}|\langle\sigma_i,\sigma^{(i)}\rangle - \frac{n^2b^3}{\beta^3}\right)\\ &+ \frac{4\beta^4}{n^4b^4}\sum_{i=1}^n\left(\langle\sigma_i,\sigma^{(i)}\rangle^2 - \left(1-\frac{N-1}{\beta}\right)\frac{(n-1)^2b^2}{\beta^2}\right)\\ &+ \frac{4\beta^4}{n^4b^4}\sum_{i=1}^n\sum_{j,k\ne i}\sigma_j^T R_i'\sigma_k,\end{aligned}$$

where

$$R_i' = \left(\frac{f(b_i)}{b_i} - \frac{1}{\beta}\right) Id - \left(\frac{Nf(b_i)}{b_i} - \frac{N}{\beta}\right) P_i - \left(f(b_i) - \frac{b}{\beta}\right)(r_i\sigma_i^T + \sigma_i r_i^T),$$

and P_i is orthogonal projection onto r_i. Therefore,

$$\frac{1}{2\lambda}E((W_n - W_n^{'})^2|\sigma)) - B^2 = \frac{2\beta^4}{n^3 b^4(1-\beta f'(b))}\left(R_2 - \frac{2b}{\beta}R_3 + R_4 + R_5\right), \tag{2.4}$$

where

$$\begin{aligned}
R_2 &= \sum_{i=1}^n \left(1 - \frac{N-1}{\beta}\right)\left(|\sigma^{(i)}|^2 - \frac{(n-1)^2 b^2}{\beta^2}\right),\\
R_3 &= \sum_{i=1}^n \left(|\sigma^{(i)}|\langle \sigma_i, \sigma^{(i)}\rangle - \frac{n^2 b^3}{\beta^3}\right),\\
R_4 &= \sum_{i=1}^n \left(\langle \sigma_i, \sigma^{(i)}\rangle^2 - \left(1 - \frac{N-1}{\beta}\right)\frac{(n-1)^2 b^2}{\beta^2}\right),\\
R_5 &= \sum_{i=1}^n \sum_{j,k\neq i} \sigma_j^T R_i' \sigma_k.
\end{aligned}$$

For R_2, noting that $|\sigma^{(i)} - S_n| \le 1$, then by Lemma A.1, we have

$$\left(E\left|\frac{\beta|\sigma^{(i)}|}{n} - b\right|\right)^2 \le E\left|\frac{\beta|\sigma^{(i)}|}{n} - b\right|^2 \le E\left|\frac{\beta|S_n|}{n} - b\right|^2 + \frac{C}{n^2} \le \frac{C}{n}. \tag{2.5}$$

Thus,

$$\begin{aligned}
E|R_2| &\le C\sum_{i=1}^n E\left||\sigma^{(i)}|^2 - \frac{(n-1)^2 b^2}{\beta^2}\right|\\
&\le Cn^2 \sum_{i=1}^n \left(E\left|\frac{\beta^2|\sigma^{(i)}|^2}{n^2} - b^2\right| + \frac{(2n-1)b^2}{n^2}\right)\\
&\le Cn^2\left(\sum_{i=1}^n E\left|\frac{\beta|\sigma^{(i)}|}{n} - b\right| + C\right) \le Cn^{5/2}.
\end{aligned} \tag{2.6}$$

For R_3, we have

$$\begin{aligned}
E|R_3| &= E\left|\sum_{i=1}^n \left(|S_n|\langle\sigma_i, S_n\rangle - \frac{n^2b^3}{\beta^3} + |\sigma^{(i)}|\langle\sigma_i, \sigma^{(i)}\rangle - |S_n|\langle\sigma_i, S_n\rangle\right)\right|\\
&\le E\left||S_n|^3 - \frac{n^3b^3}{\beta^3}\right| + E\left|\sum_{i=1}^n |\sigma^{(i)}|\langle\sigma_i, \sigma^{(i)}\rangle - |S_n|\langle\sigma_i, S_n\rangle\right|\\
&\le Cn^2 E\left||S_n| - \frac{nb}{\beta}\right| + E\left|\sum_{i=1}^n \left(|\sigma^{(i)}| - |S_n|\right)\langle\sigma_i, \sigma^{(i)}\rangle - |S_n|\langle\sigma_i, \sigma_i\rangle\right|\\
&\le Cn^3 E\left|\frac{\beta|S_n|}{n} - b\right| + E\sum_{i=1}^n \left(|\langle\sigma_i, \sigma^{(i)}\rangle| + |S_n|\right)\\
&\le Cn^3 E\left|\frac{\beta|S_n|}{n} - b\right| + Cn^2 \le Cn^{5/2}.
\end{aligned} \tag{2.7}$$

To bound $E|R_5|$, we note that

$$
\begin{aligned}
&\sum_{i=1}^n \sum_{j,k\neq i} \sigma_j^T R_i' \sigma_k \\
&= \sum_{i=1}^n \sum_{j,k\neq i} \left[\left(\frac{f(b_i)}{b_i} - \frac{1}{\beta} \right) \langle \sigma_j, \sigma_k \rangle - \left(f(b_i) - \frac{b}{\beta} \right) \sigma_j^T (r_i \sigma_i^T + \sigma_i r_i^T) \sigma_k \right] \\
&\quad - \sum_{i=1}^n \sum_{j,k\neq i} \left(\frac{N f(b_i)}{b_i} - \frac{N}{\beta} \right) \sigma_j^T P_i \sigma_k \\
&= \sum_{i=1}^n \left[\left(\frac{f(b_i)}{b_i} - \frac{1}{\beta} \right) |\sigma^{(i)}|^2 - 2 \left(f(b_i) - \frac{b}{\beta} \right) |\sigma^{(i)}| \langle \sigma^{(i)}, \sigma_i \rangle \right] \\
&\quad - \sum_{i=1}^n \left(\frac{N f(b_i)}{b_i} - \frac{N}{\beta} \right) \sum_{j,k\neq i} \mathrm{Trace}(\sigma_k \sigma_j^T r_i r_i^T) \\
&= \sum_{i=1}^n \left[\left(\frac{f(b_i)}{b_i} - \frac{1}{\beta} \right) |\sigma^{(i)}|^2 - 2 \left(f(b_i) - \frac{b}{\beta} \right) |\sigma^{(i)}| \langle \sigma^{(i)}, \sigma_i \rangle \right] \\
&\quad - \sum_{i=1}^n \left(\frac{N f(b_i)}{b_i} - \frac{N}{\beta} \right) \langle \sigma^{(i)}, r_i \rangle^2 \\
&= \sum_{i=1}^n (1-N) \left(\frac{f(b_i)}{b_i} - \frac{1}{\beta} \right) |\sigma^{(i)}|^2 - 2 \sum_{i=1}^n \left(f(b_i) - \frac{b}{\beta} \right) |\sigma^{(i)}| \langle \sigma^{(i)}, \sigma_i \rangle \\
&:= R_{51} - 2R_{52}.
\end{aligned}
$$

Since $1/\beta = f(b)/b$ and $b_i = \beta|\sigma^{(i)}|/n$, we have

$$
\begin{aligned}
E|R_{51}| &= E\left| \sum_{i=1}^n (1-N) \left(\frac{f(b_i)}{b_i} - \frac{f(b)}{b} \right) |\sigma^{(i)}|^2 \right| \\
&\leq Cn^2 \sum_{i=1}^n E|b_i - b| \text{ (by Lemma A.2 (iii) and the fact that } |\sigma^{(i)}| \leq n) \\
&\leq Cn^2 \sum_{i=1}^n E\left(\left| \frac{\beta|S_n|}{n} - b \right| + \frac{\beta}{n} \left(|\sigma^{(i)}| - |S_n| \right) \right) \\
&\leq Cn^{5/2} \text{ (by (2.5) and the fact that } ||\sigma^{(i)}| - |S_n|| \leq 1).
\end{aligned}
\tag{2.8}
$$

Similarly,

$$
\begin{aligned}
E|R_{52}| &= E\left| \sum_{i=1}^n (1-N) \left(f(b_i) - f(b) \right) |\sigma^{(i)}| \langle \sigma^{(i)}, \sigma_i \rangle \right| \\
&\leq Cn^2 \sum_{i=1}^n E|b_i - b| \text{ (by Lemma A.2 (i) and the fact that } |\sigma^{(i)}| \leq n) \\
&\leq Cn^{5/2}.
\end{aligned}
\tag{2.9}
$$

Combining (2.8) and (2.9), we have

$$
E|R_5| \leq Cn^{5/2}. \tag{2.10}
$$

Bounding $E|R_4|$ is the most difficult part. Here we follow a technique developed by Shao and Zhang [9, Proof of (5.51)]. Set

$$
a = \left(1 - \frac{N-1}{\beta}\right) \frac{(n-1)^2 b^2}{\beta^2},\ \sigma^{(1,2)} = S_n - \sigma_1 - \sigma_2, V_1 = \langle \sigma_1, \sigma^{(1,2)} \rangle^2,\ V_2 = \langle \sigma_2, \sigma^{(1,2)} \rangle^2,
$$

we have

$$\left|\langle\sigma_1,\sigma^{(1)}\rangle^2 - V_1\right| \le Cn, \ \left|\langle\sigma_1,\sigma^{(2)}\rangle^2 - V_2\right| \le Cn.$$

It follows that

$$\begin{aligned} ER_4^2 &= nE\left(\langle\sigma_1,\sigma^{(1)}\rangle^2 - a\right)^2 - n(n-1)E\left(\langle\sigma_1,\sigma^{(1)}\rangle^2 - a\right)\left(\langle\sigma_2,\sigma^{(2)}\rangle^2 - a\right) \\ &\le Cn^5 + n(n-1)\left|E\left(\langle\sigma_1,\sigma^{(1)}\rangle^2 - V_1 + V_1 - a\right)\left(\langle\sigma_2,\sigma^{(2)}\rangle^2 - V_2 + V_2 - a\right)\right| \\ &\le Cn^5 + n(n-1)|E\left(V_1 - a\right)\left(V_2 - a\right)| \qquad (2.11) \\ &\le Cn^5 + n(n-1)|E\left(V_1 - E(V_1|(\sigma_j)_{j>2})\right)\left(V_2 - E(V_2|(\sigma_j)_{j>2})\right)| \\ &\quad + n(n-1)|E\left(E(V_1|(\sigma_j)_{j>2}) - a\right)\left(E(V_2|(\sigma_j)_{j>2}) - a\right)| \\ &:= Cn^5 + n(n-1)(|R_{41}| + |R_{42}|). \end{aligned}$$

Define a probability density function

$$p_{12}(x,y) = \frac{1}{Z_{12}^2}\exp\left(\frac{\beta}{n}\langle x+y,\sigma^{(1,2)}\rangle\right), x,y \in \mathbb{S}^{N-1}, \tag{2.12}$$

where Z_{12}^2 is the normalizing constant. Let $(\xi_1,\xi_2) \sim p_{12}(x,y)$ given $(\sigma_j)_{j>2}$, and for $i=1,2$

$$\tilde{V}_i = E\left(\langle\xi_i,\sigma^{(1,2)}\rangle^2|(\sigma_j)_{j>2}\right). \tag{2.13}$$

Similar to Shao and Zhang [9, pages 97, 98], we can show that

$$R_{41} = E\left(\langle\xi_i,\sigma^{(1,2)}\rangle^2 - \tilde{V}_1\right)\left(\langle\xi_i,\sigma^{(1,2)}\rangle^2 - \tilde{V}_2\right) + H_1, \tag{2.14}$$

and

$$R_{42} = E\left(\tilde{V}_1 - a\right)\left(\tilde{V}_2 - a\right) + H_2, \tag{2.15}$$

where $|H_1| \le Cn^3$ and $|H_2| \le Cn^3$. Let

$$b_{12} = \frac{\beta|\sigma^{(1,2)}|}{n}. \tag{2.16}$$

By Lemma A.3 and the definition of a, we have

$$\begin{aligned} \left|\tilde{V}_1 - a\right| &= \left|\left(1 - \frac{(N-1)f(b_{12})}{b_{12}}\right)|\sigma^{(1,2)}|^2 - \left(1 - \frac{N-1}{\beta}\right)\frac{(n-1)^2b^2}{\beta^2}\right| \\ &= \left|\left(1 - \frac{N-1}{\beta}\right)\left(|\sigma^{(1,2)}|^2 - \frac{(n-1)^2b^2}{\beta^2}\right) + (N-1)\left(\frac{1}{\beta} - \frac{f(b_{12})}{b_{12}}\right)|\sigma^{(1,2)}|^2\right| \\ &\le Cn^2\left(\left|\frac{\beta^2|\sigma^{(1,2)}|^2}{n^2} - \frac{(n-1)^2b^2}{n^2}\right| + \left|\frac{f(b)}{b} - \frac{f(b_{12})}{b_{12}}\right|\right) \\ &\le Cn^2\left(\left|\frac{\beta^2|S_n|^2}{n^2} - b^2\right| + |b_{12} - b|\right) + Cn \\ &\le Cn^2\left(\left|\frac{\beta|S_n|}{n} - b\right| + \left|\frac{\beta|\sigma^{(1,2)}|}{n} - b\right|\right) + Cn \le Cn^2\left|\frac{\beta|S_n|}{n} - b\right| + Cn. \end{aligned}$$

Using similar estimate for $\left|\tilde{V}_2 - a\right|$, then we have

$$\begin{aligned} E\left|\left(\tilde{V}_1 - a\right)\left(\tilde{V}_2 - a\right)\right| &\le C\left(n^4E\left|\frac{\beta|S_n|}{n} - b\right|^2 + n^3E\left|\frac{\beta|S_n|}{n} - b\right| + n^2\right) \\ &\le Cn^3 \text{ (by Lemma A.1).} \end{aligned} \tag{2.17}$$

Note that given $(\sigma_j)_{j>2}$, ξ_1 and ξ_2 are conditionally independent. It implies that

$$E\left(\langle\xi_i,\sigma^{(1,2)}\rangle^2-\tilde{V}_1\right)\left(\langle\xi_i,\sigma^{(1,2)}\rangle^2-\tilde{V}_2\right)=0. \tag{2.18}$$

Combining (2.11)-(2.18), we have $ER_4^2\le Cn^5$, and so

$$E|R_4|\le Cn^{5/2}. \tag{2.19}$$

Combining (2.4), (2.6), (2.7), (2.10) and (2.19), we have

$$E\left|\frac{1}{2\lambda}E((W_n-W_n^{'})^2|W_n))-B^2\right|\le Cn^{-1/2}.$$

The proposition is proved. □

A Appendix

In this Section, we will prove the technical results that used in the proof of Theorem 1.1.

Lemma A.1. We have

$$E\Big|\frac{\beta|S_n|}{n}-b\Big|^2\le\frac{C}{n}.$$

Proof. By the large deviation for S_n/n [7, Proposition 2] and the argument in [7, p. 1126], one can prove that there exists $\varepsilon>0$ such that

$$P\left(\left|\frac{\beta|S_n|}{n}-b\right|\ge x\right)\le e^{-Cnx^2}$$

for all $0\le x\le\varepsilon$. Since $\left|\frac{\beta|S_n|}{n}-b\right|\le C$, it implies that

$$\begin{aligned}E\left|\frac{\beta|S_n|}{n}-b\right|^2&\le 2\int_0^\varepsilon xP\left(\left|\frac{\beta|S_n|}{n}-b\right|>x\right)dx\\&\quad+E\left(\left|\frac{\beta|S_n|}{n}-b\right|^2I\left(\left|\frac{\beta|S_n|}{n}-b\right|>\varepsilon\right)\right)\\&\le 2\int_0^\varepsilon xe^{-Cnx^2}dx+CP\left(\left|\frac{\beta|S_n|}{n}-b\right|>\varepsilon\right)\\&\le\frac{C}{n}+Ce^{-Cn\varepsilon^2}\le\frac{C}{n}.\end{aligned}$$

□

Lemma A.2. Let $x>0$ and $f(x)=\dfrac{I_{N/2}(x)}{I_{N/2-1}(x)}$. Then the following statements hold:

(i) $0<f'(x)<\dfrac{1}{N-1}\le 1$.

(ii) $|(xf(x))''|<6$.

(iii) $-5\le\dfrac{-5}{N-1}<\left(\dfrac{f(x)}{x}\right)'<0$.

Proof. As was showed in [7, p. 1134], we have

$$f'(x)=1-\frac{N-1}{x}f(x)-f^2(x). \tag{A.1}$$

It implies

$$\frac{f(x)}{x} = \frac{1 - f'(x) - f^2(x)}{N-1}, \tag{A.2}$$

and

$$f^2(x) = 1 - \frac{N-1}{x} f(x) - f'(x). \tag{A.3}$$

Amos [1, p. 243] proved that

$$0 < f'(x) < \frac{f(x)}{x}. \tag{A.4}$$

Combining (A.2)-(A.4), we have

$$0 < f'(x) < \frac{f(x)}{x} < \frac{1}{N-1}, \text{ and } f^2(x) < 1. \tag{A.5}$$

Therefore,

$$\begin{aligned}
|(xf(x))''| &= |2f'(x) + xf''(x)| \\
&= \left| 2f'(x) + x\left(-f'(x)\left(\frac{N-1}{x} + 2f(x)\right) + \frac{N-1}{x^2} f(x)\right)\right| \\
&\le 2 + (N-1)f'(x) + 2xf(x)f'(x) + \frac{(N-1)f(x)}{x} \\
&\le 4 + 2f^2(x) \text{ (by the first half of (A.5))} \\
&\le 6 \text{ (by the second half of (A.5))}.
\end{aligned}$$

The proof of (i) and (ii) is completed. For (iii), we have

$$\left(\frac{f(x)}{x}\right)' = \frac{1}{x}\left(f'(x) - \frac{f(x)}{x}\right). \tag{A.6}$$

Combining the first half of (A.5) and (A.6), we have $\left(\frac{f(x)}{x}\right)' < 0$. It follows from (A.1), (A.5) and (A.6) that

$$\left(\frac{f(x)}{x}\right)' = \frac{1}{x}\left(1 - \frac{Nf(x)}{x}\right) - \frac{f^2(x)}{x} > \frac{1}{x}\left(1 - \frac{Nf(x)}{x}\right) - \frac{1}{N-1}. \tag{A.7}$$

Apply Theorem 2 (a) of Nåsell [8], we can show that

$$\frac{1}{x}\left(1 - \frac{Nf(x)}{x}\right) > \frac{-4}{N-1}. \tag{A.8}$$

Combining (A.7) and (A.8), we have $\left(\frac{f(x)}{x}\right)' > \frac{-5}{N-1}$. The proof of (iii) is completed. □

Lemma A.3. With the notation in the proof of Theorem 1.1, we have

$$\tilde{V}_i = |\sigma^{(1,2)}|^2 \left(1 - \frac{(N-1)f(b_{12})}{b_{12}}\right), \ i = 1, 2.$$

Proof. Let $A_N = 2\pi^{N/2}/\Gamma(N/2)$ the Lebesgue measure of S^{N-1}. It follows from (2.12) that

$$\begin{aligned}
Z_{12}^2 &= \int_{S^{N-1}}\int_{S^{N-1}} \exp\left(\frac{\beta}{n}\langle x+y, \sigma^{(1,2)}\rangle\right) d\mu(x)d\mu(y) \\
&= \left(\int_{S^{N-1}} \exp\left(\frac{\beta}{n}\langle x, \sigma^{(1,2)}\rangle\right) d\mu(x)\right)^2 \\
&= \left(\frac{A_{N-1}}{A_N}\int_0^\pi e^{b_{12}\cos\varphi_{N-2}} \sin^{N-2}\varphi_{N-2} d\varphi_{N-2}\right)^2 \\
&= \left(\frac{A_{N-1}}{A_N}\frac{\sqrt{\pi}\Gamma(N/2-1/2)}{(b_{12}/2)^{N/2-1}} I_{N/2-1}(b_{12})\right)^2,
\end{aligned}$$

where we have used formula

$$I_\nu(z) = \frac{1}{\sqrt{\pi}\Gamma(\nu+1/2)}\left(\frac{\nu}{2}\right)^\nu \int_0^\pi \exp(z\cos\theta)\sin^{2\nu}\theta d\theta$$

(see, e.g., Exercise 11.5.4 in [2]) in the last equation. For $i = 1, 2$, we have

$$\begin{aligned}
\tilde{V}_i &= \frac{1}{Z_{12}}\int_{\mathbb{S}^{N-1}} \langle\theta, \sigma^{(1,2)}\rangle^2 \exp\left[\frac{\beta}{n}\langle\theta, \sigma^{(1,2)}\rangle\right] d\mu(\theta) \\
&= \frac{1}{Z_{12}}\int_{\mathbb{S}^{N-1}} |\sigma^{(1,2)}|^2 \left\langle\theta, \frac{\sigma^{(1,2)}}{|\sigma^{(1,2)}|}\right\rangle^2 \exp\left(\frac{\beta|\sigma^{(1,2)}|}{n}\left\langle\theta, \frac{\sigma^{(1,2)}}{|\sigma^{(1,2)}|}\right\rangle\right) d\mu(\theta) \\
&= |\sigma^{(1,2)}|^2 \frac{A_{N-1}}{A_N Z_{12}}\int_0^\pi \cos^2\varphi_{N-2}\sin^{N-2}\varphi_{N-2} e^{b_{12}\cos\varphi_{N-2}} d\varphi_{N-2} \\
&= |\sigma^{(1,2)}|^2 \frac{A_{N-1}}{A_N Z_{12}}\int_0^\pi e^{b_{12}\cos\varphi_{N-2}}\sin^{N-2}\varphi_{N-2} d\varphi_{N-2} \\
&\quad - \int_0^\pi e^{b_{12}\cos\varphi_{N-2}}\sin^N\varphi_{N-2} d\varphi_{N-2} \\
&= \left(1 - \frac{A_{N-1}}{A_N Z_{12}}\int_0^\pi e^{b_{12}\cos\varphi_{N-2}}\sin^N\varphi_{N-2} d\varphi_{N-2}\right)|\sigma^{(1,2)}|^2 \\
&= \left(1 - \frac{A_{N-1}}{A_N Z_{12}}\frac{\sqrt{\pi}\Gamma(N/2+1/2)}{(b_{12}/2)^{N/2}} I_{N/2}(b_{12})\right)|\sigma^{(1,2)}|^2 \\
&= \left(1 - \frac{(N-1)f(b_{12})}{b_{12}}\right)|\sigma^{(1,2)}|^2.
\end{aligned}$$

□

Finally, we would like to note again that Proposition 1.2 is a special case of Theorem 2.4 of Eichelsbacher and Löwe [4] or Theorem 13.1 in [3], but the constants in the bound may be different from those of Theorem 2.4 in [4] or Theorem 13.1 in [3]. Since the proof is short and simple, we will present here.

Proof of the Proposition 1.2. Let $h : \mathbb{R} \to \mathbb{R}$ such that $\|h'\| \le 1$ and $E|h(Z)| < \infty$, and let $f := f_h$ be the unique solution to the Stein's equation $f'(w) - wf(w) = h(w) - Eh(Z)$. Since (W, W') is an exchangeable pair and $E(W - W'|W) = \lambda(W + R)$,

$$\begin{aligned}
0 &= E(W - W')(f(W) + f(W')) \\
&= E(W - W')(f(W') - f(W)) + 2Ef(W)(W - W') \\
&= E(W - W')(f(W') - f(W)) + 2\lambda Ef(W)E(W - W'|W) \\
&= E\Delta(f(W') - f(W)) + 2\lambda EWf(W) + 2\lambda Ef(W)R.
\end{aligned}$$

It thus follows that

$$
\begin{aligned}
&|Eh(W) - Eh(Z)| \\
&= |E(f'(W) - Wf(W))| \\
&= \left| E\left(f'(W) + \frac{1}{2\lambda} E\Delta(f(W') - f(W)) + Ef(W)R \right) \right| \\
&= \left| E\left(f'(W)\left(1 - \frac{1}{2\lambda}E(\Delta^2|W)\right) + \frac{1}{2\lambda}\Delta\left(f(W') - f(W) + \Delta f'(W)\right) + f(W)R \right) \right| \\
&\le \|f'\| E\left|1 - \frac{1}{2\lambda}E(\Delta^2|W)\right| + \frac{1}{4\lambda}\|f''\| E\left|\Delta\right|^3 + \|f\| E|R|.
\end{aligned} \tag{A.9}
$$

By Lemma 2.4 in [3] we have

$$
\|f\| \le 2,\ \|f'\| \le \sqrt{2/\pi},\ \|f''\| \le 2. \tag{A.10}
$$

The conclusion of the proposition follows from (A.9) and (A.10). □

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Acknowledgments. We are grateful to the Associate Editor and an anonymous referee whose comments have been very useful to make our development clearer and more comprehensive.