Alignment and matching tests for high-dimensional tensor signals by tensor contraction

Ruihan Liu* Zhenggang Wang[†] Jianfeng Yao[‡]

*Department of Statistics and Actuarial Science, The University of Hong Kong.

[‡]School of Data Science, The Chinese University of Hong Kong (Shenzhen).

Abstract

We consider two hypothesis testing problems for low-rank and high-dimensional tensor signals, namely the tensor signal alignment and tensor signal matching problems. These problems are challenging due to the high dimension of tensors and lack of meaningful test statistics. By exploiting a recent tensor contraction method, we propose and validate relevant test statistics using eigenvalues of a data matrix resulting from the tensor contraction. The matrix has a long range dependence among its entries, which makes the analysis of the matrix challenging, involved and distinct from standard random matrix theory. Our approach provides a novel framework for addressing hypothesis testing problems in the context of high-dimensional tensor signals.

Keywords: high-dimensional tensors; low-rank tensors; tensor signal alignment; tensor signal matching; tensor contraction; linear spectral statistics; random matrix theory.

MSC 2010 subject classifications: Primary 62H15; Secondary 60B20,62H10

*E-mail: rhliu@connect.hku.hk †E-mail: zgwangsrmkph@gmail.com ‡E-mail: jeffyao@cuhk.edu.cn

1

1 Introduction

In the era of "big data", the analysis of high-dimensional tensor data has become increasingly important in various fields, including genomics, economics, image analysis, and machine learning. High-order tensor data often exhibit intrinsic low-rank structures [26, 41]. To capture these low-rank structures, the "signal plus noise" tensor model has been widely adopted [27, 18, 22]. Let $n_1, \ldots, n_d \in \mathbb{N}^+$ denote d dimension numbers, where $d \geq 3$, and let $N = n_1 + \cdots + n_d$. The d-fold rank-R spiked tensor model is defined as:

$$T = \sum_{r=1}^{R} \beta_r \boldsymbol{x}^{(r,1)} \otimes \cdots \otimes \boldsymbol{x}^{(r,d)} + \frac{1}{\sqrt{N}} \boldsymbol{X},$$
 (1)

where $\beta_1 \geq \cdots \geq \beta_R > 0$ are the signal-to-noise ratios (SNRs), $\{\boldsymbol{x}^{(1,l)}, \cdots, \boldsymbol{x}^{(R,l)}\}$ are mutually orthogonal unit vectors \mathbb{R}^{n_l} for each $1 \leq l \leq d$ [25], and $\boldsymbol{X} = (X_{i_1 \cdots i_d})_{n_1 \times \cdots \times n_d} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ is a noise tensor with independent and identically distributed (i.i.d.) entries, each having zero mean and unit variance. Specifically, the rank-1 spiked tensor model [35] is given by:

$$T = \beta x^{(1)} \otimes \cdots \otimes x^{(d)} + \frac{1}{\sqrt{N}} X,$$
 (2)

where $\beta > 0$ is the single SNR of the model.

The primary focus of most existing literature is on recovering the signal vectors $\{x^{(1,l)}, \ldots, x^{(R,l)}\}$, $1 \leq l \leq d$ from the observed tensor T, with a particular emphasis on the computational efficiency of recovery algorithms. In the case of the rank-one model (2) with symmetric and i.i.d. Gaussian noise X, [21] showed that computing the maximum likelihood (ML) estimator of $\beta x^{(1)} \otimes \cdots \otimes x^{(d)}$ is in general NP-hard, and [4] provided a comprehensive discussion on the relationship between the computational complexity of the ML estimator and the value of the SNR β . To reduce the computational complexity, [35] proposed the use of the power iteration method and approximate message passing (AMP) algorithms. These two methods have been extensively investigated by [27, 13, 34, 23, 9] for AMP and by [22] for power iteration. Moreover, [35] introduced the tensor unfolding method, which involves unfolding the tensor data T into matrices, enabling the recovery of signals through Principal Component Analysis (PCA). [10] conducted a comprehensive study of the tensor unfolding method for the general asymmetric model (2) under fairly general noise distribution assumptions.

However, when the SNRs fall below the phase transition threshold, these recovery methods often fail. In such cases, a less ambitious but potentially more achievable goal is to test the alignment of a signal in T with a given directional tensor $\mathbf{a}^{(1)} \otimes \cdots \otimes \mathbf{a}^{(d)}$, where $\mathbf{a}^{(j)}, 1 \leq j \leq d$ are d given directional unit vectors in \mathbb{R}^{n_j} , respectively. This leads to the following tensor signal alignment test between two hypotheses:

$$H_0: \boldsymbol{a}^{(l)} \perp \boldsymbol{x}^{(r,l)} \text{ for } 1 \leq l \leq d, \ 1 \leq r \leq R.$$

$$H_1: \text{there exists at least one } 1 \leq l \leq d, \ 1 \leq r \leq R \text{ such that } \boldsymbol{a}^{(1)} \not\perp \boldsymbol{x}^{(r,l)}.$$
(3)

Despite the tensor signal alignment test appearing more tractable than signal recovery, to the best of our knowledge, there is no established and rigorously justified procedure for addressing this problem. The difficulty stems from the high dimensionality of the tensors and the lack of a meaningful test statistic.

We leverage the tensor contraction operator Φ_d , originally proposed in [36], which maps an arbitrary tensor T and unit vectors $\{a^{(j)}\}$ to a matrix R:

$$\Phi_{d}: \mathbb{R}^{n_{1} \times \cdots \times n_{d}} \times \mathbb{S}^{n_{1}-1} \times \cdots \times \mathbb{S}^{n_{d}-1} \longrightarrow \mathbb{R}^{N \times N},
(\boldsymbol{T}, \boldsymbol{a}^{(1)}, \cdots, \boldsymbol{a}^{(d)}) \longmapsto \boldsymbol{R} = \begin{pmatrix}
\boldsymbol{0}_{n_{1} \times n_{1}} & \boldsymbol{T}^{12} & \cdots & \boldsymbol{T}^{1d} \\
(\boldsymbol{T}^{12})' & \boldsymbol{0}_{n_{2} \times n_{2}} & \cdots & \boldsymbol{T}^{2d} \\
\vdots & \vdots & \ddots & \vdots \\
(\boldsymbol{T}^{1d})' & (\boldsymbol{T}^{2d})' & \cdots & \boldsymbol{0}_{n_{d} \times n_{d}}
\end{pmatrix}.$$
(4)

Here, for a pair of indices $1 \leq j_1 < j_2 \leq d$, $T^{j_1j_2}$ is an $n_{j_1} \times n_{j_2}$ matrix, called second order contraction matrix of T along the directions $\{a^{(j_1)}, a^{(j_2)}\}$, as introduced in [28]. It is defined by:

$$\mathbf{T}^{j_1 j_2} = \left[\sum_{i_j=1, j \neq j_1, j_2}^{n_j} T_{i_1 \cdots i_d} \prod_{l=1, l \neq j_1, j_2}^{d} a_{i_l}^{(l)} \right]_{n_{j_1} \times n_{j_2}}.$$
 (5)

From a mathematical perspective, the contraction operator Φ_d has several advantages. Firstly, Φ_d is linear in T. When applied to the R-rank tensor in (1), we have

$$R = \Phi_d(T, \boldsymbol{a}^{(1)}, \dots, \boldsymbol{a}^{(d)})$$

$$= \sum_{r=1}^d \beta_r \Phi_d(\boldsymbol{x}^{(r,1)} \otimes \dots \otimes \boldsymbol{x}^{(r,d)}, \boldsymbol{a}^{(1)}, \dots, \boldsymbol{a}^{(d)}) + \frac{1}{\sqrt{N}} \Phi_d(\boldsymbol{X}, \boldsymbol{a}^{(1)}, \dots, \boldsymbol{a}^{(d)}),$$

$$= \boldsymbol{S} + \boldsymbol{M}.$$
(6)

where S is the contracted signal matrix containing the R tensor signals, and M is the residual matrix representing pure noise. Under the null hypothesis H_0 , S = 0 implying R = M. In contrast, under the alternative H_1 , $S \neq 0$, result in $R \neq M$.

Furthermore, both the contracted signal matrix S and noise matrix M are symmetric, with S having a finite rank. This allows us to analyze the contracted data matrix R using linear spectral statistics (LSS), a powerful tool from random matrix theory. Central limit theorems for LSS of random matrices have received much attention in high-dimensional statistics, see [6, 30, 5, 33, 42] for a few classical references. In our case, by employing an appropriate LSS of R with an established asymptotic distribution, we can effectively distinguish between the two hypotheses.

We first establish that the eigenvalue distribution of R has a limit ν when the d dimensions $\{n_j\}$ grow to infinity in comparable rates. Next, we introduce the following test statistic:

$$\widehat{T}_N^{(d)} = \|\mathbf{R}\|_2^2 - N \int_{-\infty}^{\infty} x^2 \nu(dx).$$
 (7)

Here, $\|\mathbf{R}\|_2^2 = \sum_{i,j=1}^N R_{i,j}^2$ is a linear spectral statistic of \mathbf{R} . As one of the main results of this paper, we establish that under the null hypothesis H_0 ,

$$\frac{\widehat{T}_N^{(d)} - \xi_N^{(d)}}{\sigma_N^{(d)}} \xrightarrow{d} \mathcal{N}(0, 1), \tag{8}$$

where $\xi_N^{(d)}$ and $\sigma_N^{(d)}$ are known parameters that can be calculated numerically. Under the alternative hypothesis H_1 ,

$$\frac{\widehat{T}_N^{(d)} - \xi_N^{(d)}}{\sigma_N^{(d)}} - \mathcal{D}^{(d)} / \sigma_N^{(d)} \xrightarrow{d} \mathcal{N}(0, 1), \tag{9}$$

where $\mathcal{D}^{(d)}/\sigma_N^{(d)}$ is a positive mean drift, the details of which are provided in §4. Consequently, the asymptotic normal distribution in (8) enables us to construct a test for a given significance level α , while the distribution in (9) guarantees a positive power for the test, which depends on the magnitude of $\mathcal{D}^{(d)}/\sigma_N^{(d)}$.

When d = 2, the tensor model (1) reduces to a finite-rank perturbed or spiked random matrix. In this context, the signal alignment test in (3) can be seen as a tensor extension of existing tests for the presence of spikes along given directions, as studied by [17, 38, 32, 37, 8].

However, when $d \geq 3$, a fundamental difference emerges: the elements $\mathbf{T}^{j_1j_2}$ in the contracted data matrix \mathbf{R} become correlated. This correlation significantly increases the complexity of studying the matrix, making the analysis more challenging compared to the d=2 case. The presence of these correlations necessitates the development of novel techniques to effectively analyze the eigenvalue distribution and establish the asymptotic properties of the test statistic $\widehat{T}_N^{(d)}$ in high dimensions.

The main contributions of this article are as follows.

- (i) We conduct an in-depth analysis of the contracted data matrix \mathbf{R} , whose entries display significant correlations and deviate from traditional random matrix models in which the elements of the noise matrix are typically assumed to be independent of one another, including
 - (a) The characterization of its limiting spectral distribution (LSD) through a vector Dyson equation, along with entrywise behaviors of the resolvent.
 - (b) The establishment of CLT for a broad class of its LSS.
- (ii) We establish a rigorous procedure for the tensor signal alignment test (3) by establishing the normality asymptotic of the test statistic and deriving its power function under a general alternative hypothesis.
- (iii) We also address the problem of testing for the matching of two high-dimensional low-rank tensor signals. To tackle this problem, we employ an approach similar to the one established for the tensor signal alignment test. The details of this test and its associated procedure are provided in §4.2

The contributions presented in this article are novel. One notable innovation is that our tensor signal model in (1) allows for non-Gaussian and non-symmetric signals. This sets our work apart from most existing literature on high-dimensional tensor data models, which typically assumes symmetry or Gaussianity for either the tensor signal, the tensor noise, or both.

The rest of this article is organized as follows. In $\S 2$, we establish several important asymptotic spectral properties of the random matrix R, including its LSD, vector Dyson equation, and entrywise behaviors. For the sake of clarity, in $\S 3$, we consider the case of 3-fold tensors and establish a CLT for linear spectral statistics (LSS) of the matrix R. The corresponding CLT for the general case of d-fold tensors is presented later in to $\S 5$. In $\S 4$, we establish new procedures for testing tensor signal alignments and tensor signal matchings. Numerical experiments are conducted in $\S 6$ to evaluate the performance our CLT and two testing procedures introduced in $\S 4$. Finally, the proofs of all our results are included in the Supplementary Materials [29].

We end this section with some useful notations.

- (i) Given $z \in \mathbb{C}$, $\Re(z)$ and $\Im(z)$ are the real and imaginary part of z, respectively.
- (ii) We use a vector in $\mathbb{R}^{n_1 \times \cdots \times n_d}$ to represent the d-fold real tensor with size $n_1 \times \cdots \times n_d$.
- (iii) Given a matrix $A = [a_{i,j}]_{n \times n}$, $\operatorname{Tr}(A) = \sum_{i=1}^n a_{i,i}$ and A' denotes the transpose of A and $\operatorname{diag}(A)$ is the diagonal matrix made with the main diagonal of A. Moreover, ||A|| denotes the spectral norm of A and $||A||_k = (\sum_{i,j} |a_{i,j}|^k)^{1/k}$ for $k \in \mathbb{N}^+$. For any tensor or matrix, $T \in \mathbb{R}^{n_1 \times \cdots \times n_d}$, $||T||_k = (\sum_{i_1 \cdots i_d} |T_{i_1 \cdots i_d}|^k)^{1/k}$.
- (iv) Given an integrable random variable $X, X^c := X \mathbb{E}[X]$ denotes its centered version.
- $\text{(v) Given } \eta>0\text{, define }\mathbb{C}_{\eta}^{+}:=\{z\in\mathbb{C}:\Im(z)>\eta\}\text{ and }\mathbb{C}^{+}:=\{z\in\mathbb{C}:\Im(z)>0\}.$
- (vi) Given two matrices A, B of size $m \times n$, when $B_{ij} \neq 0$ for all i, j,

$$\frac{A}{B} = [A_{ij}B_{ij}^{-1}]_{m \times n}. (10)$$

(vii) Let $X = (X_n)$ and $Y = (Y_n)$ be two sequences of nonnegative random variables. We say Y stochastically dominates X if for all (small) $\epsilon > 0$ and (large) D > 0,

$$\mathbb{P}(X_n > n^{\epsilon} Y_n) \le n^{-D}$$

when $n \ge n_0(\epsilon, D)$ is sufficiently large. This property is denoted by $X \prec Y$ or $X = O_{\prec}(Y)$.

2 The limiting spectral distribution of the matrix M

In this section, we explore several key spectral properties of the matrix M (6). While M is symmetric and its entries have zero mean and a variance of N^{-1} , similar to a standard Wigner matrix, a crucial difference is that the entries of M are generally correlated. For example, when

d=3, given $\{i,j,k\}=\{1,2,3\}$, the (i,j)-th block of \boldsymbol{M} is $N^{-1/2}\boldsymbol{X}^{ij}$ by (4), where the (s_1,t_1) -th entry of \boldsymbol{X}^{ij} is $X_{s_1,t_1}^{ij}=\sum_{i_k=1}^{n_k}X_{s_1t_1i_k}a_{i_k}^{(k)}$, we have

$$Cov(X_{s_1,t_1}^{ij}, X_{s_2,t_2}^{ik}) = \delta_{s_1,s_2} a_{t_1}^{(j_1)} a_{t_2}^{(j_2)}, \tag{11}$$

where δ_{s_1,s_2} is the Kronecker delta. Therefore, elements in the same row of M are dependent. Likewise, when $d \geq 4$, it can be shown that

$$Cov(X_{s_1,t_1}^{i_1j_1}, X_{s_2,t_2}^{i_2j_2}) = a_{s_1}^{(i_1)} a_{s_2}^{(i_2)} a_{t_1}^{(j_1)} a_{t_2}^{(j_2)},$$
(12)

where $1 \le i_1 < j_1 \le d, 1 \le i_2 < j_2 \le d$ such that $(i_1, j_1) \ne (i_2, j_2)$. In this case, the dependence is even more widespread.

Several recent works [12, 2, 3] have explored symmetric random matrices with correlated entries. These studies typically assume that the correlations between matrix entries decay rapidly as the distance between their indices increases. However, our model M does not satisfy such a fast decay assumption. By (11) and (12), if all $a^{(j)} = (n_j^{-1/2}, \dots, n_j^{-1/2})'$, the covariance between entries of M can be independent of their distances.

To study the LSD of M, we start by examining its resolvent matrix:

$$\mathbf{Q}(z) := (\mathbf{M} - z\mathbf{I}_N)^{-1}, \quad z \in \mathbb{C}^+. \tag{13}$$

Similar to (4), we split $Q(z) = [Q^{ij}(z)]_{d\times d}$ into $d\times d$ blocks where $Q^{ij}(z) \in \mathbb{C}^{n_i\times n_j}$. For *i*-th diagonal block $Q^{ii}(z), 1\leq i\leq d$, let

$$\begin{cases}
\rho_i(z) := N^{-1} \operatorname{Tr}(\mathbf{Q}^{ii}(z)), & \rho(z) := \sum_{i=1}^d \rho_i(z), \\
\mathfrak{m}_i(z) := \mathbb{E}[\rho_i(z)], & \mathfrak{m}(z) := \sum_{i=1}^d \mathfrak{m}_i(z) = \mathbb{E}[\rho(z)].
\end{cases}$$
(14)

Note that $\rho(z)$ is the Stieltjes transform of the empirical spectral distribution (ESD) of M. To determine the LSD of M through $\rho(z)$, we first establish the vector Dyson equation induced by M. According to Theorem 2.2, there exists $\varepsilon(z) \in \mathbb{C}^d$ such that $\lim_{N \to \infty} \|\varepsilon(z)\|_{\infty} = 0$ and

$$-\frac{\mathfrak{c}}{\boldsymbol{m}(z)} = z + \boldsymbol{S}_d \boldsymbol{m}(z) + \boldsymbol{\varepsilon}(z), \quad \boldsymbol{S}_d := \boldsymbol{1}_{d \times d} - \boldsymbol{I}_d, \tag{15}$$

where $m(z) = (\mathfrak{m}_1(z), \dots, \mathfrak{m}_d(z))'$, \mathfrak{c} is defined in (17) and $\frac{\mathfrak{c}}{m(z)}$ is understood as the entrywise division defined in (10). Taking the limit of (15) as $N \to \infty$ yields

$$-\frac{\mathfrak{c}}{g(z)} = z + S_d g(z),\tag{16}$$

where $g(z) = (g_1(z), \dots, g_d(z))'$ is the limit of m(z). (16) is the vector Dyson equation induced by the matrix M.

The following assumptions are made for the general tensor model (1).

Assumption 2.1 (Subexponential tails). The noise variables $X_{i_1 \cdots i_d}$ are i.i.d. with zero mean, unit variance and subexponential tails, that is, for some $\theta > 0$,

$$\limsup_{x \to \infty} e^{x^{\theta}} \mathbb{P}(|X_{i_1 \dots i_d}| \ge x) < \infty,$$

Assumption 2.2 (High-dimensionality scheme). The tensor dimensions n_1, \dots, n_d all tend to infinity in such a way that

$$\lim_{n_1,\cdots,n_d\to\infty}\frac{n_j}{n_1+\cdots+n_d}=\mathfrak{c}_j\in(0,1),\quad 1\leq j\leq d.$$

This limiting framework is denoted simply as $N := n_1 + \cdots + n_d \to \infty$ and we define

$$\mathfrak{c} = (\mathfrak{c}_1, \cdots, \mathfrak{c}_d)'. \tag{17}$$

Theorem 2.1. Under Assumptions 2.1 and 2.2, we have

- 1. The vector Dyson equation (16) admits a unique analytical solution $\mathbf{g}(z) = (g_1(z), \dots, g_d(z))'$ on \mathbb{C}^+ .
- 2. The function

$$g(z) = \sum_{i=1}^{d} g_i(z).$$
 (18)

is the Stieltjes transform of a probability measure ν . Furthermore, the support of ν is finite, denoted by $[-\zeta, \zeta]$, where the edge ζ is nonnegative, finite, and given by

$$\zeta := \inf \Big\{ E > 0 : \lim_{\eta \downarrow 0} \Im(g(E + \mathrm{i}\eta)) = 0 \Big\}. \tag{19}$$

- 3. The Stieltjes transform g(z) has a unique singularity at z=0, i.e. ν has a unique point mass at 0, if and only if $\max\{\mathfrak{c}_1,\cdots,\mathfrak{c}_d\}\geq 1/2$.
- 4. Let $\mathfrak{v}_d = 2(d-1)\sum_{i=1}^d \sqrt{\mathfrak{c}_i}$, then we have $\mathbb{P}(\|\mathbf{M}\| > \mathfrak{v}_d + t) = o(N^{-l})$ for any t, l > 0.

The proof of Theorem 2.1 is given in §B and §C of the supplement. Next, for any $\eta_0 > 0$, define the region

$$\mathcal{S}_{\eta_0} := \{ z \in \mathbb{C}^+ : |\Re(z)|, |\Im(z)| \le \eta_0^{-1}, \operatorname{dist}(z, [-\max\{\mathfrak{v}_d, \zeta\}, \max\{\mathfrak{v}_d, \zeta\}]) > \eta_0 \}. \tag{20}$$

The next theorem establishes the convergence of the LSD to the measure determined by (16).

Theorem 2.2. Under Assumptions 2.1 and 2.2, for any $\eta_0 > 0$ and $z \in \mathcal{S}_{\eta_0}$ in (20), the vector function $\boldsymbol{\varepsilon}(z)$

$$\boldsymbol{\varepsilon}(z) := \frac{\mathbf{c}}{\boldsymbol{m}(z)} + z + \boldsymbol{S}_d \boldsymbol{m}(z), \tag{21}$$

satisfies that for any $\omega \in (1/2 - \delta, 1/2)$, where $\delta > 0$ is a sufficiently small constant

$$\sup_{z \in \mathcal{S}_{\eta_0}} \| \boldsymbol{\varepsilon}(z) \|_{\infty} = \mathcal{O}(\eta_0^{-11} N^{-2\omega}),$$

where m(z) and S_d are defined in (14) and (15), then

$$\lim_{N\to\infty} \sup_{z\in\mathcal{S}_{\eta_0}} \|\boldsymbol{m}(z) - \boldsymbol{g}(z)\|_{\infty} = 0.$$

Consequently, the measure ν defined in Theorem 2.1 is the LSD of M.

The proof of Theorem 2.2 is given in §D.2 of the supplement.

Theorem 2.2 expresses a crucial stability of the vector Dyson equation (16): if a vector-valued function m(z) satisfies a perturbed version of the vector Dyson equation with a small perturbation term $\varepsilon(z)$ uniformly controlled over a given region \mathcal{S}_{η_0} as in (21), then the difference between m(z) and the solution g(z) of the original equation (16) is also small uniformly over \mathcal{S}_{η_0} . This stability immediately implies the asymptotic equivalence of m(z) and g(z), and the measure ν associated with g(z) is the LSD of the matrix M.

Remark 2.1. Previous studies in [15, 36] have derived the LSD ν of the matrix M for the case of a Gaussian noise tensor X. In this work, we not only generalize their results to encompass non-Gaussian noise tensors, but also provide a comprehensive analysis of several important asymptotic properties of the matrix M, including:

- 1. The support interval of the LSD ν , and the necessary and sufficient conditions for the existence of a point mass in ν ;
- 2. The existence and uniqueness of the solution to the vector Dyson equation (16) induced by the matrix M;
- 3. The stability of the vector Dyson equation (16) and the invertibility of the underlying stability operators.

Readers can refer to §B and §C in the supplement for more details.

Furthermore, we provide the following approximation for general entries of the resolvent matrix Q(z).

Theorem 2.3 (Entrywise law). Under Assumptions 2.1 and 2.2, for any $\eta_0 > 0$ and $z \in \mathcal{S}_{\eta_0}$ in (20) and $\omega \in (1/2 - \delta, 1/2)$, where $\delta > 0$ is a sufficiently small constant, and $s, t \in \{1, \dots, d\}$,

$$\left| Q_{i_s i_t}^{st}(z) - \mathfrak{c}_s^{-1} g_s(z) \left[\delta_{st} \delta_{i_s i_t} + (a_{i_s}^{(s)})^2 \sum_{k \neq s}^d (g(z) - g_s(z) - g_k(z)) W_{sk}^{(d)}(z) \right] \right| \prec \mathcal{O}(\eta_0^{-21} N^{-\omega}),$$

where $Q_{i_si_t}^{st}(z)$ is the (i_s, i_t) -th entry of \mathbf{Q}^{st} and $a_{i_s}^{(s)}$ is the i-th entry of $\mathbf{a}^{(s)}$, and $W_{sk}^{(d)}$ is defined later in (59).

The proof of Theorem 2.3 is given in §D of the supplement.

Remark 2.2. Note that the diagonal entries of the resolvent matrix Q(z) depend on both the vector g(z) and the given unit vectors $a^{(1)}, \dots, a^{(d)}$. The definition of localization is provided in (30). For delocalized a, the entries will be close to $\mathfrak{c}_s^{-1}g_s(z)$, while localized a will result in additional terms. For example, when d=3 and $a^{(1)}=(n_1^{-1/2},\dots,n_1^{-1/2})'$ (a delocalized vector), then $(a_{i_1}^{(1)})^2=n_1^{-1}$ and we can show that $(a_{i_s}^{(s)})^2|\sum_{k\neq s}^d(g(z)-g_s(z)-g_k(z))W_{sk}^{(d)}(z)|\leq O(\eta_0^{-2}N^{-1})$, then have

$$\left|Q_{ii}^{11}(z) - \mathfrak{c}_1^{-1}g_1(z)\right| \prec \mathcal{O}(\eta_0^{-21}N^{-\omega} + \eta_0^{-3}N^{-1}),$$

for all $1 \le i \le n_1$. In contrast, when $\boldsymbol{a}^{(1)} = (1, 0, \dots, 0)'$ (a localized vector), we have

$$|Q_{11}^{11}(z) - \mathfrak{c}_1^{-1}g_1(z)[1 + g_2(z)W_{13}^{(3)}(z) + g_3(z)W_{12}^{(3)}(z)]| \prec O(\eta_0^{-21}N^{-\omega}),$$

where an additional nonvanishing term $\mathfrak{c}_{1}^{-1}g_{1}(z)[g_{2}(z)W_{13}^{(3)}(z)+g_{3}(z)W_{12}^{(3)}(z)]$ appears.

Remark 2.3. If the noise in the rank-one model (2) is Gaussian, [36] showed that there exists a $\beta_s > 0$ such that when $\beta \in (\beta_s, +\infty)$, the ML estimator of $\beta \boldsymbol{x}^{(1)} \otimes \cdots \otimes \boldsymbol{x}^{(d)}$ in (2),

$$(\lambda_*, \boldsymbol{u}_*^{(1)}, \cdots, \boldsymbol{u}_*^{(d)}) := \underset{\lambda \in \mathbb{R}^+, (\boldsymbol{u}^{(1)} \cdots \boldsymbol{u}^{(d)}) \in \mathbb{S}^{n_1 - 1} \times \cdots \times \mathbb{S}^{n_d - 1}}{\operatorname{argmin}} \|\boldsymbol{T} - \lambda \boldsymbol{u}^{(1)} \otimes \cdots \otimes \boldsymbol{u}^{(d)}\|_2^2, \qquad (22)$$

satisfies that

$$\begin{cases}
\lambda_* \xrightarrow{a.s.} \lambda^{\infty}(\beta) \\
|\langle \boldsymbol{x}^{(i)}, \boldsymbol{u}_*^{(i)} \rangle| \xrightarrow{a.s.} q_i(\lambda^{\infty}(\beta))
\end{cases},$$
(23)

where

$$q_i(z) := \left(\frac{\alpha_i(z)^{d-3}}{\prod_{j \neq i} \alpha_j(z)}\right)^{\frac{1}{2d-4}} \quad \text{and} \quad \alpha_i(z) := \frac{\beta}{z + g(z) - g_i(z)},$$

and $\lambda^{\infty}(\beta)$ satisfies $f(\lambda^{\infty}(\beta), \beta) = 0$, where $f(z, \beta) = z + g(z) - \beta \prod_{i=1}^{d} q_i(z)$, and $\lambda^{\infty}(\beta)$ is a constant on $\beta \in [0, \beta_s]$. This implies that when $\beta < \beta_s$, no inference about β is possible based on λ_* . It can be shown that (23) also holds for general non-Gaussian noises satisfying Assumption 2.1 by employing the same techniques used in §D of the supplementary document to analyze the ML estimator though we do not pursue it in details in this paper.

3 CLT for linear spectral statistics of M when d=3

Recall our hypothesis test (3). Under H_0 , the contracted signal matrix $\mathbf{S} = \mathbf{\Phi}_d(\mathbf{x}^{(r,1)} \otimes \cdots \otimes \mathbf{x}^{(r,d)}, \mathbf{a}^{(1)}, \cdots, \mathbf{a}^{(d)})$ is a zero matrix, and the statistic $\widehat{T}_n^{(d)}$ in (7) reduces to $\|\mathbf{M}\|_2^2 - N \int_{-\infty}^{\infty} x^2 \nu(dx)$, which is a LSS of \mathbf{M} . In this section, we aim to establish the asymptotic distribution for general LSS of \mathbf{M} , focusing on the case of d=3 for simplicity. The main results for general $d \geq 3$, presented in Section 5, involve more complicated formulas but do not differ essentially from this special case d=3.

We first present our main results in Section 3.1, and then provide the explicit formulas for the asymptotic mean and variance, which are relatively complex and tedious, in Section 3.2. Finally, a brief outline of the proofs is given in Section 3.3.

Now consider d=3 with dimensions (n_1, n_2, n_3) satisfying Assumption 2.2. Let $\boldsymbol{a}^{(1)} \in \mathbb{R}^{n_1}, \boldsymbol{a}^{(2)} \in \mathbb{R}^{n_2}, \boldsymbol{a}^{(3)} \in \mathbb{R}^{n_3}$ be three deterministic unit vectors, and $\boldsymbol{X} = [X_{i_1 i_2 i_3}] \in \mathbb{R}^{n_1 \times n_2 \times n_3}$ be a random tensor satisfying Assumption 2.1. Denote

$$egin{aligned} m{M} &= rac{1}{\sqrt{N}} m{\Phi}_3(m{X}, m{a}^{(1)}, m{a}^{(2)}, m{a}^{(3)}), \quad m{Q}(z) = (m{M} - z m{I}_N)^{-1} = \left(egin{aligned} m{Q}^{11}(z) & m{Q}^{12}(z) & m{Q}^{13}(z) \ (m{Q}^{12}(z))' & m{Q}^{22}(z) & m{Q}^{23}(z) \ (m{Q}^{13}(z))' & (m{Q}^{23}(z))' & m{Q}^{33}(z) \end{array}
ight), \end{aligned}$$

where $z \in \mathbb{C}^+$ and $N = n_1 + n_2 + n_3$. As stated in Theorem 2.1, the support of the LSD ν is $[-\zeta, \zeta]$, defined in (19), and $\|\mathbf{M}\|$ is stochastically bounded by $\mathfrak{v}_3 = 4(\sqrt{\mathfrak{c}_1} + \sqrt{\mathfrak{c}_2} + \sqrt{\mathfrak{c}_3})$. Define $v_B^{(3)} := \max\{\zeta, \mathfrak{v}_3\}$ and consider the class of functions

$$\mathfrak{F}_3 := \left\{ f(z) : f \text{ is analytic on an open set containing } \left[-v_B^{(3)}, v_B^{(3)} \right] \right\}. \tag{24}$$

For $f \in \mathfrak{F}_3$, consider a LSS of M of the form:

$$\mathcal{L}_{\boldsymbol{M}}(f) := \frac{1}{N} \sum_{l=1}^{N} f(\lambda_l) = \int_{\mathbb{R}} f(x) \nu_N(dx), \tag{25}$$

where $\lambda_1, \dots, \lambda_N$ are the eigenvalues of M and $\nu_N = N^{-1} \sum_{j=1}^N \delta_{\lambda_j}$ is the ESD of M. By Theorem 2.2, ν_N converges to ν almost surely, we thus consider

$$G_N(f) := N \int_{-\infty}^{\infty} f(x)(\nu_N(dx) - \nu(dx)) = N \left(\mathcal{L}_{\mathbf{M}}(f) - \int_{-\infty}^{\infty} f(x)\nu(dx) \right). \tag{26}$$

Our main goal is to derive the asymptotic distribution of $G_N(f)$.

3.1 Main results

Before presenting our main theorem, we introduce some auxiliary notations. First, we define the third and fourth cumulants of $X_{i_1 \cdots i_d}$ as follows:

$$\kappa_3 := \mathbb{E}[X_{i_1 \cdots i_d}^3], \quad \text{and} \quad \kappa_4 := \mathbb{E}[X_{i_1 \cdots i_d}^4] - 3.$$

$$(27)$$

Given $k \in \{1, \dots, d\}$, define

$$\mathfrak{b}_k^{(1)} := \frac{1}{\sqrt{N}} \sum_{i_1,\dots,i_k}^{n_k} a_{i_k}^{(k)}. \tag{28}$$

Let k_1, k_2, \ldots, k_l be distinct integers in $\{1, \ldots, d\}$. Define for $r \in \mathbb{N}, r \geq 2$

$$\mathcal{A}_{i_{1}\cdots i_{d}}^{(k_{1},\cdots,k_{l})} := \prod_{j\neq k_{1}\cdots k_{l}} a_{i_{j}}^{(j)}, \quad \mathcal{B}_{(r)}^{(k_{1},\cdots,k_{l})} := \sum_{i_{j}=1,j\neq k_{1}\cdots k_{l}}^{n_{j}} (\mathcal{A}_{i_{1}\cdots i_{d}}^{(k_{1},\cdots,k_{l})})^{r}, \tag{29}$$

Moreover, we say the vector $\boldsymbol{a}^{(j)}$ is delocalized if

$$\lim_{n_j \to \infty} \|\boldsymbol{a}^{(j)}\|_{\infty} = \lim_{n_j \to \infty} \max_{1 \le i_j \le n_j} |a_{i_j}^{(j)}| = 0.$$
 (30)

Otherwise, $a^{(j)}$ is localized.

Remark 3.1. The purpose of defining $\mathfrak{b}_{k}^{(1)}$ and $\mathcal{B}_{(4)}^{(k_{1},k_{2})}$ is that they will appear in the asymptotic mean and variance of the CLTs in the forthcoming Propositions 3.1 and 3.2. For example, when d=3, we know that $\mathfrak{b}_{k}^{(1)}=N^{-1/2}\sum_{i_{k}=1}^{n_{k}}a_{i_{k}}^{(k)}\in[-\mathfrak{c}_{k},\mathfrak{c}_{k}]$ and $\mathcal{B}_{(4)}^{(1,2)}=\|\boldsymbol{a}^{(3)}\|_{4}^{4}\in[0,1]$ due to $\|\boldsymbol{a}^{(k)}\|_{2}=1$. When d=4, we have $\mathcal{B}_{(4)}^{(1,2)}=\|\boldsymbol{a}^{(3)}\|_{4}^{4}\times\|\boldsymbol{a}^{(4)}\|_{4}^{4}\in[0,1]$. Notably, by (30), if all $\boldsymbol{a}^{(l)}$ are delocalized, then $\lim_{n_{l}\to\infty}\|\boldsymbol{a}^{(l)}\|_{4}=0$, implying that all $\lim_{N\to\infty}\mathcal{B}_{(4)}^{(k_{1},k_{2})}=0$.

Theorem 3.1. Under Assumptions 2.1 and 2.2 with d=3, for any $f \in \mathfrak{F}_3$ in (24) and deterministic unit vectors $\mathbf{a}^{(1)} \in \mathbb{R}^{n_1}$, $\mathbf{a}^{(2)} \in \mathbb{R}^{n_2}$, $\mathbf{a}^{(3)} \in \mathbb{R}^{n_3}$, we have

$$\frac{G_N(f) - \xi_N^{(3)}}{\sigma_N^{(3)}} \stackrel{d}{\longrightarrow} \mathcal{N}(0, 1),$$

where

$$\xi_N^{(3)} := -\frac{1}{2\pi i} \oint_{\mathfrak{C}_1} f(z) \mu_N^{(3)}(z; \kappa_3, \kappa_4, \boldsymbol{a}^{(1)}, \boldsymbol{a}^{(2)}, \boldsymbol{a}^{(3)}) dz, \tag{31}$$

$$(\sigma_N^{(3)})^2 := -\frac{1}{4\pi^2} \oint_{\mathfrak{C}_1} \oint_{\mathfrak{C}_2} f(z_1) f(z_2) \mathcal{C}_N^{(3)}(z_1, z_2; \kappa_4, \boldsymbol{a}^{(1)}, \boldsymbol{a}^{(2)}, \boldsymbol{a}^{(3)}) dz_1 dz_2, \tag{32}$$

where \mathfrak{C}_1 and \mathfrak{C}_2 are two disjoint rectangular contours with vertices $\pm E_1 \pm i\eta_1$ and $\pm E_2 \pm i\eta_2$, respectively, such that $E_1, E_2 \geq v_B^{(3)} + t$, where t > 0 is a fixed constant and $\eta_1, \eta_2 > 0$. The mean function $\mu_N^{(3)}(z; \kappa_3, \kappa_4, \mathbf{a}^{(1)}, \mathbf{a}^{(2)}, \mathbf{a}^{(3)})$ and the variance function $\mathcal{C}_N^{(3)}(z_1, z_2; \kappa_4, \mathbf{a}^{(1)}, \mathbf{a}^{(2)}, \mathbf{a}^{(3)})$ are defined later in (38) and (46), respectively.

The proof of Theorem 3.1 is given in §F of the supplement. For notational simplicity, we denote $\mu_N^{(3)}(z; \kappa_3, \kappa_4, \boldsymbol{a}^{(1)}, \boldsymbol{a}^{(2)}, \boldsymbol{a}^{(3)})$ and $\mathcal{C}_N^{(3)}(z_1, z_2; \kappa_4, \boldsymbol{a}^{(1)}, \boldsymbol{a}^{(2)}, \boldsymbol{a}^{(3)})$ by $\mu_N^{(3)}(z)$ and $\mathcal{C}_N^{(3)}(z_1, z_2)$, respectively.

Remark 3.2. $\mu_N^{(3)}(z)$ and $\mathcal{C}_N^{(3)}(z_1, z_2)$ can be evaluated numerically for any fixed z, z_1, z_2 . The values of $\xi_N^{(3)}$ and $\sigma_N^{(3)}$ can be then obtained through contour integration. Examples of these numerical computations are provided in Section 6.1.

3.2 The asymptotic mean and variance functions $\mu_N^{(3)}$ and $\mathcal{C}_N^{(3)}$

In this section, we provide explicit formulas of $\mu_N^{(3)}(z)$ and $\mathcal{C}_N^{(3)}(z_1, z_2)$. To introduce the mean function $\mu_N^{(3)}(z)$, we first define two auxiliary functions $\boldsymbol{W}^{(3)}(z)$ and $\boldsymbol{V}^{(3)}(z_1, z_2)$ as follows:

1. For any $z \in \mathbb{C}^+$, let

$$\mathbf{\Gamma}^{(3)}(z) := (z + g(z))\mathbf{I}_3 - \operatorname{diag}(\mathbf{g}(z)) + g(z)\mathbf{S}_3 - \operatorname{diag}(g(z))\mathbf{S}_3 - \mathbf{S}_3\operatorname{diag}(g(z)).$$

And define

$$\mathbf{W}^{(3)}(z) := -\mathbf{\Gamma}^{(3)}(z)^{-1}. \tag{33}$$

2. For any $z_1, z_2 \in \mathbb{C}^+$, let

$$\mathbf{\Pi}^{(3)}(z_1, z_2) := \mathbf{I}_3 - \operatorname{diag}(\mathfrak{c}^{-1} \circ \mathbf{g}(z_1) \circ \mathbf{g}(z_2)) \mathbf{S}_3, \tag{34}$$

then define

$$V^{(3)}(z_1, z_2) := \Pi^{(3)}(z_1, z_2)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ g(z_1) \circ g(z_2)).$$
 (35)

Proposition 3.1 (Mean function $\mu_N^{(3)}(z)$ for d=3). Under Assumptions 2.1 and 2.2, for any $\eta_0 > 0$ and $z \in \mathcal{S}_{\eta_0}$ in (20), let

$$\overrightarrow{M}_{N}^{(3)}(z) = \left(M_{1,N}^{(3)}(z), M_{2,N}^{(3)}(z), M_{3,N}^{(3)}(z)\right)',$$

where for $1 \le i \le 3$

$$M_{i,N}^{(3)}(z) := g_i(z) \sum_{r \neq i}^{3} \sum_{w \neq i,r}^{3} W_{rw}^{(3)}(z) + \sum_{l \neq i}^{3} \left[(g(z) - g_i(z) - g_l(z)) W_{il}^{(3)}(z) + V_{il}^{(3)}(z,z) \right]$$

$$- 2\kappa_3 (\mathfrak{c}_1 \mathfrak{c}_2 \mathfrak{c}_3)^{-1} g_1(z) g_2(z) g_3(z) \mathfrak{b}_1^{(1)} \mathfrak{b}_2^{(1)} \mathfrak{b}_3^{(1)} + \kappa_4 \mathfrak{c}_i^{-1} g_i(z)^2 \sum_{l \neq i}^{3} \mathcal{B}_{(4)}^{(i,l)} \mathfrak{c}_l^{-1} g_l(z)^2, \tag{36}$$

and $\mathfrak{b}_{k}^{(1)}, \mathcal{B}_{(4)}^{(i,l)}, W_{jk}^{(3)}(z), V_{ij}^{(3)}(z,z)$ are defined in (28), (29), (33), (35), respectively. Then we have

$$\lim_{N \to \infty} \|N(\boldsymbol{m}(z) - \boldsymbol{g}(z)) - \boldsymbol{\Pi}^{(3)}(z, z)^{-1} \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1} \circ \boldsymbol{g}(z)) \overrightarrow{M}_{N}^{(3)}(z)\| = 0, \tag{37}$$

where $\Pi^{(3)}(z,z)$ is defined in (34). Consequently, we obtain that

$$\lim_{N \to \infty} \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}(z))] - Ng(z) - \mu_N^{(3)}(z) = 0,$$

where

$$\mu_N^{(3)}(z) := \mathbf{1}_3' \mathbf{\Pi}^{(3)}(z, z)^{-1} \operatorname{diag}(\mathbf{c}^{-1} \circ \mathbf{g}(z)) \overrightarrow{M}_N^{(3)}(z). \tag{38}$$

To introduce the covariance function $C_N^{(3)}(z_1, z_2)$, we need the functions $\mathcal{V}_{st}^{(3)}(z_1, z_2)$ and $\mathcal{U}_{st,N}^{(3)}(z_1, z_2)$ for $1 \leq s, t \leq 3$ defined as follows:

1. For any $s, t, r \in \{1, 2, 3\}$ and $z_1, z_2 \in \mathbb{C}_{\eta}^+$, define

$$\tilde{\boldsymbol{V}}_{r}^{(3)}(z_{1}, z_{2}) := \boldsymbol{\Pi}^{(3)}(z_{1}, z_{2})^{-1} \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1} \circ \boldsymbol{g}(z_{1})) [\operatorname{diag}(\boldsymbol{V}^{(3)}(z_{2}, z_{2})) + \operatorname{diag}(\boldsymbol{S}_{3} \boldsymbol{V}_{\cdot r}^{(3)}(z_{1}, z_{2})) \boldsymbol{V}^{(3)}(z_{1}, z_{2})].$$
(39)

where $V_{r}^{(3)}(z_1, z_2)$ is the r-th column of $V^{(3)}(z_1, z_2)$ defined in (35). Let $\tilde{V}_{str}^{(3)}(z_1, z_2)$ be the (s, t)-th entry of $\tilde{V}_{r}^{(3)}(z_1, z_2)$, define

$$\mathcal{V}_{st}^{(3)}(z_1, z_2) = \sum_{l \neq s}^{3} \tilde{V}_{stl}^{(3)}(z_1, z_2). \tag{40}$$

2. For any $s,t \in \{1,2,3\}$ and $z_1,z_2 \in \mathbb{C}_{\eta}^+$, let

$$\mathring{\boldsymbol{V}}^{(3)}(z_1, z_2) := \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z_1)) \boldsymbol{V}^{(3)}(z_1, z_2), \tag{41}$$

and $\mathring{V}_{st}^{(3)}(z_1,z_2)$ be the (s,t)-th entry of $\mathring{\boldsymbol{V}}^{(3)}(z_1,z_2)$, then define

$$\mathcal{U}_{st,N}^{(3)}(z_1,z_2)$$

$$:= \mathfrak{c}_s^{-1} g_s(z_1) g_s(z_2) \sum_{l \neq s}^3 \mathcal{B}_{(4)}^{(s,l)} \mathring{V}_{lt}^{(3)}(z_1, z_2) + \mathring{V}_{st}^{(3)}(z_1, z_2) \sum_{l \neq s}^3 \mathcal{B}_{(4)}^{(s,l)} \mathfrak{c}_l^{-1} g_l(z_1) g_l(z_2). \tag{42}$$

Proposition 3.2 (Covariance function $C_N^{(3)}(z_1, z_2)$ for d = 3). Under Assumptions 2.1 and 2.2, for any $\eta_0 > 0$ and $z_1, z_2 \in \mathcal{S}_{\eta_0}$ in (20), let

$$C_{st,N}^{(3)}(z_1, z_2) := \text{Cov}(\text{Tr}(\boldsymbol{Q}^{ss}(z_1)), \text{Tr}(\boldsymbol{Q}^{tt}(z_2))), \quad \boldsymbol{C}_N^{(3)}(z_1, z_2) := [C_{st,N}^{(3)}(z_1, z_2)]_{3\times 3}, \quad (43)$$

where $s, t \in \{1, 2, 3\}$. Further define

$$\boldsymbol{F}_{N}^{(3)}(z_{1}, z_{2}) = [\mathcal{F}_{st,N}^{(3)}(z_{1}, z_{2})]_{3\times3}, \quad \mathcal{F}_{st,N}^{(3)}(z_{1}, z_{2}) := 2\mathcal{V}_{st}^{(3)}(z_{1}, z_{2}) + \kappa_{4}\mathcal{U}_{st,N}^{(3)}(z_{1}, z_{2}), \tag{44}$$

where $V_{st}^{(3)}(z_1, z_2)$ and $U_{st,N}^{(3)}(z_1, z_2)$ are determined by the system of equations (40) and (42), respectively. Then we have

$$\lim_{N \to \infty} \|\boldsymbol{C}_N^{(3)}(z_1, z_2) - \boldsymbol{\Pi}^{(3)}(z_1, z_2)^{-1} \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1} \circ \boldsymbol{g}(z_1)) \boldsymbol{F}_N^{(3)}(z_1, z_2) \| = 0, \tag{45}$$

where $\Pi^{(3)}(z_1, z_2)$ is defined in (34). Consequently, $Var(Tr(\mathbf{Q}(z)))$ is bounded by $C_{\eta_0, \mathfrak{c}}$ for any $z \in \mathcal{S}_{\eta_0}$ and

$$\lim_{N \to \infty} \left| \operatorname{Cov} \left(\operatorname{Tr}(\boldsymbol{Q}(z_1)), \operatorname{Tr}(\boldsymbol{Q}(z_2)) \right) - \mathcal{C}_N^{(3)}(z_1, z_2) \right| = 0,$$

where

$$C_N^{(3)}(z_1, z_2) := \mathbf{1}_3' \mathbf{\Pi}^{(3)}(z_1, z_2)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z_1)) \boldsymbol{F}_N^{(3)}(z_1, z_2) \mathbf{1}_3. \tag{46}$$

The proofs of Propositions 3.1 and 3.2 are given in §E of the supplement.

Remark 3.3. The functions $\mu_N^{(3)}(z)$ and $\mathcal{C}_N^{(3)}(z_1, z_2)$, introduced in Propositions 3.1 and 3.2, involve the inverse of the matrix $\mathbf{\Pi}^{(3)}(z_1, z_2)$ defined in (34). Consequently, it is necessary to establish the invertibility of $\mathbf{\Pi}^{(3)}(z_1, z_2)$. Similarly, the invertibility of $\mathbf{\Gamma}(z)$ needs to be proven due to its appearance in (33). The proofs of these invertibility results can be found in §B of the supplement.

Remark 3.4. Given the Stieltjes transform g(z) and the vectors $\boldsymbol{a}^{(1)}, \boldsymbol{a}^{(2)}, \boldsymbol{a}^{(3)}$, the functions $\boldsymbol{W}^{(3)}(z), \boldsymbol{V}^{(3)}(z_1, z_2), \mathcal{V}_{st}^{(3)}(z_1, z_2)$ and $\mathcal{U}_{st,N}^{(3)}(z_1, z_2)$ can be calculated through (33), (35), (40) and (42), respectively. Combining with κ_3, κ_4 , we can further calculate the values of $\mu_N^{(3)}(z)$ and $\mathcal{C}_N^{(3)}(z_1, z_2)$. Furthermore, the Stieltjes transform g(z) can be evaluated numerically using a fixed-point algorithm, we refer the details to Lemma B.1 of the supplement.

Remark 3.5. By Propositions 3.1 and 3.2, $\mu_N^{(3)}(z)$ depends on the third and fourth cumulant κ_3, κ_4 , and the unit vectors $\boldsymbol{a}^{(1)}, \boldsymbol{a}^{(2)}, \boldsymbol{a}^{(3)}$, while $\mathcal{C}_N^{(3)}(z_1, z_2)$ depends on the fourth cumulant κ_4 and the unit vectors $\boldsymbol{a}^{(1)}, \boldsymbol{a}^{(2)}, \boldsymbol{a}^{(3)}$. Precisely, for the mean function $\mu_N^{(3)}(z)$, note that $M_{i,N}^{(3)}(z)$ contains the functions

$$\kappa_3(\mathfrak{c}_1\mathfrak{c}_2\mathfrak{c}_3)^{-1}g_1(z)g_2(z)g_3(z)\mathfrak{b}_1^{(1)}\mathfrak{b}_2^{(1)}\mathfrak{b}_3^{(1)}\quad\text{and}\quad \kappa_4\mathfrak{c}_i^{-1}g_i(z)^2\sum_{l\neq i}^3\mathcal{B}_{(4)}^{(i,l)}\mathfrak{c}_l^{-1}g_l(z)^2.$$

For example, if specifically $\mathbf{a}^{(l)} = (1, 0, \dots, 0)'$ for some $l \in \{1, 2, 3\}$, then $\mathfrak{b}_l^{(1)} = \mathrm{O}(N^{-1/2})$ and $\mu_N^{(3)}(z)$ will be independent of κ_3 ; if all $\mathbf{a}^{(l)}$ are delocalized, then $\lim_{N\to\infty} \mathcal{B}_{(4)}^{(i,l)} = 0$ by Remark

3.1 and $\mu_N^{(3)}(z)$ will be also independent of κ_4 . Similarly, for the variance function $\mathcal{C}_N^{(3)}(z_1, z_2)$, by (42), $\mathcal{U}_{st,N}^{(3)}(z_1, z_2)$ depends on $\mathcal{B}_{(4)}^{(s,l)}$, so $\lim_{N\to\infty} |\mathcal{U}_{st,N}^{(3)}(z_1, z_2)| = 0$ if all $\boldsymbol{a}^{(l)}$ are delocalized. By (45) and (44), we have

$$C_N^{(3)}(z_1, z_2) = 2\Pi^{(3)}(z_1, z_2)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z_1)) \mathcal{V}^{(3)}(z_1, z_2) + o(1) \mathbf{1}_{3 \times 3},$$

which is independent of κ_4 , so does $C_N^{(3)}(z_1, z_2)$ due to (46).

The following proposition follows from Remark 3.5.

Proposition 3.3. 1. In general, the asymptotic mean $\xi_N^{(3)} = \xi_N^{(3)}(\kappa_3, \kappa_4, \boldsymbol{a}^{(1)}, \boldsymbol{a}^{(2)}, \boldsymbol{a}^{(3)})$ of LSS in (31) depends on κ_3, κ_4 and $\boldsymbol{a}^{(1)}, \boldsymbol{a}^{(2)}, \boldsymbol{a}^{(3)}$.

- 2. In general, the asymptotic variance $\sigma_N^{(3)} = \sigma_N^{(3)}(\kappa_4, \boldsymbol{a}^{(1)}, \boldsymbol{a}^{(2)}, \boldsymbol{a}^{(3)})$ of LSS in (32) depends on κ_4 and $\boldsymbol{a}^{(1)}, \boldsymbol{a}^{(2)}, \boldsymbol{a}^{(3)}$.
- 3. If the third and fourth cumulant of random noises are zero (e.g. the noise tensor X is Gaussian), $\xi_N^{(3)}$ and $\sigma_N^{(3)}$ will be independent of $a^{(1)}, a^{(2)}, a^{(3)}$.
- 4. If all $a^{(1)}, a^{(2)}, a^{(3)}$ are delocalized, $\xi_N^{(3)}$ and $\sigma_N^{(3)}$ will be independent of κ_4 .

For further illustrations of these conclusions, readers may refer to the numerical experiments reported in Table 1 in §6 for more details.

3.3 Outline of the proof of Theorem 3.1

In this section, we outline the proof of Theorem 3.1. The general framework follows that of Chapter 9 in [7]. Consider the event $\mathcal{E}_{M} := \{ \|M\| \leq v_{B}^{(3)} + t \}$, where $v_{B}^{(3)} = \max\{\mathfrak{v}_{3}, \zeta\}$ and t > 0 is a fixed constant. By Theorem 2.1, we have $\mathbb{P}(\mathcal{E}_{M}) \geq 1 - \mathrm{o}(N^{-l})$ for any l > 0. This implies that the probability of the existence of outlier eigenvalues greater than $v_{B}^{(3)}$ is overwhelmingly small. As a result, their effect will be negligible, i.e.,

$$G_N(f)1_{\mathcal{E}_M} \stackrel{\mathbb{P}}{\longrightarrow} G_N(f),$$

Therefore, by the Cauchy integration theorem, it suffices to study the following equivalent form of $G_N(f)$,

$$-\frac{1}{2\pi i} \oint_{\sigma} f(z) \{ \operatorname{Tr}(\boldsymbol{Q}(z)) - Ng(z) \} dz,$$

where \mathfrak{C} is a rectangle contour with vertexes $\pm E_0 \pm i\eta_0$ such that $E_0 \geq v_B^{(3)} + t$, t > 0 is a fixed constant and $\eta_0 > 0$ is sufficiently small. Both E_0 and the event \mathcal{E}_M ensure that $\text{Tr}(\mathbf{Q}(z))$ and g(z) are nonsingular for all $z \in \mathfrak{C}$, making the above contour integration well-defined.

Consequently, to establish the CLT for $G_N(f)$, it is enough to establish the CLT for $\text{Tr}(\mathbf{Q}(z)) - Ng(z)$. We show that $\text{Tr}(\mathbf{Q}(z)) - \mathbb{E}[\text{Tr}(\mathbf{Q}(z))]$ weakly converges to a complex Gaussian process on \mathcal{S}_{η_0} in (20) by the following steps:

(i) The tightness of $\text{Tr}(\boldsymbol{Q}(z)) - \mathbb{E}[\text{Tr}(\boldsymbol{Q}(z))]$:

Proposition 3.4. Under Assumptions 2.1 and 2.2, for any $\eta_0 > 0$, $\text{Tr}(\mathbf{Q}(z)) - \mathbb{E}[\text{Tr}(\mathbf{Q}(z))]$ is tight on S_{η_0} in (20), i.e.

$$\sup_{\substack{z_1, z_2 \in \mathcal{S}_{\eta_0} \\ z_1 \neq z_2}} \frac{\mathbb{E}\left[|\operatorname{Tr}(\boldsymbol{Q}(z_1) - \boldsymbol{Q}(z_2)) - \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}(z_1) - \boldsymbol{Q}(z_2))|^2\right]}{|z_1 - z_2|^2} < C_{\eta_0}.$$

(ii) Characteristic function: prove that the joint characteristic function of the real part and imaginary part of $\text{Tr}(\mathbf{Q}(z)) - \mathbb{E}[\text{Tr}(\mathbf{Q}(z))]$ converges to the characteristic function of a normal vector. Combining with Theorem 3.4, we have

Proposition 3.5. Under Assumptions 2.1 and 2.2, for any sufficiently small constant $\eta_0 > 0$, $\text{Tr}(\mathbf{Q}(z)) - \mathbb{E}[\text{Tr}(\mathbf{Q}(z))]$ asymptotically weakly converges to a Gaussian random process on \mathcal{S}_{η_0} .

Readers can refer to §F in the supplement for the proofs of Propositions 3.4 and 3.5. Note that the rectangular contour $\mathfrak{C} = \mathfrak{C}^h \cup \mathfrak{C}^v$, where $\mathfrak{C}^h := \{x \pm i\eta_0 : x \in [-E_0, E_0]\}$ and $\mathfrak{C}^v := \mathfrak{C} \setminus \mathfrak{C}^h$. Since $\mathfrak{C}^h \subset \mathcal{S}_{\eta_0}$, by Propositions 3.1, 3.2 and 3.5, we have

$$-\frac{1}{2\pi \mathrm{i}\sigma_N^{(3)}}\oint_{\mathfrak{C}^h}f(z)\{\mathrm{Tr}(\boldsymbol{Q}(z))-Ng(z)\}dz-\xi_N^{(3)}/\sigma_N^{(3)}\stackrel{d}{\longrightarrow}\mathcal{N}(0,1).$$

Finally, we can complete the proof of Theorem 3.1 by showing that

$$\lim_{\eta_0\downarrow 0} \limsup_{N\to\infty} \mathbb{E} \left| \oint_{\mathfrak{C}^v} f(z) \{ \operatorname{Tr}(\boldsymbol{Q}(z)) - Ng(z) \} dz \right|^2 = 0.$$

4 Tests about tensor signals when d = 3

In this section, we propose new procedures for two tensor signal testing problems: testing for signal alignments and testing for signal matchings. These problems are formulated in equations (3) and (55), respectively.

4.1 Testing for tensor signal alignments

When d = 3, recall our spiked tensor model (1):

$$T = \sum_{r=1}^{R} \beta_r \boldsymbol{x}^{(r,1)} \otimes \boldsymbol{x}^{(r,2)} \otimes \boldsymbol{x}^{(r,3)} + \frac{1}{\sqrt{N}} \boldsymbol{X}.$$

Given three unit vectors $\boldsymbol{a}^{(1)} \in \mathbb{R}^{n_1}, \boldsymbol{a}^{(2)} \in \mathbb{R}^{n_2}, \boldsymbol{a}^{(3)} \in \mathbb{R}^{n_3}$, we construct the following statistic:

$$\widehat{T}_{N}^{(3)} := \widehat{T}_{N}^{(3)}(\boldsymbol{a}^{(1)}, \boldsymbol{a}^{(2)}, \boldsymbol{a}^{(3)}) := \|\boldsymbol{R}\|_{2}^{2} - N \int_{-\infty}^{\infty} x^{2} \nu(dx), \tag{47}$$

where ν is the LSD of M, and R and M are defined in (6). The following proposition is provide:

Proposition 4.1. Under Assumptions 2.1 and 2.2, for the spiked tensor model (1) and three unit vectors $\mathbf{a}^{(1)} \in \mathbb{R}^{n_1}$, $\mathbf{a}^{(2)} \in \mathbb{R}^{n_2}$, $\mathbf{a}^{(3)} \in \mathbb{R}^{n_3}$, the statistic $\widehat{T}_N^{(3)}$ in (47) satisfies that

$$(\widehat{T}_N^{(3)} - \xi_N^{(3)} - \mathcal{D}^{(3)}) / \sigma_N^{(3)} \stackrel{d}{\longrightarrow} \mathcal{N}(0, 1),$$

where

$$\mathcal{D}^{(3)} := 2\sum_{r=1}^{R} \beta_r^2 \sum_{l=1}^{3} \langle \boldsymbol{x}^{(r,l)}, \boldsymbol{a}^{(l)} \rangle^2 \ge 0, \tag{48}$$

and $\xi_N^{(3)}, \sigma_N^{(3)}$ are derived from (31) and (32) by setting $f(z) = z^2$, i.e.

$$\begin{split} \xi_N^{(3)} &= -\frac{1}{2\pi \mathrm{i}} \oint_{\mathfrak{C}_1} z^2 \mu_N^3(z; \kappa_3, \kappa_4, \boldsymbol{a}^{(1)}, \boldsymbol{a}^{(2)}, \boldsymbol{a}^{(3)}) dz, \\ (\sigma_N^{(3)})^2 &= -\frac{1}{4\pi^2} \oint_{\mathfrak{C}_1} \oint_{\mathfrak{C}_2} z_1^2 z_2^2 \mathcal{C}_N^{(3)}(z_1, z_2; \kappa_4, \boldsymbol{a}^{(1)}, \boldsymbol{a}^{(2)}, \boldsymbol{a}^{(3)}) dz_1 dz_2. \end{split}$$

Proof. Note that $\mathbf{R} = \mathbf{M} + \sum_{r=1}^{R} \beta_r \Delta^{(r)}$, where

$$\Delta^{(r)} = \boldsymbol{U}_r \left(\begin{array}{ccc} 0 & \langle \boldsymbol{a}^{(3)}, \boldsymbol{x}^{(r,3)} \rangle & \langle \boldsymbol{a}^{(2)}, \boldsymbol{x}^{(r,2)} \rangle \\ \langle \boldsymbol{a}^{(3)}, \boldsymbol{x}^{(r,3)} \rangle & 0 & \langle \boldsymbol{a}^{(1)}, \boldsymbol{x}^{(r,1)} \rangle \\ \langle \boldsymbol{a}^{(2)}, \boldsymbol{x}^{(r,2)} \rangle & \langle \boldsymbol{a}^{(1)}, \boldsymbol{x}^{(r,1)} \rangle & 0 \end{array} \right) \boldsymbol{U}_r', \quad \boldsymbol{U}_r := \left(\begin{array}{ccc} \boldsymbol{x}^{(r,1)} & \boldsymbol{0}_{n_1} & \boldsymbol{0}_{n_2} \\ \boldsymbol{0}_{n_2} & \boldsymbol{x}^{(r,2)} & \boldsymbol{0}_{n_2} \\ \boldsymbol{0}_{n_3} & \boldsymbol{0}_{n_3} & \boldsymbol{x}^{(r,3)} \end{array} \right),$$

since $\{\boldsymbol{x}^{(1,l)},\cdots,\boldsymbol{x}^{(R,l)}\}$ are orthogonal in \mathbb{R}^{n_l} for $1 \leq l \leq 3$, then we have $\boldsymbol{U}_{r_1}\boldsymbol{U}'_{r_2} = \boldsymbol{0}_{N \times N}$ for $r_1 \neq r_2$ and

$$\|\mathbf{R}\|_{2}^{2} = \|\mathbf{M}\|_{2}^{2} + \sum_{r=1}^{R} \beta_{r}^{2} \|\Delta^{(r)}\|_{2}^{2} + 2 \sum_{r=1}^{R} \beta_{r} \operatorname{Tr}(\mathbf{M}\Delta^{(r)}).$$

Moreover, for each $1 \le r \le R$, since

$$\text{Tr}(\boldsymbol{M}\Delta^{(r)}) = \frac{2}{\sqrt{N}} (\langle \boldsymbol{x}^{(r,3)}, \boldsymbol{a}^{(3)} \rangle (\boldsymbol{x}^{(r,1)})' \boldsymbol{X}(\boldsymbol{a}^{(3)}) \boldsymbol{x}^{(r,2)} + \langle \boldsymbol{x}^{(r,2)}, \boldsymbol{a}^{(2)} \rangle (\boldsymbol{x}^{(r,1)})' \boldsymbol{X}(\boldsymbol{a}^{(2)}) \boldsymbol{x}^{(r,3)}$$

$$+ \langle \boldsymbol{x}^{(r,1)}, \boldsymbol{a}^{(1)} \rangle (\boldsymbol{x}^{(r,2)})' \boldsymbol{X}(\boldsymbol{a}^{(1)}) \boldsymbol{x}^{(r,3)}) = \frac{2}{\sqrt{N}} \sum_{i_1, i_2, i_3 = 1}^{n_1, n_2, n_3} X_{i_1 i_2 i_3} (\langle \boldsymbol{x}^{(r,3)}, \boldsymbol{a}^{(3)} \rangle x_{i_1}^{(r,1)} x_{i_2}^{(r,2)} a_{i_3}^{(3)}$$

$$+ \langle \boldsymbol{x}^{(r,2)}, \boldsymbol{a}^{(2)} \rangle x_{i_1}^{(r,1)} a_{i_2}^{(2)} x_{i_3}^{(r,3)} + \langle \boldsymbol{x}^{(r,1)}, \boldsymbol{a}^{(1)} \rangle a_{i_1}^{(1)} x_{i_2}^{(r,2)} x_{i_3}^{(r,3)}),$$

then we have $\mathbb{E}[\text{Tr}(\boldsymbol{M}\Delta^{(r)})] = 0$ and

$$\operatorname{Var}(\operatorname{Tr}(\boldsymbol{M}\Delta^{(r)}))$$

$$\begin{split} &\leq \frac{4}{N} \sum_{i_1,i_2,i_3=1}^{n_1,n_2,n_3} \left(\langle \boldsymbol{x}^{(r,3)},\boldsymbol{a}^{(3)} \rangle x_{i_1}^{(r,1)} x_{i_2}^{(r,2)} a_{i_3}^{(3)} + \langle \boldsymbol{x}^{(r,2)},\boldsymbol{a}^{(2)} \rangle x_{i_1}^{(r,1)} a_{i_2}^{(2)} x_{i_3}^{(r,3)} + \langle \boldsymbol{x}^{(r,1)},\boldsymbol{a}^{(1)} \rangle a_{i_1}^{(1)} x_{i_2}^{(r,2)} x_{i_3}^{(r,3)} \right)^2 \\ &\leq \frac{12}{N} \sum_{i_1,i_2,i_3=1}^{n_1,n_2,n_3} \left[(x_{i_1}^{(r,1)} x_{i_2}^{(r,2)} a_{i_3}^{(3)})^2 + (x_{i_1}^{(r,1)} a_{i_2}^{(2)} x_{i_3}^{(r,3)})^2 + (a_{i_1}^{(1)} x_{i_2}^{(r,2)} x_{i_3}^{(r,3)})^2 \right] \leq \frac{36}{N}. \end{split}$$

Hence, by the Chebyshev's inequality, $\operatorname{Tr}(\boldsymbol{M}\Delta^{(r)}) \stackrel{\mathbb{P}}{\longrightarrow} 0$ and

$$\widehat{T}_{N}^{(3)} \stackrel{\mathbb{P}}{\longrightarrow} \|\boldsymbol{M}\|_{2}^{2} - N \int_{-\infty}^{\infty} x^{2} \nu(dx) + \sum_{r=1}^{R} \beta_{r}^{2} \|\Delta^{(r)}\|_{2}^{2}.$$
(49)

According to Theorem 3.1, since $N^{-1}||M||_2^2$ is an LSS of M, we have

$$\frac{\|\boldsymbol{M}\|_2^2 - N \int_{-\infty}^{\infty} x^2 \nu(dx) - \xi_N^{(3)}}{\sigma_N^{(3)}} \xrightarrow{d} \mathcal{N}(0, 1).$$

Finally, recall that $|\langle \boldsymbol{x}^{(r_1,l)}, \boldsymbol{x}^{(r_2,l)} \rangle| = \delta_{r_1,r_2}$ for $1 \leq l \leq 3$, we can derive that $\|\Delta\|_2^2 = 2\sum_{l=1}^3 \langle \boldsymbol{x}^{(r,l)}, \boldsymbol{a}^{(l)} \rangle^2$, which concludes this proposition.

Here, let $\tilde{T}_N^{(3)} := (\hat{T}_N^{(3)} - \xi_N^{(3)})/\sigma_N^{(3)}$. Under H_0 , since $\boldsymbol{a}^{(l)} \perp \boldsymbol{x}^{(r,l)}$ for all $1 \leq r \leq R, 1 \leq l \leq d$, then $\mathcal{D}^{(3)} = 0$; under H_1 , since there exists at least one $1 \leq r \leq R$ and $1 \leq l \leq d$ such that $\boldsymbol{a}^{(l)} \not\perp \boldsymbol{x}^{(r,l)}$, then it implies that $\mathcal{D}^{(3)} > 0$. We conclude from Proposition 4.1 that

$$\begin{cases}
\tilde{\mathcal{T}}_N^{(3)} \xrightarrow{d} \mathcal{N}(0,1) & \text{under } H_0, \\
\tilde{\mathcal{T}}_N^{(3)} - \mathcal{D}^{(3)} / \sigma_N^{(3)} \xrightarrow{d} \mathcal{N}(0,1) & \text{under } H_1.
\end{cases}$$
(50)

Given a significance level $\alpha \in (0,1)$, the rejection region of our test procedure is

{Reject
$$H_0$$
 if $\tilde{\mathcal{T}}_N^{(3)} > z_{\alpha}$ }, (51)

where z_{α} is α -th upper quantile of the standard normal. Moreover, the asymptotic power of our test satisfies that

$$\lim_{N \to \infty} \mathbb{P}(\tilde{\mathcal{T}}_N^{(3)} > z_\alpha | H_1) - 1 + \Phi(z_\alpha - \mathcal{D}^{(3)} / \sigma_N^{(3)}) = 0, \tag{52}$$

where $\Phi(\cdot)$ is the cumulative distribution function of the standard normal.

The implementation of the test procedure requires numerical values of $\xi_N^{(3)}$, $\sigma_N^{(3)}$, which can be found following Remarks 3.2 and 3.4. This procedure needs also the values of κ_3 , κ_4 , we can estimate κ_3 , κ_4 using straightforward moment estimators:

$$\hat{\kappa}_{3} = \frac{(\mathfrak{c}_{1}\mathfrak{c}_{2}\mathfrak{c}_{3})^{-1}}{N^{3/2}} \sum_{i_{1},i_{2},i_{3}=1}^{n_{1},n_{2},n_{3}} T_{i_{1}i_{2}i_{3}}^{3},$$

$$\hat{\kappa}_{4} = \frac{(\mathfrak{c}_{1}\mathfrak{c}_{2}\mathfrak{c}_{3})^{-1}}{N} \sum_{i_{1},i_{2},i_{3}=1}^{n_{1},n_{2},n_{3}} T_{i_{1}i_{2}i_{3}}^{4} - 3.$$
(53)

We can show that $\hat{\kappa}_3 \xrightarrow{\mathbb{P}} \kappa_3$ by the large law of numbers, so does $\hat{\kappa}_4$. For $\hat{\kappa}_3$, note that

$$T_{i_1 i_2 i_3}^3 = \frac{X_{i_1 i_2 i_3}^3}{N^{3/2}} + \frac{3X_{i_1 i_2 i_3}^2}{N} \sum_{r=1}^R \beta_r x_{i_1}^{(r,1)} x_{i_2}^{(r,2)} x_{i_3}^{(r,3)} + \frac{3X_{i_1 i_2 i_3}}{N^{1/2}} \left(\sum_{r=1}^R \beta_r x_{i_1}^{(r,1)} x_{i_2}^{(r,2)} x_{i_3}^{(r,3)} \right)^2 + \left(\sum_{r=1}^R \beta_r x_{i_1}^{(r,1)} x_{i_2}^{(r,2)} x_{i_3}^{(r,3)} \right)^3.$$

Since $\boldsymbol{x}^{(r,1)}, \boldsymbol{x}^{(r,2)}, \boldsymbol{x}^{(r,3)}$ are unit vectors for $1 \leq r \leq R$, then by the Holder's inequality, it yields that

$$\frac{1}{N^{3/2}} \sum_{i_1, i_2, i_3 = 1}^{n_1, n_2, n_3} \left| \sum_{r=1}^R \beta_r x_{i_1}^{(r,1)} x_{i_2}^{(r,2)} x_{i_3}^{(r,3)} \right|^3 \le \frac{R^2}{N^{3/2}} \sum_{r=1}^R \beta_r^3 \prod_{l=1}^3 \|\boldsymbol{a}^{(r,l)}\|_3^3 = \mathcal{O}(N^{-3/2}).$$

Moreover, $N^{-2} \sum_{i_1,i_2,i_3=1}^{n_1,n_2,n_3} X_{i_1i_2i_3} \left(\sum_{r=1}^R \beta_r x_{i_1}^{(r,1)} x_{i_2}^{(r,2)} x_{i_3}^{(r,3)} \right)^2$ have zero mean and its variance equals to $N^{-4} \sum_{i_1,i_2,i_3=1}^{n_1,n_2,n_3} \left(\sum_{r=1}^R \beta_r x_{i_1}^{(r,1)} x_{i_2}^{(r,2)} x_{i_3}^{(r,3)} \right)^4 \leq \mathcal{O}(N^{-4})$. Similarly, the absolute mean of

$$N^{-5/2} \sum_{i_1, i_2, i_3=1}^{n_1, n_2, n_3} X_{i_1 i_2 i_3}^2 \sum_{r=1}^R \beta_r x_{i_1}^{(r,1)} x_{i_2}^{(r,2)} x_{i_3}^{(r,3)}$$

is upper bounded by $N^{-5/2} \sum_{r=1}^{R} \beta_r \sum_{i_1,i_2,i_3=1}^{n_1,n_2,n_3} |x_{i_1}^{(r,1)} x_{i_2}^{(r,2)} x_{i_3}^{(r,3)}| \leq \mathcal{O}(N^{-1})$, and its variance is equal to $N^{-5} \sum_{i_1,i_2,i_3=1}^{n_1,n_2,n_3} \left(\sum_{r=1}^{R} \beta_r x_{i_1}^{(r,1)} x_{i_2}^{(r,2)} x_{i_3}^{(r,3)} \right)^2 \leq \mathcal{O}(N^{-5})$. Therefore, we have

$$\frac{(\mathfrak{c}_1\mathfrak{c}_2\mathfrak{c}_3)^{-1}}{N^{3/2}}\sum_{i_1,i_2,i_3=1}^{n_1,n_2,n_3}T^3_{i_1i_2i_3} \overset{\mathbb{P}}{\longrightarrow} \frac{1}{n_1n_2n_3}\sum_{i_1,i_2,i_3=1}^{n_1,n_2,n_3}X^3_{i_1i_2i_3} = \hat{\kappa}_3 \overset{\mathbb{P}}{\longrightarrow} \kappa_3,$$

so does $\hat{\kappa}_4$.

To summarize, we propose the following test procedure:

- (i) Given the observation $T \in \mathbb{R}^{n_1 \times n_2 \times n_2}$ such that the dimensions (n_1, n_2, n_3) satisfy Assumption 2.2, we first compute $\hat{\kappa}_3$, $\hat{\kappa}_4$ using (53).
- (ii) Based on $(\mathfrak{c}_1,\mathfrak{c}_2,\mathfrak{c}_3) = N^{-1}(n_1,n_2,n_3)$, given any $z \in \mathbb{C}^+$, solve g(z) by the iterative method mentioned in Remark 3.4. After obtaining $g(z) = \sum_{j=1}^3 g_j(z)$, the LSD $\nu(E) = \lim_{\eta \downarrow 0} \pi^{-1} \Im(g(E+i\eta))$, which allows us to compute $\int_{-\infty}^{\infty} x^2 \nu(dx)$ numerically.
- (iii) Based on $\boldsymbol{g}(z)$ and $\boldsymbol{a}^{(1)}, \boldsymbol{a}^{(2)}, \boldsymbol{a}^{(3)}$, compute $\boldsymbol{W}^{(3)}(z), \boldsymbol{V}^{(3)}(z,z), \mathcal{V}_{st}^{(3)}(z_1,z_2)$ and $\mathcal{U}_{st,N}^{(3)}(z_1,z_2)$ by (33), (35), (40) and (42); combining with $\hat{\kappa}_3, \hat{\kappa}_4$ in (53), we further obtain $\mu_N^{(3)}(z)$ and $\mathcal{C}_N^{(3)}(z_1,z_2)$ by (38) and (46), then the asymptotic mean and variance of $\widehat{T}_N^{(3)}$ can be numerically estimated by

$$\hat{\xi}_N^{(3)} = -\frac{1}{2\pi \mathrm{i}} \oint_{\mathfrak{C}_1} z^2 \mu_N^{(3)}(z) dz \quad (\hat{\sigma}_N^{(3)})^2 = -\frac{1}{4\pi^2} \oint_{\mathfrak{C}_1} \oint_{\mathfrak{C}_2} z_1^2 z_2^2 \mathcal{C}_N^{(3)}(z_1, z_2) dz_1 dz_2,$$

where the precise definitions of contours $\mathfrak{C}_1, \mathfrak{C}_2$ are given in Theorem 3.1.

(iv) Given a significance level $\alpha \in (0,1)$, we reject H_0 if

$$\tilde{\mathcal{T}}_N^{(3)} = \frac{\hat{T}_N^{(3)} - \hat{\xi}_N^{(3)}}{\hat{\sigma}_N^{(3)}} > z_{\alpha}.$$

4.2 Testing for tensor signal matching

Consider two independent tensor observations $T^{(0)}$ and $T^{(1)}$ from the model (1):

$$\begin{cases}
\mathbf{T}^{(0)} = \sum_{r_0=1}^{R_0} \beta_{r_0,0} \mathbf{x}^{(r_0,1)} \otimes \mathbf{x}^{(r_0,2)} \otimes \mathbf{x}^{(r_0,3)} + \frac{1}{\sqrt{N}} \mathbf{X}^{(0)}, \\
\mathbf{T}^{(1)} = \sum_{r_1=1}^{R_1} \beta_{r_1,1} \mathbf{y}^{(r_1,1)} \otimes \mathbf{y}^{(r_1,2)} \otimes \mathbf{y}^{(r_1,3)} + \frac{1}{\sqrt{N}} \mathbf{X}^{(1)},
\end{cases} (54)$$

where $\boldsymbol{X}^{(0)}$ and $\boldsymbol{X}^{(1)}$ are independent and $\boldsymbol{x}^{(r_0,l)}, \boldsymbol{y}^{(r_1,l)} \in \mathbb{R}^{n_l}$ are deterministic unit vectors for $1 \leq l \leq 3$ and $1 \leq r_0 \leq R_0, 1 \leq r_1 \leq R_1$. We are interested in testing whether $\boldsymbol{T}^{(0)}$ and

 $T^{(1)}$ partially share the same signal structure. This problem can be formulated as the following hypothesis test:

$$H_0: \boldsymbol{x}^{(r_0,l)} \perp \boldsymbol{y}^{(r_1,l)} \text{ for any } 1 \leq r_0 \leq R_0, 1 \leq r_1 \leq R_1 \text{ and } 1 \leq l \leq 3,$$

 $H_1: \text{ there } \exists \text{ at least one } 1 \leq r_0 \leq R_0, 1 \leq r_1 \leq R_1 \text{ and } 1 \leq l \leq 3 \text{ s.t. } \boldsymbol{x}^{(r_0,l)} \not\perp \boldsymbol{y}^{(r_1,l)}.$ (55)

In neuroimaging analysis, the hypothesis test (55) often appears in classification problems, that is, determining whether a person suffers from certain brain diseases based on their neuroimage signals. Typically, the neurological research relies on the functional magnetic resonance imaging (fMRI) data, which is a 3-fold high-dimensional tensor of fractional amplitude of low-frequency fluctuations (fALFF). Many existing literature (e.g. [14, 19, 39, 20]) assumed that the fMRI data from patients suffering certain brain diseases have a low-rank representation (1). For the classification problems, one commonly used method is the supervised tensor learning method (see [40, 43, 11, 20]). The key idea is to first recover the low-rank structures of given labeled samples in database (e.g. the patient groups and normal groups), then classify the new samples based on these estimated low rank structures. In other words, this procedure is equivalent to testing whether the low-rank signals of fMRI data from new samples are the same as those from patient or normal groups, which aligns with the hypothesis test (55).

To build our test procedure, define for $1 \le r_0 \le R_0$,

$$m{R}^{(r_0,1)} := m{\Phi}_d(m{T}^{(1)},m{x}^{(r_0,1)},m{x}^{(r_0,2)},m{x}^{(r_0,3)}),$$

and

$$\widehat{T}_{r_0,N}^{(3)} = \widehat{T}_{r_0,N}^{(3)}(\boldsymbol{x}^{(r_0,1)}, \boldsymbol{x}^{(r_0,2)}, \boldsymbol{x}^{(r_0,3)}) := \|\boldsymbol{R}^{(r_0,1)}\|_2^2 - N \int_{-\infty}^{\infty} x^2 \nu(dx).$$
 (56)

Similar to Proposition 4.1, the following proposition establishes the asymptotic normality of the statistic $\widehat{T}_{r_0,N}^{(3)}$.

Proposition 4.2. Under Assumptions 2.1 and 2.2, for two tensor data $\mathbf{T}^{(0)}$ and $\mathbf{T}^{(1)}$ in (54) and $1 \leq r_0 \leq R_0$, the statistic $\widehat{T}_{r_0,N}^{(3)}$ (56) satisfies that

$$(\widehat{T}_{r_0,N}^{(3)} - \xi_N^{(r_0,3)} - \mathcal{D}^{(r_0,3)}) / \sigma_N^{(r_0,3)} \stackrel{d}{\longrightarrow} \mathcal{N}(0,1),$$

where

$$\mathcal{D}^{(r_0,3)} := 2 \sum_{r_1=1}^{R_1} \beta_{r_1,1}^2 \sum_{l=1}^3 \langle \boldsymbol{x}^{(r_0,l)}, \boldsymbol{y}^{(r_1,l)} \rangle^2 \ge 0,$$

and $\xi_N^{(r_0,3)}, \sigma_N^{(r_0,3)}$ are derived from (31) and (32) by setting $f(z)=z^2$, i.e.

$$\xi_N^{(r_0,3)} = -\frac{1}{2\pi i} \oint_{\mathfrak{C}_1} z^2 \mu_N^{(3)}(z; \kappa_3, \kappa_4, \boldsymbol{x}^{(r_0,1)}, \boldsymbol{x}^{(r_0,2)}, \boldsymbol{x}^{(r_0,3)}) dz,$$

$$(\sigma_N^{(r_0,3)})^2 = -\frac{1}{4\pi^2} \oint_{\mathfrak{C}_1} \oint_{\mathfrak{C}_2} z_1^2 z_2^2 \mathcal{C}_N^{(3)}(z_1, z_2; \kappa_4, \boldsymbol{x}^{(r_0,1)}, \boldsymbol{x}^{(r_0,2)}, \boldsymbol{x}^{(r_0,3)}) dz_1 dz_2.$$

The proof of above proposition is the same as Proposition 4.1. We omit the details here. For the hypothesis test (55), the key task is to estimate $\boldsymbol{x}^{(r_0,l)}$. Note that $\boldsymbol{X}^{(0)}$ and $\boldsymbol{X}^{(1)}$ are independent, then $\boldsymbol{T}^{(0)}$ and $\boldsymbol{T}^{(1)}$ are also independent. We can apply some existing algorithms in the literature, e.g. the tensor unfolding method [35, 10], to estimate $\boldsymbol{x}^{(r_0,1)} \otimes \boldsymbol{x}^{(r_0,2)} \otimes \boldsymbol{x}^{(r_0,3)}$. After obtaining the estimation $\hat{\boldsymbol{x}}^{(r_0,1)} \otimes \hat{\boldsymbol{x}}^{(r_0,2)} \otimes \hat{\boldsymbol{x}}^{(r_0,2)}$ for $1 \leq r_0 \leq R_0$, with the statistic $\hat{T}_{r_0,N}^{(3)}$ in Proposition 4.2, we can test

$$H_0^{(r_0)}: \hat{\boldsymbol{x}}^{(r_0,l)} \perp \boldsymbol{y}^{(r_1,l)}$$
 for any $1 \leq r_1 \leq R_1$ and $1 \leq l \leq 3$, $H_1^{(r_0)}:$ there exists at least one $1 \leq r_1 \leq R_1$ and $1 \leq l \leq 3$ such that $\hat{\boldsymbol{x}}^{(r_0,l)} \not\perp \boldsymbol{y}^{(r_1,l)}$,

through the procedures in §4.1. We accept H_0 in (55) only if we accept $H_0^{(r_0)}$ for all $1 \le r_0 \le R_0$.

Remark 4.1. The above test procedure requires that

$$\widehat{T}_{r_0,N}^{(3)}(\hat{\boldsymbol{x}}^{(r_0,1)},\hat{\boldsymbol{x}}^{(r_0,2)},\hat{\boldsymbol{x}}^{(r_0,3)}) \stackrel{\mathbb{P}}{\longrightarrow} \widehat{T}_{r_0,N}^{(3)}(\boldsymbol{x}^{(r_0,1)},\boldsymbol{x}^{(r_0,2)},\boldsymbol{x}^{(r_0,3)}). \tag{57}$$

Many existing works in the literature have established convergence rate bounds of the form $1 - |\langle \boldsymbol{x}^{(r_0,l)}, \hat{\boldsymbol{x}}^{(r_0,l)} \rangle| \prec \mathfrak{r}_{r_0,l}$, for $1 \leq l \leq 3$ when the SNR $\beta_{r_0,0}$ is sufficiently large, where the convergence rate $\mathfrak{r}_{r_0,l} = \mathfrak{r}_{r_0,l}(\beta_{r_0,0},N)$ depends on the SNR $\beta_{r_0,0}$ and dimension N. Without loss of generality, we assume that such a bound holds. By (49), we know that

$$\begin{split} \widehat{T}_{r_0,N}^{(3)}(\boldsymbol{x}^{(r_0,1)},\boldsymbol{x}^{(r_0,2)},\boldsymbol{x}^{(r_0,3)}) \\ \stackrel{\mathbb{P}}{\longrightarrow} \|\boldsymbol{M}(\boldsymbol{x}^{(r_0,1)},\boldsymbol{x}^{(r_0,2)},\boldsymbol{x}^{(r_0,3)})\|_2^2 - N \int_{-\infty}^{\infty} x^2 \nu(dx) + 2 \sum_{r_1=1}^{R_1} \beta_{r_1}^2 \sum_{l=1}^{3} \langle \boldsymbol{x}^{(r_0,l)},\boldsymbol{y}^{(r_1,l)} \rangle^2. \end{split}$$

Since $T^{(0)}$ and $T^{(1)}$ are independent, similarly we obtain that

$$\begin{split} \widehat{T}_{r_0,N}^{(3)}(\hat{\boldsymbol{x}}^{(r_0,1)},\hat{\boldsymbol{x}}^{(r_0,2)},\hat{\boldsymbol{x}}^{(r_0,3)}) \\ &\stackrel{\mathbb{P}}{\longrightarrow} \|\boldsymbol{M}(\hat{\boldsymbol{x}}^{(r_0,1)},\hat{\boldsymbol{x}}^{(r_0,2)},\hat{\boldsymbol{x}}^{(r_0,3)})\|_2^2 - N \int_{-\infty}^{\infty} x^2 \nu(dx) + 2 \sum_{r_1=1}^{R_1} \beta_{r_1}^2 \sum_{l=1}^3 \langle \hat{\boldsymbol{x}}^{(r_0,l)},\boldsymbol{y}^{(r_1,l)} \rangle^2. \end{split}$$

It is easy to see that

$$\begin{aligned} & \left| \langle \hat{\boldsymbol{x}}^{(r_0,l)}, \boldsymbol{y}^{(r_1,l)} \rangle^2 - \langle \boldsymbol{x}^{(r_0,l)}, \boldsymbol{y}^{(r_1,l)} \rangle^2 \right| \leq \left| \langle \hat{\boldsymbol{x}}^{(r_0,l)} - \boldsymbol{x}^{(r_0,l)}, \boldsymbol{y}^{(r_1,l)} \rangle \right| \cdot \left| \langle \hat{\boldsymbol{x}}^{(r_0,l)} + \boldsymbol{x}^{(r_0,l)}, \boldsymbol{y}^{(r_1,l)} \rangle \right| \\ & \leq \sqrt{2} \min\{ \|\hat{\boldsymbol{x}}^{(r_0,l)} - \boldsymbol{x}^{(r_0,l)}\|_2, \|\hat{\boldsymbol{x}}^{(r_0,l)} + \boldsymbol{x}^{(r_0,l)}\|_2 \} \leq 2(1 - \left| \langle \boldsymbol{x}^{(r_0,l)}, \hat{\boldsymbol{x}}^{(r_0,l)} \rangle \right|)^{1/2} = 2\mathfrak{r}_{r_0,l}^{1/2}. \end{aligned}$$

Moreover, similar to the block decomposition in (4), we define

$$\begin{split} \Delta M_{i_1 i_2}^{12} &:= M_{i_1 i_2}^{12} (\boldsymbol{x}^{(r_0,1)}, \boldsymbol{x}^{(r_0,2)}, \boldsymbol{x}^{(r_0,3)})^2 - M_{i_1 i_2}^{12} (\hat{\boldsymbol{x}}^{(r_0,1)}, \hat{\boldsymbol{x}}^{(r_0,2)}, \hat{\boldsymbol{x}}^{(r_0,3)})^2 \\ &= N^{-1} \sum_{i_3 = 1}^{n_3} X_{i_1 i_2 i_3} (x_{i_3}^{(r_0,3)} - \hat{x}_{i_3}^{(r_0,3)}) \cdot \sum_{i_3 = 1}^{n_3} X_{i_1 i_2 i_3} (x_{i_3}^{(r_0,3)} + \hat{x}_{i_3}^{(r_0,3)}). \end{split}$$

By Proposition 1.1 in [16] and Assumption 2.1, we can prove that

$$\mathbb{P}(|\Delta M_{i_1,i_2}^{12}| > t) \le C \exp(-C_{\theta}(Nt\mathfrak{r}_{r_0,l}^{-1/2})^{\theta}).$$

then for any fixed $\epsilon > 0$ and $t = O(\mathfrak{r}_{r_0,l}^{1/2} N^{\epsilon-1})$, we have

$$\begin{split} & \mathbb{P}\big(\big|\|\boldsymbol{M}(\hat{\boldsymbol{x}}^{(r_0,1)},\hat{\boldsymbol{x}}^{(r_0,2)},\hat{\boldsymbol{x}}^{(r_0,3)})\|_2^2 - \|\boldsymbol{M}(\boldsymbol{x}^{(r_0,1)},\boldsymbol{x}^{(r_0,2)},\boldsymbol{x}^{(r_0,3)})\|_2^2\big| > \mathfrak{r}_{r_0,l}^{1/2}N^{\epsilon+1}\big) \\ & \leq 2\sum_{i_1,i_2=1}^{n_1,n_2} \mathbb{P}(|\Delta M_{i_1,i_2}^{12}| > t) + 2\sum_{i_1,i_3=1}^{n_1,n_3} \mathbb{P}(|\Delta M_{i_1,i_3}^{13}| > t) + 2\sum_{i_2,i_3=1}^{n_2,n_3} \mathbb{P}(|\Delta M_{i_2,i_3}^{23}| > t) \\ & \leq \mathrm{O}(N^2 \exp(-C_{\theta}N^{-\epsilon\theta})). \end{split}$$

Therefore, we only require the convergence rate $\mathfrak{r}_{r_0,l} = \mathrm{o}(N^{-2(1+\epsilon)})$. For the d-fold tensor unfolding method, let $\beta_{r_0,0} = \lambda n^{(d-2)/4}$ and $\lambda > 1 + \mathrm{O}(1)$, [10] proved that $\mathfrak{r}_{r_0,l} \leq \mathrm{O}(n^{\delta - d/4}(\lambda - 1)^{-3/2})$ for any sufficiently small $\delta > 0$. Consequently, when d = 3 and $\beta_{r_0,0} = \mathrm{O}(N^{5/6+\epsilon+\delta})$, we can conclude (57). Readers may also refer to §6.3 for a numerical experiment about the power of $\widehat{T}_{r_0,N}^{(3)}(\hat{x}^{(r_0,1)},\hat{x}^{(r_0,2)},\hat{x}^{(r_0,3)})$ under different values of $\beta_{r_0,0}$.

5 The general case of d-fold tensors $(d \ge 3)$

5.1 CLT for LSS of M

In this section, we extend Theorem 3.1 in §3 for general $d \geq 3$. Let

$$\boldsymbol{M} = \frac{1}{\sqrt{N}} \boldsymbol{\Phi}_d(\boldsymbol{X}, \boldsymbol{a}^{(1)}, \cdots, \boldsymbol{a}^{(d)}) \quad \text{and} \quad \boldsymbol{Q}(z) = (\boldsymbol{M} - z\boldsymbol{I}_N)^{-1}, \tag{58}$$

where $\boldsymbol{a}^{(i)}, 1 \leq i \leq d$ are d deterministic unit vectors and $N = \sum_{i=1}^{d} n_i$ where the dimension n_1, \dots, n_d satisfy Assumption 2.2. $\boldsymbol{X} = [X_{i_1 \dots i_d}]_{n_1 \times \dots \times n_d} \in \mathbb{R}^{n_1 \times \dots \times n_d}$ is a random tensor with entries satisfying Assumption 2.1. Similarly to §3.2, we define the mean function $\mu_N^{(d)}(z)$ and covariance function $\mathcal{C}_N^{(d)}(z_1, z_2)$ using the following functions, which are defined for any sufficiently small $\eta > 0$ and $z, z_1, z_2 \in \mathbb{C}_{\eta}^+$:

1. Let

$$\boldsymbol{\Gamma}^{(d)}(z) := (z + g(z))\boldsymbol{I}_d - \operatorname{diag}(\boldsymbol{g}(z)) + g(z)\boldsymbol{S}_d - \operatorname{diag}(\boldsymbol{g}(z))\boldsymbol{S}_d - \boldsymbol{S}_d\operatorname{diag}(\boldsymbol{g}(z))$$

and

$$\mathbf{W}^{(d)}(z) = [W_{st}^{(d)}(z)]_{d \times d} = -\mathbf{\Gamma}^{(d)}(z)^{-1}.$$
 (59)

2. Let $\Pi^{(d)}(z_1, z_2) = I_d - \operatorname{diag}(\mathfrak{c}^{-1} \circ g(z_1) \circ g(z_2)) S_d$ and

$$V^{(d)}(z_1, z_2) := \Pi^{(d)}(z_1, z_2)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ g(z_1) \circ g(z_2)). \tag{60}$$

3. Given $r, k_1, k_2 \in \{1, \dots, d\}$, let

$$\begin{split} \tilde{\boldsymbol{V}}_r^{(d)}(z_1, z_2) := & \, \boldsymbol{\Pi}^{(d)}(z_1, z_2)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z_1)) [\operatorname{diag}(\boldsymbol{V}^{(d)}(z_2, z_2)) \\ & + \operatorname{diag}(\boldsymbol{S}_d \boldsymbol{V}_{\cdot r}^{(d)}(z_1, z_2)) \boldsymbol{V}^{(d)}(z_1, z_2)], \end{split}$$

where $V_{r}^{(d)}(z_1, z_2)$ is the r-th column of $V^{(d)}(z_1, z_2)$. Moreover, denote

$$\mathcal{V}_{k_1 k_2}^{(d)}(z_1, z_2) := \sum_{l \neq k_1}^d \tilde{V}_{k_1 k_2 l}^{(d)}(z_1, z_2). \tag{61}$$

4. Given $k_1, k_2 \in \{1, \dots, d\}$, let $\mathring{\boldsymbol{V}}^{(d)}(z_1, z_2) := \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z_1)) \boldsymbol{V}^{(d)}(z_2, z_2)$ and

$$\mathcal{U}_{k_1 k_2, N}^{(d)}(z_1, z_2) \tag{62}$$

$$:= \mathfrak{c}_{k_1}^{-1} g_{k_1}(z_1) g_{k_1}(\bar{z}_2) \sum_{l \neq k_1}^d \mathcal{B}_{(4)}^{(k_1,l)} \mathring{V}_{lk_2}^{(d)}(z_1,z_2) + \mathring{V}_{k_1k_2}^{(d)}(z_1,z_2) \sum_{l \neq k_1}^d \mathcal{B}_{(4)}^{(k_1,l)} \mathfrak{c}_l^{-1} g_l(z_1) g_l(\bar{z}_2),$$

where $\mathcal{B}_{(4)}^{(k_1,l)}$ is defined in (29).

Similar to (24), let $v_B^{(d)} := \max\{\mathfrak{v}_d, \zeta\}$ and

$$\mathfrak{F}_d := \{f(z) : f \text{ is analytic on an open set containing } \left[-v_B^{(d)}, v_B^{(d)} \right] \}.$$

Now, for any $f \in \mathfrak{F}_d$, we present the extension of Theorem 3.1 as follows:

Theorem 5.1. Under Assumptions 2.1 and 2.2, for any $f \in \mathfrak{F}_d$ and deterministic unit vectors $\boldsymbol{a}^{(1)} \in \mathbb{R}^{n_1}, \cdots, \boldsymbol{a}^{(d)} \in \mathbb{R}^{n_d}$, let

$$G_N(f) = N \int_{-\infty}^{\infty} f(x) (\nu_N(dx) - \nu(dx)),$$

where ν_N and ν are the ESD and LSD of M in (58), respectively. Then we have

$$\frac{G_N(f) - \mu_N^{(d)}}{\sigma_N^{(d)}} \xrightarrow{d} \mathcal{N}(0,1).$$

where

$$\xi_N^{(d)} := -\frac{1}{2\pi i} \oint_{\sigma_1} f(z) \mu_N^{(d)}(z) dz, \tag{63}$$

$$(\sigma_N^{(d)})^2 := -\frac{1}{4\pi^2} \oint_{\sigma_1} \oint_{\sigma_2} f(z_1) f(z_2) \mathcal{C}_N^{(d)}(z_1, z_2) dz_1 dz_2, \tag{64}$$

where \mathfrak{C}_1 and \mathfrak{C}_2 are two disjoint rectangular contours with vertices $\pm E_1 \pm i\eta_1$ and $\pm E_2 \pm i\eta_2$, respectively, such that $E_1, E_2 \geq v_B^{(d)} + t$, where t > 0 is fixed and $\eta_1, \eta_2 > 0$. Here, the mean function $\mu_N^{(d)}(z)$ is defined as follows:

$$\mu_N^{(d)}(z) := \mathbf{1}_d' \mathbf{\Pi}^{(d)}(z, z)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ g(z)) \overrightarrow{M}_N^{(d)}(z),$$

where $\overrightarrow{M}_N^{(d)}(z) = (M_{1,N}^{(d)}(z), \cdots, M_{d,N}^{(d)}(z))'$ and for $1 \le i \le d$

$$M_{i,N}^{(d)}(z) := g_i(z) \sum_{r \neq i}^{d} \sum_{w \neq i,r}^{d} W_{rw}^{(d)}(z) + \sum_{l \neq i}^{d} \left[(g(z) - g_l(z) - g_l(z)) W_{il}^{(d)}(z) + V_{il}^{(d)}(z, z) \right]$$

$$-2\kappa_3 \sum_{l\neq i}^d \sum_{t\neq l,i}^d \mathcal{B}^{(i,l,t)}_{(3)}(\mathfrak{c}_i \mathfrak{c}_l \mathfrak{c}_t)^{-1} g_i(z) g_l(z) g_t(z) \mathfrak{b}^{(1)}_i \mathfrak{b}^{(1)}_l \mathfrak{b}^{(1)}_t \mathfrak{b}^{(1)}_t + \kappa_4 \mathfrak{c}_i^{-1} g_i(z)^2 \sum_{l\neq i}^d \mathcal{B}^{(i,l)}_{(4)} \mathfrak{c}_l^{-1} g_l(z)^2,$$

and $\mathfrak{b}_{i}^{(1)}$, $\mathcal{B}_{(3)}^{(i,l,t)}$, $W_{il}^{(d)}(z)$, $V_{il}^{(d)}(z,z)$ are defined in (28), (29), (59) and (60), respectively. The variance function $\mathcal{C}_{N}^{(d)}(z_{1},z_{2})$ is defined as follows:

$$C_N^{(d)}(z_1, z_2) := \mathbf{1}_d' \mathbf{\Pi}^{(d)}(z_1, z_2)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z_1)) \boldsymbol{F}_N^{(d)}(z_1, z_2) \mathbf{1}_d,$$

where

$$\boldsymbol{F}_{N}^{(d)}(z_{1}, z_{2}) = [\mathcal{F}_{st,N}^{(d)}(z_{1}, z_{2})]_{d \times d} \quad \mathcal{F}_{st,N}^{(d)}(z_{1}, z_{2}) := 2\mathcal{V}_{st}^{(d)}(z_{1}, z_{2}) + \kappa_{4}\mathcal{U}_{st,N}^{(d)}(z_{1}, z_{2}),$$

and $\mathcal{V}_{st}^{(d)}(z_1,z_2),\mathcal{U}_{st,N}^{(d)}(z_1,z_2)$ are defined in (61) and (62), respectively.

The proof of Theorem 5.1 is given in §G of the supplement.

5.2 Testing for tensor signals

Given the tensor data T generated by (1) and d deterministic unit vectors $\mathbf{a}^{(l)} \in \mathbb{R}^{n_l}$ for $1 \leq l \leq d$, let's define

$$R = R(a^{(1)}, \cdots, a^{(d)}) = \Phi_d(T, a^{(1)}, \cdots, a^{(d)}),$$

and

$$\widehat{T}_N^{(d)} = \widehat{T}_N^{(d)}(\boldsymbol{a}^{(1)}, \cdots, \boldsymbol{a}^{(d)}) = \|\boldsymbol{R}\|_2^2 - N \int_{-\infty}^{\infty} x^2 \nu(dx).$$

Now, we present the generalization of Proposition 4.1 for $d \geq 3$.

Proposition 5.1. Under Assumptions 2.1 and 2.2, for any deterministic unit vectors $\mathbf{a}^{(1)} \in \mathbb{R}^{n_1}, \dots, \mathbf{a}^{(d)} \in \mathbb{R}^{n_d}$, we have

$$(\widehat{T}_N^{(d)} - \xi_N^{(d)} - \mathcal{D}^{(d)}) / \sigma_N^{(d)} \xrightarrow{d} \mathcal{N}(0, 1),$$

where

$$\mathcal{D}^{(d)} = \sum_{r=1}^{R} \beta_r^2 \sum_{k \neq l}^{d} \prod_{j \neq k}^{d} \langle \boldsymbol{x}^{(r,j)}, \boldsymbol{a}^{(j)} \rangle^2 \ge 0,$$

and $\xi_N^{(d)}$, $\sigma_N^{(d)}$ are derived from (63) and (64) as follows:

$$\begin{split} \xi_N^{(d)} &= -\frac{1}{2\pi \mathrm{i}} \oint_{\mathfrak{C}_1} z^2 \mu_N^{(d)}(z) dz, \\ (\sigma_N^{(d)})^2 &= -\frac{1}{4\pi^2} \oint_{\mathfrak{C}_1} \oint_{\mathfrak{C}_2} z_1^2 z_2^2 \mathcal{C}_N^{(d)}(z_1, z_2) dz_1 dz_2. \end{split}$$

The proof of the above proposition follows the same steps as the proof of Proposition 4.1 and is thus omitted. The key step is to show that $\mathbf{R} = \mathbf{M} + \sum_{r=1}^{R} \beta_r \mathbf{U}_r \mathbf{B}^{(r)} \mathbf{U}'_r$, where $\mathbf{B}^{(r)} = [B_{k,l}^{(r)}] \in \mathbb{R}^{d \times d}$ such that $B_{k,l} = (1 - \delta_{k,l}) \prod_{j \neq k,l}^{d} \langle \mathbf{x}^{(r,j)}, \mathbf{a}^{(j)} \rangle$ and

$$oldsymbol{U}_r = \left(egin{array}{cccc} oldsymbol{x}^{(r,1)} & oldsymbol{0}_{n_1} & \cdots & oldsymbol{0}_{n_1} \ oldsymbol{0}_{n_2} & oldsymbol{x}^{(r,2)} & \cdots & oldsymbol{0}_{n_2} \ dots & \ddots & \ddots & dots \ oldsymbol{0}_{n_d} & \cdots & oldsymbol{0}_{n_d} & oldsymbol{x}^{(r,3)} \end{array}
ight) \in \mathbb{R}^{N imes d}.$$

Let $\tilde{\mathcal{T}}_N^{(d)} := (\hat{T}_N^{(d)} - \xi_N^{(d)})/\sigma_N^{(d)}$, Proposition 4.1 implies that

$$\begin{cases} \tilde{\mathcal{T}}_N^{(d)} \stackrel{d}{\longrightarrow} \mathcal{N}(0,1) & \text{under } H_0, \\ \tilde{\mathcal{T}}_N^{(d)} - \mathcal{D}^{(d)} / \sigma_N^{(d)} \stackrel{d}{\longrightarrow} \mathcal{N}(0,1) & \text{under } H_1. \end{cases}$$

The test procedures for general $d \geq 3$ are nearly identical to those introduced in §4.1, with the only difference being the estimations of $\hat{\kappa}_3$, $\hat{\kappa}_4$, which now become:

$$\begin{cases} \hat{\kappa}_3 = \prod_{l=1}^d \mathfrak{c}_l \times N^{3/2 - d} \sum_{i_1 \cdots i_d = 1}^{n_1 \cdots n_d} T^3_{i_1 \cdots i_d} \\ \hat{\kappa}_4 = \prod_{l=1}^d \mathfrak{c}_l \times N^{2 - d} \sum_{i_1 \cdots i_d = 1}^{n_1 \cdots n_d} T^4_{i_1 \cdots i_d} - 3 \end{cases}.$$

One can show that $\hat{\kappa}_3 \xrightarrow{\mathbb{P}} \kappa_3$ and $\hat{\kappa}_4 \xrightarrow{\mathbb{P}} \kappa_4$ using the same arguments as in §4.1, we omit the details here.

6 Numerical Experiments

In this section, we conduct numerical experiments to investigate the performance of our theorems and hypothesis tests. First, we provide several examples to demonstrate the validity of our CLT results presented in Theorem 3.1. Next, we compute the empirical power of our test statistic for (3) under different values of β . Finally, we present an experiment to demonstrate the performance of the tensor signal matching test described in §4.2.

For simplicity of presentation, we focus on the case d=3 and $n_1=n_2=n_3=100$, i.e., $\mathfrak{c}_1=\mathfrak{c}_2=\mathfrak{c}_3=1/3$. The LSD $\nu(x)$ is obtained by solving (16). We have

$$g(z) = \frac{3}{4} \left(\sqrt{z^2 - \frac{8}{3}} - z \right), \text{ and } \nu(x) = \frac{3}{4\pi} \sqrt{\frac{8}{3} - x^2}, \quad |x| \le \sqrt{\frac{8}{3}}.$$
 (65)

6.1 Experiment 1: verification of the CLT

In this subsection, we compare the empirical values of $\mathbb{E}[G_N(f)]$ and $\text{Var}(G_N(f))$ with their theoretical limiting values given in Equations (31) and (32), respectively. Additionally, we assess the normality of the statistics using quantile-quantile plots.

To further illustrate the influence of unit vectors $\boldsymbol{a}^{(1)}, \boldsymbol{a}^{(2)}, \boldsymbol{a}^{(3)}$ and the cumulants κ_3 and κ_4 of random noises on the asymptotic mean $\xi_N^{(d)}$ and variance $\sigma_N^{(3)}$ of the CLT for the LSS, as discussed in Proposition 3.3 and Remark 3.5, we consider several different test functions, two types of vector selection and two distributions for entries of noise tensors. The results are summarized in Table 1.

Specifically, for vector selection, we consider $\mathbf{a}^{(l)} = (1, 0, \dots, 0)', l = 1, 2, 3$, which we abbreviate as "localized" vectors, and $\mathbf{a}^{(l)} = n_l^{-1/2}(1, \dots, 1)', l = 1, 2, 3$, abbreviated as "delocalized" vectors. When $\mathbf{a}^{(l)} = (1, 0, \dots, 0)', l = 1, 2, 3, \mu_N^{(3)}$ will be asymptotically independent of κ_3 . If all $\mathbf{a}^{(l)}$ are delocalized, both $\mu_N^{(3)}$ and $\sigma_N^{(3)}$ become independent of κ_4 as $N \to \infty$. For the noise tensors, we consider those with elements following a standard normal distribution, $\mathcal{N}(0,1)$, which have zero

third and fourth cumulants, and those with elements uniformly distributed on $[-\sqrt{3}, \sqrt{3}]$, denoted as Unif $(\pm\sqrt{3})$, which have a third cumulant of 0 and a fourth cumulant of -1.2. When the noise follows a normal distribution, the influence of κ_3 and κ_4 on the asymptotic mean $\xi_N^{(d)}$ and variance $\sigma_N^{(3)}$ of LSS vanishes.

Table 1: Empirical values of $\mathbb{E}[G_N(f)]$ and $\text{Var}(G_N(f))$ from 100 independent repetitions compared to their respective limiting values in (31) and (32), with different test functions, types of vectors $\{a^{(1)}, a^{(2)}, a^{(3)}\}$ and random tensors X for $n_1 = n_2 = n_3 = 100$.

			$\mathbb{E}[G_N(f)]$		$Var(G_N(f))$	
f(x)	Noise type	Vector type	Empirical	Limit	Empirical	Limit
x^2	$\mathcal{N}(0,1)$	all types	0.0132	0	2.6907	2.6339
e^x	$\mathcal{N}(0,1)$	all types	0.1013	0.0961	1.0841	1.0667
$\cos(x)$	$\mathcal{N}(0,1)$	all types	0.0767	0.0720	0.4046	0.4195
$\frac{\exp(x^2)}{\sqrt{1+x^4}}$	$\mathcal{N}(0,1)$	all types	1.0823	1.1148	6.0429	6.0941
x^2	$\operatorname{Unif}(\pm\sqrt{3})$	localized	-0.0127	0	1.0584	1.0524
e^x	$\mathrm{Unif}(\pm\sqrt{3})$	localized	0.0486	0.0581	0.4508	0.4498
$\cos(x)$	$\mathrm{Unif}(\pm\sqrt{3})$	localized	0.0395	0.0429	0.1825	0.1723
$\frac{\exp(x^2)}{\sqrt{1+x^4}}$	$\mathrm{Unif}(\pm\sqrt{3})$	localized	0.7308	0.7119	2.5070	2.3745
x^2	$\operatorname{Unif}(\pm\sqrt{3})$	delocalized	0.0129	0	2.7312	2.6339
e^x	$\mathrm{Unif}(\pm\sqrt{3})$	delocalized	0.0987	0.0961	1.0757	1.0667
$\cos(x)$	$\mathrm{Unif}(\pm\sqrt{3})$	delocalized	0.0786	0.0720	0.4286	0.4195
$\frac{\exp(x^2)}{\sqrt{1+x^4}}$	$\mathrm{Unif}(\pm\sqrt{3})$	delocalized	1.1406	1.1148	6.0004	6.0941

As shown in Table 1, the empirical results closely match the theoretical values. The results also confirm the intuitions stated in Proposition 3.3. Moreover, the QQ plots of $G_N(f)$ in Figure 1 demonstrate that the asymptotic normality of the LSS holds well.

6.2 Experiment 2: tensor signal alignment test

This experiment focuses on the tensor signal alignment test (3). We generate the observation T using (2) with varying values of β . We are particularly interested in the test's performance when the signal is below the phase transition threshold, i.e., $\beta \in (0, \beta_s]$. For the case $\mathfrak{c}_1 = \mathfrak{c}_2 = \mathfrak{c}_3 = 1/3$, the phase transition threshold is $\beta_s = 2/\sqrt{3}$, as stated in Corollary 3 of [36]. According to (50), we then have

$$\begin{cases} \tilde{\mathcal{T}}_N^{(3)}(\boldsymbol{x}^{(1)},\boldsymbol{x}^{(2)},\boldsymbol{x}^{(3)}) \stackrel{d}{\longrightarrow} \mathcal{N}(0,1), & \text{under } H_0, \\ \tilde{\mathcal{T}}_N^{(3)}(\boldsymbol{x}^{(1)},\boldsymbol{x}^{(2)},\boldsymbol{x}^{(3)}) - 6\beta^2/\sigma_N^{(3)} \stackrel{d}{\longrightarrow} \mathcal{N}(0,1), & \text{under } H_1. \end{cases}$$

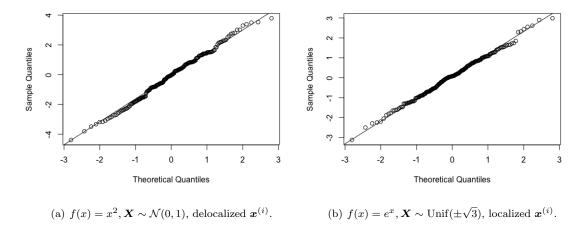


Figure 1: QQ plots of $G_N(f)$ from 100 independent repetitions.

In Table 2 and Figure 2, we use the same settings as in §6.1, with a significance level of $\alpha = 0.05$. We compute the test's empirical power for different β values with 200 repetitions.

Table 2: Empirical sizes $(\beta = 0)$ and powers of $\tilde{\mathcal{T}}_N^{(3)}(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \boldsymbol{x}^{(3)})$ under different β 's and types of noises \boldsymbol{X} and vectors $\boldsymbol{x}^{(i)}$.

β	$\mathcal{N}(0,1),$	$\mathcal{N}(0,1),$	Unif($\pm\sqrt{3}$),	Unif($\pm\sqrt{3}$),
	delocalized	localized	delocalized	localized
0	0.045	0.050	0.045	0.055
0.2	0.075	0.055	0.075	0.090
0.4	0.135	0.115	0.145	0.230
0.6	0.345	0.355	0.340	0.685
0.8	0.745	0.730	0.735	0.975
1	0.970	0.980	0.965	1
1.2	1	1	1	1

Table 2 and Figure 2 provide several insights into the performance of the tensor signal alignment test. Firstly, the empirical sizes are close to the nominal level of 5%.

This suggests that the test maintains the desired significance level reasonably well. Secondly, as the SNR β increases, the power of the test rapidly approaches 1 in all four scenarios. This indicates that the test is highly effective in detecting the presence of a signal when the SNR is sufficiently large. Most notably, even for β values below the critical transition value $\beta_s = 2/\sqrt{3}$, such as $\beta = 1$, the test achieves a power close to one. The test's ability to detect the presence of a signal in such challenging conditions highlights its sensitivity and effectiveness.

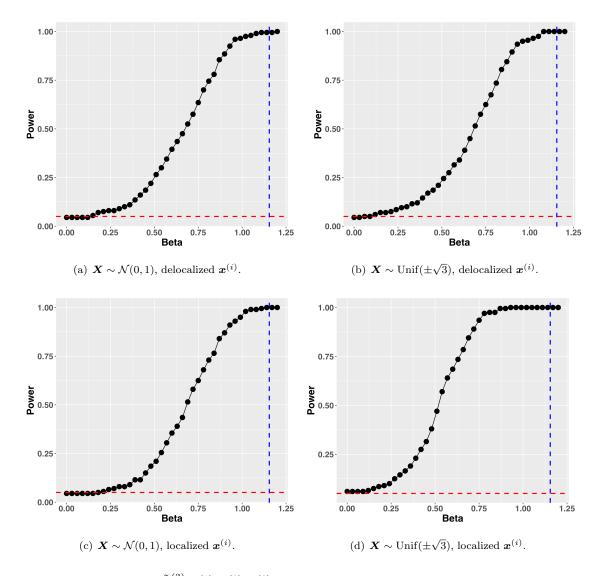


Figure 2: Power plots of $\tilde{\mathcal{T}}_N^{(3)}(\boldsymbol{x}^{(1)},\boldsymbol{x}^{(2)},\boldsymbol{x}^{(3)})$ under different β 's and types of noises \boldsymbol{X} and vectors $\boldsymbol{x}^{(i)}$, where the dashed red line is the significance level $\alpha=0.05$ and the dashed blue line is the threshold of phase transition.

6.3 Experiment 3: tensor signal matching test

In this subsection, We focus on the tensor signal matching test (55). We generate two independent samples, $T^{(0)}$ and $T^{(1)}$, using the following model:

$$\begin{cases} \boldsymbol{T}^{(0)} = \beta_0 \boldsymbol{x}^{(1)} \otimes \boldsymbol{x}^{(2)} \otimes \boldsymbol{x}^{(3)} + \frac{1}{\sqrt{N}} \boldsymbol{X}^{(0)}, \\ \boldsymbol{T}^{(1)} = \beta_1 \boldsymbol{x}^{(1)} \otimes \boldsymbol{x}^{(2)} \otimes \boldsymbol{x}^{(3)} + \frac{1}{\sqrt{N}} \boldsymbol{X}^{(1)}, \end{cases}$$

where the noise tensors $\boldsymbol{X}^{(0)}$ and $\boldsymbol{X}^{(1)}$ are independent, and the two rank-1 tensor signals are parallel but have different strengths. Following the procedures described in §4.2, we first apply the tensor unfolding method to estimate the $\hat{\boldsymbol{x}}^{(1)} \otimes \hat{\boldsymbol{x}}^{(2)} \otimes \hat{\boldsymbol{x}}^{(3)}$ using the first tensor data $\boldsymbol{T}^{(0)}$.

Then, we test whether $T^{(1)}$ contains a signal along $\hat{x}^{(1)} \otimes \hat{x}^{(2)} \otimes \hat{x}^{(3)}$ or not.

The main objective of this experiment is to investigate how the values of β_0 and β_1 affect the power of (55) and to compare it with the power of $\tilde{\mathcal{T}}_N^{(3)}(\boldsymbol{x}^{(1)},\boldsymbol{x}^{(2)},\boldsymbol{x}^{(3)})$ when using known directional vectors.

We set $\beta_0 = 2, 2.5, 3$ and estimate $\hat{x}^{(1)}, \hat{x}^{(2)}, \hat{x}^{(3)}$ for each β_0 . The rest of the setting is essentially the same as in §6.2, with the addition of $\beta_1 \in [0, 1.2]$. We compute the empirical power of $\tilde{\mathcal{T}}_N^{(3)}(\hat{x}^{(1)}, \hat{x}^{(2)}, \hat{x}^{(3)})$ and present the power plots in Figure 3.

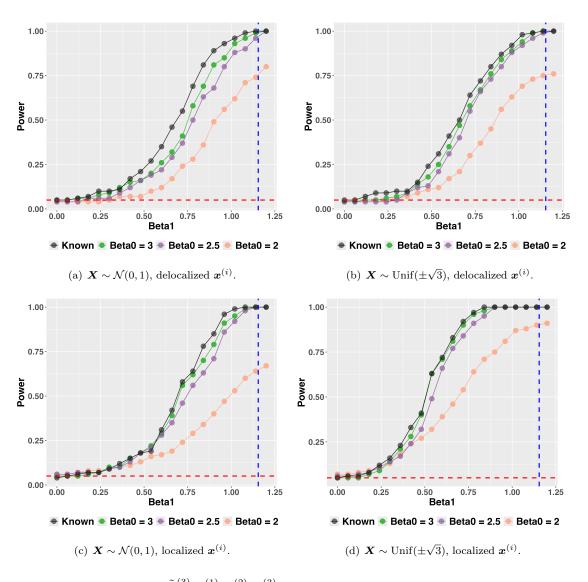


Figure 3: Power plots of $\tilde{\mathcal{T}}_N^{(3)}(\hat{\boldsymbol{x}}^{(1)},\hat{\boldsymbol{x}}^{(2)},\hat{\boldsymbol{x}}^{(3)})$ under different β_0,β_1 and types of noises \boldsymbol{X} and vectors $\boldsymbol{x}^{(i)}$. "Known" denotes the empirical power of $\tilde{\mathcal{T}}_N^{(3)}(\boldsymbol{x}^{(1)},\boldsymbol{x}^{(2)},\boldsymbol{x}^{(3)})$, while "Beta0=a" represents the empirical power of $\tilde{\mathcal{T}}_N^{(3)}(\hat{\boldsymbol{x}}^{(1)},\hat{\boldsymbol{x}}^{(2)},\hat{\boldsymbol{x}}^{(3)})$ when $\beta_0=a,\ a=2,2.5,3$. The dashed red line and blue line indicate the significance level $\alpha=0.05$ and the threshold of phase transition $\beta_s=2/\sqrt{3}=1.1547$, respectively.

Figure 3 reveals several key findings regarding the empirical powers of using $\tilde{\mathcal{T}}_N^{(3)}(\hat{\boldsymbol{x}}^{(1)},\hat{\boldsymbol{x}}^{(2)},\hat{\boldsymbol{x}}^{(3)})$ compared to those using $\tilde{\mathcal{T}}_N^{(3)}(\boldsymbol{x}^{(1)},\boldsymbol{x}^{(2)},\boldsymbol{x}^{(3)})$. In general, the empirical powers of $\tilde{\mathcal{T}}_N^{(3)}(\hat{\boldsymbol{x}}^{(1)},\hat{\boldsymbol{x}}^{(2)},\hat{\boldsymbol{x}}^{(3)})$, which rely on estimated directional vectors, are lower than those of $\tilde{\mathcal{T}}_N^{(3)}(\boldsymbol{x}^{(1)},\boldsymbol{x}^{(2)},\boldsymbol{x}^{(3)})$, which use known directional vectors. This observation holds true across all the situations considered in the experiment. However, when the signal strength in $\boldsymbol{T}^{(0)}$ is sufficiently strong, such as when $\beta_0 = 2.5$ or 3, the performance of $\tilde{\mathcal{T}}_N^{(3)}(\hat{\boldsymbol{x}}^{(1)},\hat{\boldsymbol{x}}^{(2)},\hat{\boldsymbol{x}}^{(3)})$ becomes comparable to that of $\tilde{\mathcal{T}}_N^{(3)}(\boldsymbol{x}^{(1)},\boldsymbol{x}^{(2)},\boldsymbol{x}^{(3)})$. This suggests that the accuracy of the estimated directional vectors improves as the signal strength in $\boldsymbol{T}^{(0)}$ increases, leading to a better performance of the tensor signal matching test.

Remarkably, in cases where $\beta_0 = 2.5$ or 3, even when the signal strength β_1 in $T^{(1)}$ is below the phase transition threshold (e.g., $\beta_1 = 1$), our test still maintains a high power close to 1 for detecting a potential signal matching. This highlights the sensitivity and robustness of the test in identifying signal matching even in challenging scenarios where the signal strength is relatively weak.

Supplementary Materials of the paper "Alignment and matching tests for high-dimensional tensor signals via tensor contraction"

This supplementary document provides all the technical proofs of the results of this paper. It is self-contained without using the results of the main paper.

A Basic settings

For the sake of completeness and readability of this supplement, we start by introducing some notations, definitions and assumptions, even though they may have been encountered earlier in the manuscript.

- (i) Given $z \in \mathbb{C}$, $\Re(z)$ and $\Im(z)$ are the real and imaginary part of z respectively.
- (ii) We use a vector in $\mathbb{R}^{n_1 \times \cdots \times n_d}$ to represent the d-fold real tensor with size $n_1 \times \cdots \times n_d$.
- (iii) Given $A = [a_{ij}]_{n \times n}$, $\operatorname{Tr}(A) = \sum_{i=1}^n a_{ii}$ and A' denotes the transpose of A and $\operatorname{diag}(A)$ is the diagonal matrix made with the main diagonal of A. Moreover, ||A|| denotes the spectral norm of A and $||A||_k = (\sum_{i,j} |a_{ij}|^k)^{1/k}$ for any $k \in \mathbb{N}^+$.
- (iv) Given a matrix $A = [a_{ij}]_{n \times n}$, A_i and $A_{\cdot j}$ denotes the *i*-th row and *j*-th column of A, respectively.
- (v) The *n*-dimensional unit sphere is defined as $\mathbb{S}^{n-1} := \{ \boldsymbol{x} \in \mathbb{R}^n : \|\boldsymbol{x}\|_2 = 1 \}.$
- (vi) C_{η} represents a positive constant which depends on some parameters η .
- (vii) Given an integrable random variable X, we define its centered version as $X^c := X \mathbb{E}[X]$.
- (viii) Given $\eta > 0$, define $\mathbb{C}_{\eta}^+ := \{z \in \mathbb{C} : \Im(z) > \eta\}$ and $\mathbb{C}^+ := \{z \in \mathbb{C} : \Im(z) > 0\}$.
- (ix) For a real sequence $\{a_n\}$, $a_n = \mathrm{o}(n^{-r})$ for $r \ge 0$ means that $\lim_{n \to \infty} a_n n^r = 0$; $a_n = \mathrm{O}(n^{-r})$ means $a_n n^r$ is bounded.
- (x) The asymptotic almost surely convergence, converges in probability and in distribution are denoted by $\xrightarrow{a.s.}$, $\xrightarrow{\mathbb{P}}$ and \xrightarrow{d} , respectively.
- (xi) Given two matrices A, B of size $m \times n$, when $B_{ij} \neq 0$ for all i, j

$$\frac{A}{B} = [A_{ij}B_{ij}^{-1}]_{m \times n}.\tag{A.1}$$

(xii) Let $X = \{X_n\}$ and $Y = \{Y_n\}$ be two sequences of nonnegative random variables. We say Y stochastically dominates X if for all (small) $\epsilon > 0$ and (large) D > 0,

$$\mathbb{P}(X_n > n^{\epsilon} Y_n) \le n^{-D} \tag{A.2}$$

for all $n \geq n_0(\epsilon, D)$, which is denoted by $X \prec Y$ or $X \prec O(Y)$.

Let $d \in \mathbb{N}^+$ and $d \geq 3$, $n_1, \dots, n_d \in \mathbb{N}^+$ be d positive integers, the d-fold rank-R spiked tensor model is defined as:

$$T = \sum_{r=1}^{R} \beta_r \boldsymbol{x}^{(r,1)} \otimes \cdots \otimes \boldsymbol{x}^{(r,d)} + \frac{1}{\sqrt{N}} \boldsymbol{X},$$
 (A.3)

where $\beta_r > 0$, $\boldsymbol{x}^{(r,i)} \in \mathbb{S}^{n_i-1}$, $N := \sum_{j=1}^d n_j$ and $\boldsymbol{X} = [X_{i_1 \dots i_d}]_{n_1 \times \dots \times n_d} \in \mathbb{R}^{n_1 \times \dots \times n_d}$ is a random tensor such that $X_{i_1 \dots i_d}$ are i.i.d. with a subexponential distribution X, that is

Assumption A.1.

$$\limsup_{x>0} e^{x^{\theta}} \mathbb{P}(|X| \ge x) < \infty,$$

where $\theta > 0$. Moreover, $\mathbb{E}[X] = 0$, Var(X) = 1, and its third and forth cumulants are denoted by

$$\kappa_3 := \mathbb{E}[X^3] \quad \text{and} \quad \kappa_4 := \mathbb{E}[X^4] - 3.$$

Assumption A.2. The tensor dimensions n_1, \dots, n_d all tend to infinity such that

$$\lim_{n_1, \dots, n_d \to \infty} \frac{n_j}{n_1 + \dots + n_d} = \mathfrak{c}_j \in (0, 1), \quad 1 \le j \le d.$$

This limiting framework is simply denoted as $N \to \infty$ (where $N := n_1 + \cdots + n_d$) and let

$$\mathfrak{c} = (\mathfrak{c}_1, \cdots, \mathfrak{c}_d)'.$$

Let $\boldsymbol{a}^{(1)} \in \mathbb{S}^{n_1-1}, \dots, \boldsymbol{a}^{(d)} \in \mathbb{S}^{n_d-1}$ be d deterministic unit vectors such that the vector dimensions n_1, \dots, n_d satisfy Assumption A.2. Next, we further define several auxiliary notations as follows:

• Given $k \in \{1, \dots, d\}$, define

$$\mathfrak{b}_k^{(1)} := \sum_{i_1,\dots,i_k}^{n_k} a_{i_k}^{(k)}. \tag{A.4}$$

• For any l distinct integers $k_1, k_2, \dots, k_l \in \{1, \dots, d\}$, i.e. $k_1 \neq k_2 \neq \dots \neq k_l$, define

$$\mathcal{B}_{(r)}^{(k_1,\dots,k_l)} := \sum_{i_j=1, j\neq k_1\dots k_l}^{n_j} (\mathcal{A}_{i_1\dots i_d}^{(k_1,\dots,k_l)})^r, \tag{A.5}$$

where $r \geq 2, r \in \mathbb{N}$ and

$$\mathcal{A}_{i_1\cdots i_d}^{(k_1,\cdots,k_l)} := \prod_{j \neq k_1\cdots k_l} a_{i_j}^{(j)}. \tag{A.6}$$

Moreover, we say $a^{(j)}$ is delocalized if

$$\lim_{n_{j} \to \infty} \|\boldsymbol{a}^{(j)}\|_{\infty} = \lim_{n_{j} \to \infty} \max_{1 \le i_{j} \le n_{j}} |a_{i_{j}}^{(j)}| = 0, \tag{A.7}$$

otherwise, $a^{(j)}$ is localized.

As the core tool of this article, for any a d-fold tensor $T \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ and vectors $\boldsymbol{a}^{(j)} = (a_1^{(j)}, \cdots, a_{n_j}^{(j)})' \in \mathbb{R}^{n_j}, 1 \leq j \leq d$ the d-fold blockwise tensor contraction operator $\boldsymbol{\Phi}_d$ is defined by

$$\Phi_d: \mathbb{R}^{n_1 \times \cdots \times n_d} \times \mathbb{S}^{n_1 - 1} \times \cdots \times \mathbb{S}^{n_d - 1} \longrightarrow \mathbb{R}^{N \times N},$$

$$\Phi_{d}(\boldsymbol{T}, \boldsymbol{a}^{(1)}, \cdots, \boldsymbol{a}^{(d)}) \longrightarrow \begin{pmatrix}
\mathbf{0}_{n_{1} \times n_{1}} & \boldsymbol{T}^{12} & \cdots & \boldsymbol{T}^{1d} \\
(\boldsymbol{T}^{12})' & \mathbf{0}_{n_{2} \times n_{2}} & \cdots & \boldsymbol{T}^{2d} \\
\vdots & \vdots & \ddots & \vdots \\
(\boldsymbol{T}^{1d})' & (\boldsymbol{T}^{2d})' & \cdots & \mathbf{0}_{n_{d} \times n_{d}}
\end{pmatrix}, \tag{A.8}$$

where

$$T^{ij} = T(a^{(1)}, \dots, a^{(i-1)}, a^{(i+1)}, \dots, a^{(j-1)}, a^{(j+1)}, \dots, a^{(d)}) \in \mathbb{R}^{n_i \times n_j}$$
 for $i < j$.

and

$$T(\{\boldsymbol{a}^{(1)}, \cdots, \boldsymbol{a}^{(d)}\} \setminus \{\boldsymbol{a}^{(j_1)}, \boldsymbol{a}^{(j_2)}\}) := \left[\sum_{i_j=1, j \neq j_1, j_2}^{n_j} T_{i_1, \cdots, i_d} \mathcal{A}_{i_1 \cdots i_d}^{(j_1, j_2)}\right]_{n_{j_1} \times n_{j_2}}$$
(A.9)

is second order contraction matrix for any $1 \le j_1 \ne j_2 \le d$. In this article, we will study the asymptotic spectral properties of

$$M := \frac{1}{\sqrt{N}} \Phi_d(X, a^{(1)}, \dots, a^{(d)})$$
 and $Q(z) = (M - zI_N)^{-1}$, (A.10)

where Q(z) is the resolvent of M for any $z \in \mathbb{C}^+$. Similar as (A.8), we also split $Q(z) = [Q^{ij}(z)]_{d \times d}$ into $d \times d$ blocks such that $Q^{ij}(z) \in \mathbb{C}^{n_i \times n_j}$, then for each diagonal block, let

$$\rho_i(z) := N^{-1} \operatorname{Tr}(\boldsymbol{Q}^{ii}(z)), \quad \rho(z) := \sum_{i=1}^d \rho_i(z), \quad \mathfrak{m}_i(z) := \mathbb{E}\left[\rho_i(z)\right], \quad \mathfrak{m}(z) := \mathbb{E}[\rho(z)], \quad (A.11)$$

and

$$\boldsymbol{m}(z) := (\mathfrak{m}_1(z), \cdots, \mathfrak{m}_d(z))' \quad \text{and} \quad \mathfrak{c} := (\mathfrak{c}_1, \cdots, \mathfrak{c}_d)'.$$
 (A.12)

B Properties of vector Dyson equation induced by the matrix M

In this section, we will investigate several important properties of the vector Dyson equation derived by M, which is defined as follows:

$$-\frac{\mathfrak{c}}{g(z)} = z + \mathbf{S}_d g(z),\tag{B.1}$$

where $g(z) = (g_1(z), \dots, g_d(z))'$ is the solution of (B.1) and " $\frac{\mathfrak{c}}{g(z)}$ " is the entrywise division as in (A.1) and

$$S_d := \mathbf{1}_{d \times d} - I_d. \tag{B.2}$$

The main reason of studying the vector Dyson equation (B.1) is that the mean of the trace of resolvent Q(z) satisfies that (see Theorem D.2 for more details of (B.3))

$$-\frac{\mathbf{c}}{\boldsymbol{m}(z)} = z + \boldsymbol{S}_d \boldsymbol{m}(z) + \boldsymbol{\delta}(z), \tag{B.3}$$

where $\boldsymbol{m}(z) = (N^{-1}\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{11}(z))], \cdots, N^{-1}\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{dd}(z))])'$ defined in (A.12) and $\boldsymbol{\delta}(z)$ is a small perturbation term such that $\lim_{N\to\infty} \|\boldsymbol{\varepsilon}(z)\|_{\infty} = 0$. It is easy to see that (B.1) is the limiting form of (B.3). Therefore, the vector Dyson equation (B.1) is an important tool to investigate the asymptotic properties of $N^{-1}\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}(z))]$. In precise, we investigate the following properties of the vector Dyson equation (B.1):

- 1. (B.1) admits a unique analytical solution on \mathbb{C}^+ ;
- 2. For any vector-valued function $\mathbf{v}(z) \in \mathbb{C}^d$ satisfying $-\frac{\mathfrak{c}}{\mathbf{v}(z)} = z + \mathbf{S}_d \mathbf{v}(z) + \boldsymbol{\varepsilon}(z)$, $\boldsymbol{\varepsilon}(z)$ here is a small perturbation term uniformly controlled over a given region, then $\|\mathbf{g}(z) \mathbf{v}(z)\|_{\infty}$ is also small uniformly over the same region.

Particularly, the property 2 above is called the *stability of the vector Dyson equation* (B.1). This stability immediately implies the asymptotic equivalence of m(z) and g(z). Further combining the fact that there exists a probability measure ν associated with g(z) (see Theorem C.2), we can determine ν is indeed the limiting spectral distribution of the matrix M.

Technically, to establish the stability of the vector Dyson equation (B.1), we prove that the stability operator of (B.1), which is a $d \times d$ complex matrix (see (B.6) later), is invertible in §B.2. Moreover, this stability operator also appears in the asymptotic mean and variance of the linear spectral statistics of the matrix M.

For a comprehensive discussion of the Dyson equation of random matrices, readers can refer to [1]. Without loss of generality, we assume $\mathfrak{c}_1 = \max_{1 \leq l \leq d} \mathfrak{c}_l$ in §B.

B.1 Existence and uniqueness for the solution of (B.1)

Theorem B.1. Under Assumption A.2, (B.1) admits a unique analytical solution on \mathbb{C}^+ .

First, we will show that (B.1) has a unique solution in the domain of

$$\mathscr{B}_{\eta_0}^d := \left\{ \boldsymbol{u}(z) \in \mathscr{B}_+^d : \|\boldsymbol{u}\|_{\infty} \le \eta_0^{-1} \mathfrak{c}_1, \quad \min_{1 \le i \le d} \Im(u_i(z)) \ge \frac{\eta_0^3 \mathfrak{c}_d^2 \mathfrak{c}_1^{-1}}{[1 + \mathfrak{c}_1(d-1)]^2} \right\},$$

where

$$\mathscr{B}_+^d := \left\{ \boldsymbol{u}(z) \in \mathbb{C}^d \text{ is analytical for } z \in \mathbb{C}^+ \text{ and } \min_{1 \leq i \leq d} \Im(u_i(z)) > 0 \right\}.$$

Here, we introduce the following metric:

$$D_{\mathbb{C}^+}(z_1, z_2) = \frac{|z_1 - z_2|^2}{\Im(z_1)\Im(z_2)}$$
 for $\forall z_1, z_2 \in \mathbb{C}^+$.

Besides, we define a function mapping $\Psi_d: \mathscr{B}^d_+ \to \mathscr{B}^d_+$ as follows:

$$\Psi_d(z, \boldsymbol{u}) = -\frac{\mathfrak{c}}{z + \boldsymbol{S}_d \boldsymbol{u}(z)}.$$

Then we give the following result:

Lemma B.1 (Ψ_d is a contraction mapping). Under Assumption A.2, for any $\eta_0 > 0$, let

$$\mathbb{H}_{\eta_0} := \{ z \in \mathbb{C}_{\eta_0}^+, |z| \le \eta_0^{-1} \}, \tag{B.4}$$

then $\Psi_d(z,\cdot)$ maps $\mathscr{B}^d_{\eta_0}$ to itself such that

$$\max_{1 \le j \le d} D_{\mathbb{C}^+}(\boldsymbol{\Psi}_d(z, \boldsymbol{u})_j, \boldsymbol{\Psi}_d(z, \boldsymbol{w})_j) \le (1 + \eta_0^2 \|\boldsymbol{S}_d\|^{-1})^{-2} \max_{1 \le j \le d} D_{\mathbb{C}^+}(u_j(z), w_j(z)),$$

for any $z \in \mathbb{H}_{\eta_0}$ and $\boldsymbol{u}, \boldsymbol{w} \in \mathscr{B}_{\eta_0}^+$, where $\Psi_d(z, \boldsymbol{u})_j$ represents the j-th entry of $\Psi_d(z, \boldsymbol{u})$.

Proof. First, notice that

$$|\Psi_d(z,\boldsymbol{u})_j| \leq \Im(z+\boldsymbol{S}_d\boldsymbol{u})_j^{-1} \max_{1 \leq i \leq d} \mathfrak{c}_i \leq \eta_0^{-1} \mathfrak{c}_1$$

and

$$|\Psi_d(z, \boldsymbol{u})_j| \ge rac{\min_{1 \le i \le d} \mathfrak{c}_i}{|z| + |(\boldsymbol{S}_d \boldsymbol{u})_j|} \ge rac{\eta_0 \mathfrak{c}_d}{1 + \mathfrak{c}_1 (d-1)},$$

where the last inequality is valid due to $|z| \leq \eta_0^{-1}$ for $z \in \mathbb{H}_{\eta_0}$, $\|\boldsymbol{u}\|_{\infty} \leq \mathfrak{c}_{(1)}\eta_0^{-1}$ and $|(\boldsymbol{S}_d\boldsymbol{u})_j| \leq \sum_{k=1, k \neq j}^d |u_k|$ for $\boldsymbol{u} \in \mathcal{B}_{\eta_0}^d$, which implies that

$$\Im(\boldsymbol{\Psi}_{d}(z,\boldsymbol{u})_{j}) = \frac{\mathfrak{c}_{j}\Im(z+\boldsymbol{S}_{d}\boldsymbol{u})_{j}}{|z+(\boldsymbol{S}_{d}\boldsymbol{u})_{j}|^{2}} \geq \Im(z)|\boldsymbol{\Psi}_{d}(z,\boldsymbol{u})_{j}|^{2}\mathfrak{c}_{j}^{-1} \geq \frac{\eta_{0}^{3}\mathfrak{c}_{d}^{2}\mathfrak{c}_{1}^{-1}}{[1+\mathfrak{c}_{1}(d-1)]^{2}}.$$

Hence, $\Psi_d(z,\cdot)$ maps $\mathscr{B}_{\eta_0}^+$ to itself. Next, for any $u, w \in \mathscr{B}_{\eta_0}^+$, we have

$$\begin{split} &D_{\mathbb{C}^{+}}(\boldsymbol{\Psi}_{d}(z,\boldsymbol{u})_{j},\boldsymbol{\Psi}_{d}(z,\boldsymbol{w})_{j}) = D_{\mathbb{C}^{+}}(z+(\boldsymbol{S}_{d}\boldsymbol{u})_{j},z+(\boldsymbol{S}_{d}\boldsymbol{w})_{j}) \\ &= D_{\mathbb{C}^{+}}(\mathrm{i}\ \mathrm{Im}z+(\boldsymbol{S}_{d}\boldsymbol{u})_{j},\mathrm{i}\ \mathrm{Im}z+(\boldsymbol{S}_{d}\boldsymbol{w})_{j}) \\ &\leq \left(1+\frac{\Im(z)}{(\boldsymbol{S}_{d}\boldsymbol{u})_{j}}\right)^{-1}\left(1+\frac{\Im(z)}{(\boldsymbol{S}_{d}\boldsymbol{w})_{j}}\right)^{-1}D_{\mathbb{C}^{+}}((\boldsymbol{S}_{d}\boldsymbol{u})_{j},(\boldsymbol{S}_{d}\boldsymbol{w})_{j}) \\ &\leq (1+\eta_{0}^{2}\|\boldsymbol{S}_{d}\|^{-1})^{-2}\max_{1\leq i\leq d}D_{\mathbb{C}^{+}}(u_{j}(z),w_{j}(z)), \end{split}$$

where we use some basic properties of $D_{\mathbb{C}^+}(\cdot,\cdot)$ in proving above inequalities, readers can refer to Lemma 4.2 in [1] for details.

Now, the existence and uniqueness of (B.1) for $z \in \mathbb{H}_{\eta_0}$ can be proved by Lemma B.1 and Banach fixed-point theorem. Since η_0 is an arbitrary positive number, we can extend this conclusion to \mathcal{B}^d_+ by letting $\eta_0 \to 0$, which concludes Theorem B.1.

B.2 The invertibility of stability operators

The study of the stability operator induced by the vector Dyson equation (B.1) is for the sake of later Theorem B.2. To introduce it, we first define the self-energy operator as follows:

$$\mathbf{F}^{(d)} := \mathbf{F}^{(d)}(z) = \operatorname{diag}(|\mathbf{c}^{-1} \circ \mathbf{g}(z)|) \mathbf{S}_d \operatorname{diag}(|\mathbf{g}(z)|) = [F_{ij}(z)]_{d \times d}, \tag{B.5}$$

where $F_{ii}(z) \equiv 0$ and $F_{ij}(z) = \mathfrak{c}_i^{-1}|g_i(z)g_j(z)|$ for $i \neq j$. Then the stability operator of (B.1) is defined as

$$\boldsymbol{B}^{(d)} := \boldsymbol{B}^{(d)}(z) = \boldsymbol{I}_d - \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1} \circ \boldsymbol{g}(z)^{\circ 2}) \boldsymbol{S}_d = \operatorname{diag}(|\boldsymbol{g}|) (\boldsymbol{I}_d - \operatorname{diag}(e^{2i\boldsymbol{q}}) \boldsymbol{F}) \operatorname{diag}(|\boldsymbol{g}|)^{-1}. \quad (B.6)$$

In this section, we first prove that

Proposition B.1. Under Assumption A.2, for any $\eta_0 > 0$ and $z \in \mathbb{H}_{\eta_0}$ in (B.4), the stability operator (B.6) is invertible.

For simplicity, we simplify $\mathbf{F}^{(d)}$ and $\mathbf{B}^{(d)}$ by \mathbf{F} and \mathbf{B} , respectively. Before proving above proposition, we need some preliminaries. Notice that all entries of \mathbf{F} are non-negative, then according to the Perron-Frobenius theorem, there exists a positive vector $\mathbf{f} := \mathbf{f}(z)$ such that $\mathbf{F}\mathbf{f} = \|\mathbf{F}\|\mathbf{f}$. In addition, taking the imaginary part of (B.1), i.e.

$$(B.1) \Rightarrow \frac{\mathfrak{c} \circ \Im(\boldsymbol{g})}{|\boldsymbol{g}|^2} = \Im(z) + \boldsymbol{S}_d \Im(\boldsymbol{g}), \tag{B.7}$$

which yields that

$$\sin \mathbf{q} = \Im(z)\mathbf{c}^{-1} \circ |\mathbf{g}| + \mathbf{F}\sin \mathbf{q},\tag{B.8}$$

where $g = e^{iq} \circ |g|$ and $\sin q = \frac{\Im(g)}{|g|}$. Therefore, we can obtain

$$\langle \mathbf{f}, \sin \mathbf{q} \rangle = \Im(z) \langle \mathbf{f}, \mathbf{c}^{-1} \circ |\mathbf{g}| \rangle + ||\mathbf{F}|| \langle \mathbf{f}, \sin \mathbf{q} \rangle,$$

i.e.

$$\|F\| = 1 - \frac{\Im(z)\langle f, \mathfrak{c}^{-1} \circ |g|\rangle}{\langle f, \sin q\rangle} < 1, \text{ for } z \in \mathbb{C}^+.$$
(B.9)

Hence, $I_d - F$ is invertible. Moreover, by (B.6), we have

$$\boldsymbol{B}(z) = \operatorname{diag}(\mathfrak{c}^{-1/2} \circ \boldsymbol{g}(z)) (\boldsymbol{I}_d - \operatorname{diag}(\mathfrak{c}^{-1/2} \circ \boldsymbol{g}(z)) \boldsymbol{S}_d \operatorname{diag}(\mathfrak{c}^{-1/2} \circ \boldsymbol{g}(z))) \operatorname{diag}(\mathfrak{c}^{-1/2} \circ \boldsymbol{g}(z))^{-1} \boldsymbol{S}_d \boldsymbol{S}$$

where

$$\begin{split} & \boldsymbol{I}_{d} - \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1/2} \circ \boldsymbol{g}(z)) \boldsymbol{S}_{d} \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1/2} \circ \boldsymbol{g}(z)) \\ & = \operatorname{diag}(e^{\mathrm{i}\boldsymbol{q}(z)}) (\operatorname{diag}(e^{-2\mathrm{i}\boldsymbol{q}(z)}) - \operatorname{diag}(|\boldsymbol{\mathfrak{c}}^{-1/2} \circ \boldsymbol{g}(z)|) \boldsymbol{S}_{d} \operatorname{diag}(|\boldsymbol{\mathfrak{c}}^{-1/2} \circ \boldsymbol{g}(z)|)) \operatorname{diag}(e^{\mathrm{i}\boldsymbol{q}(z)}). \end{split}$$

to prove that B(z) is invertible, it is enough to prove that

$$\operatorname{diag}(e^{-2\mathrm{i}\boldsymbol{q}(z)}) - \operatorname{diag}(|\mathfrak{c}^{-1/2} \circ \boldsymbol{g}(z)|) \boldsymbol{S}_d \operatorname{diag}(|\mathfrak{c}^{-1/2} \circ \boldsymbol{g}(z)|)$$

is invertible. In fact, we can prove the above matrix is invertible by showing the spectral gap of $\operatorname{diag}(|\mathfrak{c}^{-1/2} \circ g(z)|) S_d \operatorname{diag}(|\mathfrak{c}^{-1/2} \circ g(z)|)$ is positive. To make this precise, we start with a definition:

Definition B.1. For any matrix A, the spectral gap Gap(A) is the difference between the two largest eigenvalues of $\sqrt{AA^*}$.

Next, we need the following lemma:

Lemma B.2. Let $\mathbf{v} = (v_1, \dots, v_d)' \in \mathbb{R}^d$ such that $0 < v_d \le \dots \le v_1$, where $d \ge 3$, then

$$\operatorname{Gap}(\boldsymbol{v}\boldsymbol{v}' - \operatorname{diag}(\boldsymbol{v}^{\circ 2})) > \sum_{i=3}^{d} v_i^2.$$

Proof. First, let t^{-1} be the eigenvalue of $vv' - \text{diag}(v^{\circ 2})$, by the matrix determinant lemma, it implies that

$$0 = \det(t(\boldsymbol{v}\boldsymbol{v}' - \operatorname{diag}(\boldsymbol{v}^{\circ 2})) - \boldsymbol{I}_d) = (-1)^d \det(\boldsymbol{I}_d + t\operatorname{diag}(\boldsymbol{v}^{\circ 2}))(1 - t\boldsymbol{v}'(\boldsymbol{I}_d + t\operatorname{diag}(\boldsymbol{v}^{\circ 2}))^{-1}\boldsymbol{v}).$$

In fact, $vv' - \operatorname{diag}(v^{\circ 2})$ always has one positive eigenvalue due to $\mathbf{1}'_d(vv' - \operatorname{diag}(v^{\circ 2}))\mathbf{1}_d = \sum_{k \neq l}^d v_k v_l > 0$. Suppose t > 0, that is, t^{-1} is a positive eigenvalue, we can obtain $1 - tv'(\mathbf{I}_d + t\operatorname{diag}(v^{\circ 2}))^{-1}v = 0$, and the equation

$$\sum_{i=1}^{d} \frac{1}{1 + tv_i^2} = d - 1$$

has total d-1 negative roots denoted by t_i such that $0 > t_2 > \cdots > t_d$, where $v_i^2 < -t_i^{-1} < v_{i-1}^2$ for $i = 2, \dots, d$ and one positive zero t_1 , hence we conclude that $\boldsymbol{v}\boldsymbol{v}' - \operatorname{diag}(\boldsymbol{v}^{\circ 2})$ only has one positive eigenvalue t_1^{-1} . Let $l = t^{-1}$, then we obtain

$$\prod_{i=1}^{d} (l + v_i^2) - \sum_{i=1}^{d} v_i^2 \prod_{j \neq i}^{d} (l + v_j^2) = 0.$$

Since the coefficient of l^{d-1} is zero, then $\sum_{i=1}^d t_i^{-1} = 0$. Next, suppose $s^{-1} < 0$ is a negative eigenvalue of $vv' - \operatorname{diag}(v^2)$ such that $1 - sv'(I_d + s\operatorname{diag}(v^2))^{-1}v = 0$, then we have

$$t_1^{-1} + s^{-1} \ge t_1^{-1} + t_2^{-1} = -\sum_{i=3}^d t_i^{-1} \ge \sum_{i=3}^d v_i^2.$$

On the other hand, if $\det(\mathbf{I}_d + s \operatorname{diag}(\mathbf{v}^{\circ 2})) = 0$, which implies that $s = -v_i^{-2}$. Let's consider two possible cases. First, if $v_1 = v_2$, then

$$t_1^{-1} + s^{-1} \ge -\sum_{i=2}^d t_i^{-1} - v_1^2 \ge \sum_{i=2}^d v_i^2 - v_1^2 = \sum_{i=3}^d v_i^2.$$

Second, if $v_1 > v_2$, then we claim that $s \neq -v_1^{-2}$. Otherwise, there exists a nonzero $\boldsymbol{x} \in \mathbb{R}^d$ such that

$$(\boldsymbol{v}\boldsymbol{v}' - \operatorname{diag}(\boldsymbol{v}^{\circ 2}) + v_1^2 \boldsymbol{I}_d)\boldsymbol{x} = 0 \implies v_1^2 x_k + v_k \sum_{j \neq k}^d v_j x_j = 0.$$

Let k = 1, it implies that $\langle \boldsymbol{v}, \boldsymbol{x} \rangle = 0$. When k > 1, notice that

$$(v_1^2 - v_k^2)x_k = -v_k \sum_{j=1}^d v_j x_j = 0,$$

since $v_1 > v_k$ for k > 1, it gives that $x_k = 0$ for k > 1, which further implies that $x_1 = 0$ due to $\langle \boldsymbol{v}, \boldsymbol{x} \rangle = 0$. It is a contradiction since \boldsymbol{x} is nonzero. As a result, we obtain that

$$t_1^{-1} + s^{-1} \ge -\sum_{i=2}^d t_i^{-1} - v_2^2 \ge \sum_{i=2}^d v_i^2 - v_2^2 = \sum_{i=3}^d v_i^2.$$

By the Definition B.1, we have

 $\operatorname{Gap}(\boldsymbol{v}\boldsymbol{v}' - \operatorname{diag}(\boldsymbol{v}^2)) = \min\{t_1^{-1} + s^{-1} : s < 0 \text{ and } s^{-1} \text{ is an eigenvalue of } \boldsymbol{v}\boldsymbol{v}' - \operatorname{diag}(\boldsymbol{v}^2)\} \ge \sum_{i=3}^d v_i^2,$ which completes our proof.

Remark B.1. Since F(z) in (B.5) and diag($|\mathfrak{c}^{-1/2} \circ g(z)|$) S_d diag($|\mathfrak{c}^{-1/2} \circ g(z)|$) are similar, then the largest eigenvalue of diag($|\mathfrak{c}^{-1/2} \circ g(z)|$) S_d diag($|\mathfrak{c}^{-1/2} \circ g(z)|$) is the same as F(z), which is strictly less than 1, then by Lemma B.2, we have

$$\sum_{i=1}^{d} \mathbf{c}_{i}^{-1} |g_{i}(z)|^{2} - \max_{1 \leq i \leq d} \mathbf{c}_{i}^{-1} |g_{i}(z)|^{2} < ||\mathbf{F}(z)|| < 1.$$

Therefore, it implies that $|g_i(z)| < \sqrt{\mathfrak{c}_i}$ for all $i = 1, \dots, d$ except $i = \arg\max_{1 \le i \le d} \mathfrak{c}_i^{-1} |g_i(z)|^2$.

Now, let's prove Proposition B.1 as follows:

Proof of Proposition B.1. By (B.6), since

$$\boldsymbol{B}(z) = \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1/2} \circ \boldsymbol{g}(z)) (\boldsymbol{I}_d - \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1/2} \circ \boldsymbol{g}(z)) \boldsymbol{S}_d \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1/2} \circ \boldsymbol{g}(z))) \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1/2} \circ \boldsymbol{g}(z))^{-1},$$
 and

$$\begin{split} & \boldsymbol{I}_{d} - \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1/2} \circ \boldsymbol{g}(z)) \boldsymbol{S}_{d} \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1/2} \circ \boldsymbol{g}(z)) \\ & = \operatorname{diag}(e^{\mathrm{i}\boldsymbol{q}(z)}) (\operatorname{diag}(e^{-2\mathrm{i}\boldsymbol{q}(z)}) - \operatorname{diag}(|\boldsymbol{\mathfrak{c}}^{-1/2} \circ \boldsymbol{g}(z)|) \boldsymbol{S}_{d} \operatorname{diag}(|\boldsymbol{\mathfrak{c}}^{-1/2} \circ \boldsymbol{g}(z)|)) \operatorname{diag}(e^{\mathrm{i}\boldsymbol{q}(z)}), \end{split}$$

then $\boldsymbol{B}(z)$ is invertible if and only if $\operatorname{diag}(e^{-2i\boldsymbol{q}(z)}) - \operatorname{diag}(|\mathfrak{c}^{-1/2} \circ \boldsymbol{g}(z)|) \boldsymbol{S}_d \operatorname{diag}(|\mathfrak{c}^{-1/2} \circ \boldsymbol{g}(z)|)$ is invertible. Based on Lemma B.2, we have

$$\operatorname{Gap}(\operatorname{diag}(|\mathfrak{c}^{-1/2}\circ\boldsymbol{g}(z)|)\boldsymbol{S}_d\operatorname{diag}(|\mathfrak{c}^{-1/2}\circ\boldsymbol{g}(z)|)) > \sum_{i=2}^d \mathfrak{c}_{(i)}^{-1}|g_{(i)}(z)|^2,$$

where $\mathfrak{c}_{(i)}^{-1}|g_{(i)}(z)|^2$ is the *i*-th largest entries in $|\mathfrak{c}^{-1/2} \circ g(z)|^2$. Recall that $|g_i(z)| \geq C_{\eta_0,d,\mathfrak{c}}$ when $z \in \mathbb{H}_{\eta_0}$, see Lemma B.1, so the spectral gap of $\operatorname{diag}(|\mathfrak{c}^{-1/2} \circ g(z)|) S_d \operatorname{diag}(|\mathfrak{c}^{-1/2} \circ g(z)|)$ is positive for $z \in \mathbb{H}_{\eta_0}$. By the Remark B.1, we know that the largest eigenvalue of $\operatorname{diag}(|\mathfrak{c}^{-1/2} \circ g(z)|) S_d \operatorname{diag}(|\mathfrak{c}^{-1/2} \circ g(z)|)$ is strictly smaller than 1, which can further implies that

$$\operatorname{diag}(e^{-2\mathrm{i}\boldsymbol{q}}) - \operatorname{diag}(|\mathfrak{c}^{-1/2} \circ \boldsymbol{g}(z)|) \boldsymbol{S}_d \operatorname{diag}(|\mathfrak{c}^{-1/2} \circ \boldsymbol{g}(z)|)$$

is invertible for $z \in \mathbb{C}^+$. In fact, denote λ^{\pm} to be the largest positive (+) and smallest negative (-) eigenvalue of diag($|\mathfrak{c}^{-1/2} \circ g(z)|$) S_d diag($|\mathfrak{c}^{-1/2} \circ g(z)|$), then

$$\min_{1 \le i \le d} |e^{-2iq_i} - \lambda^-| > |-1 - \lambda^-| > |\lambda^+ + \lambda^-| = \operatorname{Gap}(\operatorname{diag}(|\mathfrak{c}^{-1/2} \circ \boldsymbol{g}(z)|) \boldsymbol{S}_d \operatorname{diag}(|\mathfrak{c}^{-1/2} \circ \boldsymbol{g}(z)|))$$

which suggests all e^{-2iq_i} are not the eigenvalues of \mathbf{F} .

After establishing the invertibility of B(z), we further need the following more general results.

Proposition B.2. Under Assumption A.2, for any $\eta_0 > 0$ and $z_1, z_2 \in \mathbb{H}_{\eta_0}$ in (B.4),

$$\boldsymbol{\Lambda}^{(d)}(z_1, z_2) := \boldsymbol{I}_d - \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1/2} \circ \boldsymbol{g}(z_1)) \boldsymbol{S}_d \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1/2} \circ \boldsymbol{g}(z_2))$$
(B.10)

$$\mathbf{\Pi}^{(d)}(z_1, z_2) := \mathbf{I}_d - \operatorname{diag}(\mathfrak{c}^{-1} \circ \mathbf{g}(z_1) \circ \mathbf{g}(z_2)) \mathbf{S}_d$$
(B.11)

are invertible.

Remark B.2. In particular, when $z_1 = z_2$, we have $\Pi^{(d)}(z, z) = B^{(d)}(z)$. The purpose of proving above proposition is that $\Pi^{(d)}(z, z)^{-1}$ will appear in the asymptotic mean and variance of the LSS of the matrix M.

Similarly, we will simplify $\Pi^{(d)}(z,z)$ by $\Pi(z,z)$ in following proofs, so does others.

Proof of Proposition B.2. Notice that $\Lambda^{(d)}(z_1, z_2)$ and $\Pi^{(d)}(z_1, z_2)$ are similar, so it is enough to prove that one of them is invertible. We have already shown that $\operatorname{diag}(e^{-2iq}) - \mathbf{F}$ is invertible in Proposition B.1, which implies that

$$\operatorname{diag}(e^{-2\mathrm{i}\boldsymbol{q}}) - \operatorname{diag}(|\mathfrak{c}^{-1/2} \circ \boldsymbol{g}(z)|) \boldsymbol{S}_d \operatorname{diag}(|\mathfrak{c}^{-1/2} \circ \boldsymbol{g}(z)|) = \operatorname{diag}(e^{-\mathrm{i}\boldsymbol{q}}) \boldsymbol{\Lambda}(z,z) \operatorname{diag}(e^{-\mathrm{i}\boldsymbol{q}})$$

is also invertible. Next, let's further consider the case of $\Lambda(z_1, z_2)$ for $z_1 \neq z_2 \in \mathbb{H}_{\eta_0}$. Notice that

$$\Lambda(z_1, z_2) = \operatorname{diag}(\mathbf{g}(z_1))^{1/2} \operatorname{diag}(\mathbf{g}(z_2))^{-1/2} (\mathbf{I}_d - \Gamma(z_1, z_2)) \operatorname{diag}(\mathbf{g}(z_2))^{1/2} \operatorname{diag}(\mathbf{g}(z_1))^{-1/2}, \text{ (B.12)}$$

where

$$\Gamma(z_1, z_2) := \operatorname{diag}(\mathfrak{c}^{-1/2} \circ \sqrt{|\boldsymbol{g}(z_1) \circ \boldsymbol{g}(z_2)|}) \boldsymbol{S}_d \operatorname{diag}(\mathfrak{c}^{-1/2} \circ \sqrt{|\boldsymbol{g}(z_1) \circ \boldsymbol{g}(z_2)|}).$$

Hence, $\Lambda(z_1, z_2)$ is invertible if and only if $I_d - \Gamma(z_1, z_2)$ is invertible. For any unit vector $\mathbf{x} \in \mathbb{R}^d$, we have

$$\begin{split} \| \mathbf{\Gamma}(z_{1}, z_{2}) \mathbf{x} \|_{2}^{2} &= \sum_{i=1}^{d} \Big(\sum_{j \neq i}^{d} (\mathbf{c}_{i} \mathbf{c}_{j})^{-1/2} |g_{i}(z_{1}) g_{i}(z_{2}) g_{j}(z_{1}) g_{j}(z_{2})|^{1/2} x_{j} \Big)^{2} \\ &\leq \sum_{i=1}^{d} \Big(\sum_{j \neq i}^{d} (\mathbf{c}_{i} \mathbf{c}_{j})^{-1/2} |g_{i}(z_{1}) g_{j}(z_{1}) x_{j}| \Big) \Big(\sum_{j \neq i}^{d} (\mathbf{c}_{i} \mathbf{c}_{j})^{-1/2} |g_{i}(z_{2}) g_{j}(z_{2}) x_{j}| \Big) \\ &\leq \left[\sum_{i=1}^{d} \Big(\sum_{j \neq i}^{d} (\mathbf{c}_{i} \mathbf{c}_{j})^{-1/2} |g_{i}(z_{1}) g_{j}(z_{1}) x_{j}| \Big)^{2} \times \sum_{i=1}^{d} \Big(\sum_{j \neq i}^{d} (\mathbf{c}_{i} \mathbf{c}_{j})^{-1/2} |g_{i}(z_{2}) g_{j}(z_{2}) x_{j}| \Big)^{2} \right]^{1/2} \\ &= \| \mathbf{\Gamma}(z_{1}, z_{1}) |\mathbf{x}| \|_{2} \times \| \mathbf{\Gamma}(z_{2}, z_{2}) |\mathbf{x}| \|_{2} \leq \| \mathbf{\Gamma}(z_{1}, z_{1}) \| \times \| \mathbf{\Gamma}(z_{2}, z_{2}) \|. \end{split}$$

Since $F(z_1)$ in (B.5) and

$$\Gamma(z_1, z_1) = \operatorname{diag}(|\mathfrak{c}^{-1/2} \circ \boldsymbol{g}(z_1)|) \boldsymbol{S}_d \operatorname{diag}(|\mathfrak{c}^{-1/2} \circ \boldsymbol{g}(z_1)|)$$

are similar, their eigenvalues are coincide. By (B.9) and the symmetry of $\Gamma(z_1, z_1)$, we conclude that $\|\Gamma(z_1, z_1)\| \leq \|F(z_1)\| < 1$, so does $\|\Gamma(z_2, z_2)\|$ and $\|\Gamma(z_1, z_2)\|$. Furthermore, by Lemma B.2, we can also conclude that $\operatorname{Gap}(\Gamma(z_1, z_2)) > \sum_{i=3}^d \mathfrak{c}_{(i)}^{-1} |g_{(i)}(z_1)g_{(i)}(z_2)|$, so we can show that $\Lambda(z_1, z_2)$ is invertible for any $z_1, z_2 \in \mathbb{C}^+$ by the same arguments as those in Proposition B.1. \square

Finally, we need the upper bound of the spectral norm of $\Pi^{(d)}(z_1, z_2)^{-1}$, i.e.

Proposition B.3. Under Assumption A.2, for any $\eta_0 > 0$ and $z_1, z_2 \in \mathbb{H}_{\eta_0}$ in (B.4), we have

$$\|\mathbf{\Pi}^{(d)}(z_1, z_2)^{-1}\|, \|\mathbf{\Lambda}^{(d)}(z_1, z_2)^{-1}\| \le C_{d, \mathfrak{c}} \eta_0^{-4}.$$

Proof. Let's first prove $\|\mathbf{\Lambda}(z_1, z_2)^{-1}\| \leq C_{d,\epsilon} \eta_0^{-4}$. By (B.12), we know that

$$\|\mathbf{\Lambda}(z_1, z_2)^{-1}\| \le C_{d, \mathfrak{c}} \eta_0^{-2} (1 - \|\mathbf{\Gamma}(z_1, z_2)\|)^{-1}.$$

where we use the fact that $C_{d,\mathfrak{c}}\eta_0 \leq |g_i(z)| \leq \eta_0^{-1}$ by Lemma B.1. Since we have shown that $\|\mathbf{\Gamma}(z_1,z_2)\|^2 \leq \|\mathbf{F}(z_1)\| \cdot \|\mathbf{F}(z_2)\|$ in proofs of Proposition B.2, then

$$(1 - \|\mathbf{\Gamma}(z_1, z_2)\|)^{-1} \le \max_{i=1,2} (1 - \|\mathbf{F}(z_i)\|)^{-1}$$

By (B.9), we know that

$$(1 - ||F(z)||)^{-1} = \frac{\langle f, \sin q \rangle}{\Im(z)\langle f, \mathfrak{c}^{-1} \circ |g|\rangle},$$

since $|g_i(z)| \geq C_{d,\mathfrak{c}}\eta_0$, then due to f is a positive vector, we have

$$\frac{\langle \boldsymbol{f}, \sin \boldsymbol{q} \rangle}{\Im(z) \langle \boldsymbol{f}, \mathfrak{c}^{-1} \circ \boldsymbol{g} \rangle} \leq \frac{\langle \boldsymbol{f}, \mathbf{1}_d \rangle}{\eta_0 \min_{1 \leq i \leq d} \mathfrak{c}_i^{-1} |g_i(z)| \langle \boldsymbol{f}, \mathbf{1}_d \rangle} \leq C_{d,\mathfrak{c}} \eta_0^{-2},$$

which implies that $\|\mathbf{\Lambda}(z_1, z_2)^{-1}\| \leq C_{d,\epsilon} \eta_0^{-4}$. Similarly, for $\mathbf{\Pi}(z_1, z_2)$, since

$$\Pi(z_1, z_2) = \operatorname{diag}(\mathfrak{c}^{1/2} \circ \boldsymbol{g}(z_2)^{-1/2} \circ \boldsymbol{g}(z_2)^{-1/2}) (\boldsymbol{I}_d - \boldsymbol{\Gamma}(z_1, z_2)) \operatorname{diag}(\mathfrak{c}^{-1/2} \circ \boldsymbol{g}(z_2)^{1/2} \circ \boldsymbol{g}(z_2)^{1/2}),$$

we can complete our proof by repeating previous arguments.

B.3 Stability of the vector Dyson equation (B.1)

Roughly speaking, the stability of the vector Dyson equation (B.1) refers that if a vector-valued function v(z) satisfies a perturbed version of the vector Dyson equation with a small perturbation term $\varepsilon(z)$ uniformly controlled over a given region $\tilde{\mathcal{S}}_{\eta_0}$ as in (B.13) later, then the difference between v(z) and the solution g(z) of the original equation (B.1) is also small uniformly over $\tilde{\mathcal{S}}_{\eta_0}$. This stability is a key tool to derive the empirical spectral distribution (ESD) of the matrix M asymptotically converges to the measure ν associated with g(z), which will be proven as the limiting spectral distribution (LSD) of the matrix M later. Here, we first define a region in the upper complex plane as follows:

$$\tilde{\mathcal{S}}_{\eta_0} := \left\{ z \in \mathbb{C}^+ : \text{dist}(z, [-\zeta, \zeta]) \ge \eta_0, |\Re(z)| \le \eta_0^{-1} \right\},$$
 (B.13)

where ζ is the right and left boundary of the limiting spectral distribution $\nu(\cdot)$ of the matrix M in (C.17) later and

$$\operatorname{dist}(z, [-\zeta, \zeta]) := \min\{|z - x| : x \in [-\zeta, \zeta]\}.$$

Here, we require $\eta_0 > 0$ is sufficiently small so that $\zeta < \eta_0^{-1}$. Next, let's show that

Theorem B.2 (Stability). For any $\eta_0 > 0$ and $z \in \tilde{\mathcal{S}}_{\eta_0}$ in (B.13), let $\mathbf{v}(z) = (v_1(z), \dots, v_d(z))'$ be a d-dimensional analytical function on \mathbb{C}^+ such that

$$\varepsilon(z) = \frac{\mathfrak{c}}{\boldsymbol{v}(z)} + z + \boldsymbol{S}_d \boldsymbol{v}(z),$$

satisfies $\sup_{z \in \tilde{\mathcal{S}}_{\eta_0}} \| \boldsymbol{\varepsilon}(z) \|_{\infty} = \mathrm{O}(\eta_0^{-\beta} N^{-\alpha})$ for some $\alpha, \beta > 0$, then we have

$$\sup_{z \in \tilde{\mathcal{S}}_{\eta_0}} \|\boldsymbol{g}(z) - \boldsymbol{v}(z)\|_{\infty} \le \mathcal{O}(\eta_0^{-(\beta+4)} N^{-\alpha}),$$

where g(z) is the solution of (B.1).

Proof. First, let's split the region $\tilde{\mathcal{S}}_{\eta_0}$ into two parts, let's define

$$\tilde{\mathcal{S}}_{\eta_0}^1 := \{z \in \tilde{\mathcal{S}}_{\eta_0} : \Im(z) \le \eta_0^{-1}\} \quad \text{and} \quad \tilde{\mathcal{S}}_{\eta_0}^2 := \tilde{\mathcal{S}}_{\eta_0} \backslash \tilde{\mathcal{S}}_{\eta_0}^1.$$

For $z \in \tilde{\mathcal{S}}_{\eta_0}^2$, we have

$$\begin{split} |v_i(z) - g_i(z)| &= \left| \frac{\mathfrak{c}_i}{z + \sum_{j \neq i} g_j(z)} - \frac{\mathfrak{c}_i}{z + \sum_{j \neq i} v_j(z) + \varepsilon_i} \right| \\ &= \mathfrak{c}_i \left| \frac{\sum_{j \neq i} v_j(z) - g_j(z) + \varepsilon_i}{(z + \sum_{j \neq i} g_j(z))(z + \sum_{j \neq i} v_j(z) + \varepsilon_i)} \right| \\ &\leq \frac{\mathfrak{c}_i}{\Im(z)^2} \sum_{j \neq i} |v_j(z) - g_j(z)| + \frac{\mathfrak{c}_i |\varepsilon_i|}{\Im(z)^2} \\ &\leq \mathfrak{c}_i \eta_0^2 \sum_{j \neq i} |v_j(z) - g_j(z)| + \eta_0^2 |\varepsilon_i|. \end{split}$$

In other words, we conclude that

$$|\boldsymbol{v}(z) - \boldsymbol{g}(z)| \le \eta_0^2 \operatorname{diag}(\boldsymbol{\mathfrak{c}}) \boldsymbol{S}_d |\boldsymbol{v}(z) - \boldsymbol{g}(z)| + \eta_0^2 \boldsymbol{\varepsilon}.$$

Since $\|\operatorname{diag}(\mathbf{c})\mathbf{S}_d\| = C_{d,\mathbf{c}}$, we can choose sufficiently small η_0 such that $\eta_0^2 \|\operatorname{diag}(\mathbf{c})\mathbf{S}_d\| \ll 1$, so $(\mathbf{I}_d - \eta_0^2 \operatorname{diag}(\mathbf{c})\mathbf{S}_d)^{-1}$ exists and

$$\|(\boldsymbol{I}_d - \eta_0^2 \mathrm{diag}(\boldsymbol{\mathfrak{c}}) \boldsymbol{S}_d)^{-1}\| \leq (1 - \eta_0^2 \|\mathrm{diag}(\boldsymbol{\mathfrak{c}}) \boldsymbol{S}_d\|)^{-1} < 2,$$

Consequently, we have

$$\|\boldsymbol{v}(z) - \boldsymbol{g}(z)\|_{\infty} < \|\boldsymbol{v}(z) - \boldsymbol{g}(z)\|_{2} < 2\eta_{0}^{2}\sqrt{d}\|\boldsymbol{\varepsilon}\|_{\infty} = C_{d}\eta_{0}^{-\beta+2}N^{-\alpha}.$$

Next, for $z \in \tilde{\mathcal{S}}^1_{\eta_0}$, define $\boldsymbol{h}(z) := \boldsymbol{v}(z) - \boldsymbol{g}(z)$, we have

$$(\operatorname{diag}(e^{-2\mathrm{i}\boldsymbol{q}}) - \boldsymbol{F})\frac{\boldsymbol{h}}{|\boldsymbol{g}|} = \mathfrak{c}^{-1} \circ (e^{-\mathrm{i}\boldsymbol{q}} \circ \boldsymbol{h} \circ \boldsymbol{S}_d \boldsymbol{h} + (|\boldsymbol{g}| + e^{-\mathrm{i}\boldsymbol{q}} \circ \boldsymbol{h}) \circ \boldsymbol{\varepsilon}),$$

where $\mathbf{F} = \operatorname{diag}(\mathfrak{c}^{-1} \circ |\mathbf{g}|) \mathbf{S}_d \operatorname{diag}(|\mathbf{g}|)$ is defined in (B.5). In fact, notice that

$$\begin{split} &e^{-\mathrm{i}\boldsymbol{q}}\circ\boldsymbol{h}\circ\boldsymbol{S}_{d}\boldsymbol{h}=e^{-\mathrm{i}\boldsymbol{q}}\circ(\boldsymbol{v}-\boldsymbol{g})\circ\boldsymbol{S}_{d}(\boldsymbol{v}-\boldsymbol{g})\\ &=e^{-\mathrm{i}\boldsymbol{q}}\circ\boldsymbol{v}\circ\boldsymbol{S}_{d}(\boldsymbol{v}-\boldsymbol{g})+|\boldsymbol{g}|\circ\boldsymbol{S}_{d}\boldsymbol{g}-|\boldsymbol{g}|\circ\boldsymbol{S}_{d}\boldsymbol{v}\\ &=-e^{-\mathrm{i}\boldsymbol{q}}\circ\boldsymbol{v}\circ\boldsymbol{\varepsilon}-e^{-\mathrm{i}\boldsymbol{q}}\circ\boldsymbol{\mathfrak{c}}+e^{-\mathrm{i}\boldsymbol{q}}\circ\boldsymbol{\mathfrak{c}}\circ\frac{\boldsymbol{v}}{\boldsymbol{g}}+|\boldsymbol{g}|\circ\boldsymbol{S}_{d}\boldsymbol{g}-|\boldsymbol{g}|\circ\boldsymbol{S}_{d}\boldsymbol{v}\\ &=\mathfrak{c}\circ e^{-2\mathrm{i}\boldsymbol{q}}\circ\frac{\boldsymbol{h}}{|\boldsymbol{g}|}-\mathfrak{c}\circ\boldsymbol{F}\frac{\boldsymbol{h}}{|\boldsymbol{g}|}-e^{-\mathrm{i}\boldsymbol{q}}\circ\boldsymbol{v}\circ\boldsymbol{\varepsilon}\\ &=\mathfrak{c}\circ(\mathrm{diag}(e^{-2\mathrm{i}\boldsymbol{q}})-\boldsymbol{F})\frac{\boldsymbol{h}}{|\boldsymbol{g}|}-e^{-\mathrm{i}\boldsymbol{q}}\circ\boldsymbol{h}\circ\boldsymbol{\varepsilon}-|\boldsymbol{g}|\circ\boldsymbol{\varepsilon}, \end{split}$$

where we use the fact that

$$-rac{\mathfrak{c}}{oldsymbol{v}}-z-oldsymbol{arepsilon}=oldsymbol{S}_doldsymbol{v} \quad ext{and}\quad -rac{\mathfrak{c}}{oldsymbol{q}}-z=oldsymbol{S}_doldsymbol{g}$$

in the second equality. For simplicity, denote

$$\mathbb{B} := \operatorname{diag}(e^{-2i\boldsymbol{q}}) - \boldsymbol{F},\tag{B.14}$$

so we derive that

$$h = |g| \circ \mathbb{B}^{-1} (\mathfrak{c}^{-1} \circ (e^{-iq} \circ h \circ S_d h + (|g| + e^{-iq} \circ h) \circ \varepsilon)).$$

According to Proposition B.1, we know that \mathbb{B} is invertible and $\|\mathbb{B}^{-1}\| \leq C_{d,\mathfrak{c}}\eta_0^{-2}$ by Proposition B.3, then we have

$$\begin{aligned} \|\boldsymbol{h}\|_{\infty} &\leq \mathfrak{c}_{d}^{-1} \eta_{0}^{-1} \sqrt{d} \|\mathbb{B}^{-1}\| \left(\sqrt{d} \|\boldsymbol{S}_{d}\| \|\boldsymbol{h}\|_{\infty}^{2} + (\eta_{0}^{-1} + \|\boldsymbol{h}\|_{\infty}) \|\boldsymbol{\varepsilon}\|_{\infty} \right) \\ &\leq C_{d,\mathfrak{c}}^{(1)} \eta_{0}^{-3} \|\boldsymbol{h}\|_{\infty}^{2} + C_{d,\mathfrak{c}}^{(3)} \eta_{0}^{-(3+\beta)} N^{-\alpha} \|\boldsymbol{h}\|_{\infty} + C_{d,\mathfrak{c}}^{(2)} \eta_{0}^{-(4+\beta)} N^{-\alpha}, \end{aligned}$$

where $C_{d,\mathfrak{c}}^{(l)}$ are three constants depending on d and \mathfrak{c} for l=1,2,3. Hence, we obtain that $\|\boldsymbol{h}(z)\|_{\infty} \leq x^{-}$ or $\|\boldsymbol{h}(z)\|_{\infty} \geq x^{+}$ for all $z \in \tilde{\mathcal{S}}_{\eta_{0}}^{1}$, where

$$x^{\pm} := \frac{\eta_0^3 - C_{d,\mathfrak{c}}^{(3)} \eta_0^{-\beta} N^{-\alpha} \pm \sqrt{\left(\eta_0^3 - C_{d,\mathfrak{c}}^{(3)} \eta_0^{-\beta} N^{-\alpha}\right)^2 - 4C_{d,\mathfrak{c}}^{(1)} C_{d,\mathfrak{c}}^{(2)} \eta_0^{-(1+\beta)} N^{-\alpha}}}{2C_{d,\mathfrak{c}}^{(1)}}.$$

For any fixed η_0 , as $N \to \infty$, it implies that $\eta_0^{-\beta} N^{-\alpha}$, $\eta_0^{-(\beta+1)} N^{-\alpha} = o(\eta_0^3)$ and

$$x^+ = \mathcal{O}(\eta_0^3).$$

On the other hand, since

$$x^{-} = \frac{2C_{d,\mathfrak{c}}^{(2)}\eta_{0}^{-(1+\beta)}N^{-\alpha}}{\eta_{0}^{3} - C_{d,\mathfrak{c}}^{(3)}\eta_{0}^{-\beta}N^{-\alpha} + \sqrt{\left(\eta_{0}^{3} - C_{d,\mathfrak{c}}^{(3)}\eta_{0}^{-\beta}N^{-\alpha}\right)^{2} - 4C_{d,\mathfrak{c}}^{(1)}C_{d,\mathfrak{c}}^{(2)}\eta_{0}^{-(1+\beta)}N^{-\alpha}}},$$

where the denominator has the same order as $x^+ = O(\eta_0^3)$. Hence, it implies that

$$x^{-} = O(\eta_0^{-(\beta+4)} N^{-\alpha}).$$

Since $\|\boldsymbol{h}(z)\|_{\infty}$ is continuous on $z \in \tilde{\mathcal{S}}_{\eta_0}$ and we have shown that $\|\boldsymbol{h}(z)\|_{\infty} = \mathrm{O}(\eta_0^{-\beta+2}N^{-\alpha})$ for all $z \in \tilde{\mathcal{S}}_{\eta_0}^2$, it implies that $\|\boldsymbol{h}(z)\|_{\infty} \leq x^-$ for all $z \in \tilde{\mathcal{S}}_{\eta_0}^1$, so $\|\boldsymbol{h}(z)\|_{\infty} \leq x^- = \mathrm{O}(\eta_0^{-(\beta+4)}N^{-\alpha})$, which completes our proof.

C Properties of spectral distribution

In this section, we will derive several important properties of the empirical spectral distribution (ESD) and limiting spectral distribution (LSD) of M. Without loss of generality, we assume, as before, that $\mathfrak{c}_1 = \max_{1 \leq l \leq d} \mathfrak{c}_l$.

C.1 Support of the empirical spectral distribution

Theorem C.1. Under Assumptions A.1 and A.2, define $\mathfrak{v}_d := 2(d-1)\sum_{l=1}^d \sqrt{\mathfrak{c}_l}$, then for any t, l > 0, we have

$$\mathbb{P}(\|\boldsymbol{M}\| > \boldsymbol{v}_d + t) = o(N^{-l}). \tag{C.15}$$

For preliminaries, we need the following two results:

Lemma C.1 (Chapter 9.12.5 of [7]). Let $X = [X_{ij}]_{p \times n}$ be a random matrix with size of $p \times n$, whose entries $\{X_{ij}\}$ are i.i.d. complex random variables with mean zero, variance one, and finite fourth moments, and $|X_{ij}| \leq n^{1/4}$. If $\frac{p}{n} \to y \in (0,1)$, then for any $x > (1 + \sqrt{y})^2$ and l > 0, the spectral norm of $S_n = n^{-1}XX^*$ satisfies that

$$\mathbb{P}(\|\boldsymbol{S}_n\| > x) = o(n^{-l}).$$

Lemma C.2 ([16]). Let X_1, \dots, X_n be a set of independent random variables with $||X_i||_{\Psi_{\theta}} \leq M$ for some $\theta \in (0, 1]$. Let $\mathbf{a} = (a_1, \dots, a_n)' \in \mathbb{R}^n$, then

$$\mathbb{P}\left(\left|\sum_{i=1}^{n} a_{i}\left(X_{i} - \mathbb{E}[X_{i}]\right)\right| > t\right) \leq 2 \exp\left(-C_{\theta} \min\left\{\frac{t^{2}}{M\|\boldsymbol{a}\|_{2}^{2}}, \frac{t^{\alpha}}{M^{\alpha} \max_{1 \leq i \leq n} |a_{i}|^{\alpha}}\right\}\right),$$

where $\|\cdot\|_{\Psi_{\theta}}$ is the Orlicz norms with parameter θ .

Now, let's prove that

Proof of Theorem C.1. Since $\|\mathbf{M}\| = \sup_{\|\mathbf{x}\|_2=1} \|\mathbf{M}\mathbf{x}\|_2$, let's split \mathbf{x} by blocks, i.e. $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)'$ and $\mathbf{M}\mathbf{x} = \sum_{i=1}^d \sum_{j \neq i}^d \mathbf{M}^{ji} \mathbf{x}_i$. By the Minkowski inequality, we have

$$\|oldsymbol{M}oldsymbol{x}\|_2 \leq \sum_{i=1}^d \sum_{j
eq i}^d \|oldsymbol{M}^{ji}oldsymbol{x}_i\|_2 \quad \Longrightarrow \quad \|oldsymbol{M}\| \leq \sum_{i=1}^d \sum_{j
eq i}^d \|oldsymbol{M}^{ji}\| = \sum_{i
eq j}^d \|oldsymbol{M}^{ij}\|.$$

Next, we will show that $\mathbb{P}(\|\boldsymbol{M}^{ij}\| > \sqrt{c_i} + \sqrt{c_j}) = o(N^{-l})$ for any l > 0. Since the proofs for each block are the same, consider i = 1, j = 2, we have

$$M_{j_1j_2}^{12} = \frac{1}{\sqrt{N}} \sum_{i_3 \cdots i_d}^{n_3 \cdots n_d} X_{j_1j_2i_3 \cdots i_d} \mathcal{A}_{i_1 \cdots i_d}^{(1,2)},$$

where $\mathcal{A}_{i_1\cdots i_d}^{(1,2)}$ is defined in (A.6). By Lemma C.2 and Assumption A.1, we have

$$\mathbb{P}\left(\left|\sum_{i_3\cdots i_d}^{n_3\cdots n_d} X_{j_1j_2i_3\cdots i_d} \mathcal{A}_{i_1\cdots i_d}^{(1,2)}\right| > N^{1/4}\right) \le 2\exp(-C_{\theta}N^{1/4}),$$

then

$$\mathbb{P}\left(\left|\sum_{i_3\cdots i_d}^{n_3\cdots n_d} X_{j_1j_2i_3\cdots i_d} \mathcal{A}_{i_1\cdots i_d}^{(1,2)}\right| > N^{1/4} \middle| \exists j_1, j_2\right) \leq \sum_{j_1, j_2}^{n_1, n_2} \mathbb{P}\left(\left|\sum_{i_3\cdots i_d}^{n_3\cdots n_d} X_{j_1j_2i_3\cdots i_d} \mathcal{A}_{i_1\cdots i_d}^{(1,2)}\right| > N^{1/4}\right) \\
\leq 2n_1n_2 \exp(-C_{\theta}N^{1/4}) = o(N^{-l}).$$

By Lemma C.1, for any t > 0, we can show that

$$\mathbb{P}(\|\boldsymbol{M}^{12}\| > \sqrt{\mathfrak{c}_1} + \sqrt{\mathfrak{c}_2} + t) = \mathbb{P}(\|\boldsymbol{M}^{12}\| > \sqrt{\mathfrak{c}_1} + \sqrt{\mathfrak{c}_2} + t |\forall |M_{j_1j_2}^{12}| < N^{-1/4}) \mathbb{P}(\forall |M_{j_1j_2}^{12}| < N^{-1/4}) + \mathbb{P}(\exists |M_{j_1j_2}^{12}| < N^{-1/4}) = o(N^{-l}).$$

For other M^{ij} , we also have $\mathbb{P}(\|M^{ij}\| > \sqrt{\mathfrak{c}_i} + \sqrt{\mathfrak{c}_j} + t) = o(N^{-l})$, then we can conclude that

$$\mathbb{P}(\|\boldsymbol{M}\| \ge \boldsymbol{v}_d + d^2t) \le \sum_{i \ne j}^d \mathbb{P}(\|\boldsymbol{M}^{ij}\| \ge \sqrt{\boldsymbol{\mathfrak{c}}_i} + \sqrt{\boldsymbol{\mathfrak{c}}_j} + t) = \mathrm{o}(N^{-l}),$$

note that d is fixed integer, then we can conclude (C.15).

C.2 Support of the limit spectral distribution

Theorem C.2. Let g(z) be the solution of (B.1) on \mathbb{C}^+ and $g(z) = \sum_{i=1}^d g_i(z)$, then there exists a probability measure ν with bounded supports such that its Stieltjes transform is g(z).

Proof. Define

$$g(z) = \sum_{j=1}^{d} g_j(z)$$
 and $\nu(E) := \lim_{\eta \downarrow 0^+} \pi^{-1} g(E + i\eta),$ (C.16)

where $g_j(z)$ is the j-th entry of $\boldsymbol{g}(z)$ defined in (B.1) and $E \in \mathbb{R}$. We will show that g(z) is the Stieltjes transform of the probability measure ν , which has finite support. For a holomorphic function $\phi: \mathbb{C}^+ \to \mathbb{C}^+$ on the complex upper half plane, it is a Stieltjes transform of a measure ν_{ϕ} on the real line such that $\nu_{\phi}(\mathbb{R}) = \alpha > 0$ if and only if $|i\eta\phi(i\eta) + \alpha| \to 0$ as $\eta \to \infty$, see Theorem B.9 in [7]. Besides, ν_{ϕ} can be explicitly determined by $\nu_{\phi}(x) = \pi^{-1}\Im(\phi(x))$ for $x \in \mathbb{R}$. Therefore, let $\boldsymbol{g}(z) = (g_1(z), \cdots, g_d(z))'$ be the unique analytical solution (B.1) of on \mathbb{C}^+ , since $\mathfrak{c}_j + zg_j(z) = -g_j(z) \sum_{k \neq j} g_k(z)$, it implies that $|\mathfrak{c}_j + i\eta g_j(i\eta)| \leq (d-1)\eta^{-2} \to 0$ as $\eta \to \infty$, i.e. the deduced measure of $g_j(z)$ has mass of \mathfrak{c}_j . Hence, g(z) is a Stieltjes transform of a probability measure due to $\sum_{i=1}^d \mathfrak{c}_i = 1$. Next, suppose $\|\boldsymbol{g}(z)\|_{\infty} \leq \frac{|z|}{2(d-1)}$, then

$$|g_i(z)| = \frac{\mathfrak{c}_i}{|z + \sum_{j \neq i} g_j(z)|} \le \frac{\mathfrak{c}_i}{|z| - \sum_{j \neq i} |g_j(z)|} \le \frac{2\mathfrak{c}_j}{|z|} \Longrightarrow \|g(z)\|_{\infty} \le \min\{|z|/(2(d-1)), 2/|z|\}.$$

Let $H_0 := \{z \in \mathbb{C}^+ : |z| > 2\sqrt{d-1}(1+\epsilon)\}$, where $\epsilon > 0$, then $z \to \sqrt{d-1}\|\boldsymbol{g}(z)\|_{\infty}$ will map H_0 into two disjoint regions, i.e.

$$z \to \sqrt{d-1} \|g(z)\|_{\infty} : H_0 \to [0, (1+\epsilon)^{-1}] \cup [1+\epsilon, +\infty].$$

In fact, if we divide H_0 into two disjoint parts, $H_{0,1} := \{z \in H_0 : \|\boldsymbol{g}(z)\|_{\infty} \le |z|/(2(d-1))\}$ and $H_{0,2} := H_0 \setminus H_{0,1}$, then $\sqrt{d-1}\|\boldsymbol{g}(z)\|_{\infty} > 1 + \epsilon$ for $z \in H_{0,2}$ and $\sqrt{d-1}\|\boldsymbol{g}(z)\|_{\infty} < (1+\epsilon)^{-1}$ for $z \in H_{0,1}$. Since $z \to \|\boldsymbol{g}(z)\|_{\infty}$ is continuous for $z \in H_0$ and $\|\boldsymbol{g}(z)\|_{\infty} \le \Im(z)^{-1} \to 0$ when $\Im(z)$ is sufficiently large, then $z \to \sqrt{d-1}\|\boldsymbol{g}(z)\|_{\infty}$ maps H_0 to $[0, (1+\epsilon)^{-1}]$, i.e. $\|\boldsymbol{g}(z)\|_{\infty} \le 2|z|^{-1}$ for $z \in H_0$. Now, based on the (B.7), it gives that

$$\Im(g_i(z)) = \Im(z)\mathfrak{c}_i^{-1}|g_i(z)|^2 + \mathfrak{c}_i^{-1}|g_i(z)|^2 \sum_{j \neq i} \Im(g_j(z)) \iff \Im(g_i(z)) = \frac{\mathfrak{c}_i^{-1}|g_i(z)|^2}{1 + \mathfrak{c}_i^{-1}|g_i(z)|^2} \Im(z + g(z)),$$

which implies that

$$\Im(g_i(z)) \leq \frac{4\mathfrak{c}_i}{|z|^2 + 4\mathfrak{c}_i} \Im(z + g(z)) < \frac{4\mathfrak{c}_i}{|z|^2} \Im(z + g(z)), \quad \text{for } \forall z \in H_0,$$

where the first inequality is valid due to $|g_i(z)| \leq \frac{2\mathfrak{c}_i}{|z|}$. As a result, by summing all $\Im(g_i(z))$, we have

$$\Im(g(z))<\frac{4}{|z|^2}\Im(z+g(z))\quad\Rightarrow\quad\Im(g(z))<\frac{4\Im(z)}{|z|^2-4},$$

where we use the fact that |z| > 4 for $z \in H_0$, then

$$\Im(g(z)) < \frac{\Im(g(z))}{\epsilon(2+\epsilon)} \to 0 \text{ as } \Im(g(z)) \to 0,$$

Hence the deduced measure $\nu(E)$ of g(z) has 0 mass for all $E>2\sqrt{d-1}$, i.e. ν has finite support.

Here, let

$$\zeta := \inf \left\{ E > 0 : \lim_{\eta \to 0} \Im(g(E + i\eta)) = 0, \eta > 0 \right\},$$
 (C.17)

be the right boundary of the support of ν . Due to the symmetry of ν , the absolute value of the left boundary is the same as the right one. Now, combining (C.15) and (C.17), we give the following stable region for the spectral distribution of M:

$$S_{\eta_0} := \{ z \in \mathbb{C}^+ : \text{dist}(z, [-\max(\mathfrak{v}_3, \zeta), \max(\mathfrak{v}_3, \zeta)]) \ge \eta_0, |\Re(z)|, |\Im(z)| \le \eta_0^{-1} \},$$
 (C.18)

where η_0 is sufficiently small such that $\eta_0^{-1} > \max(\mathfrak{v}_3, \zeta)$. Consequently, since $\mathbb{P}(\|\boldsymbol{M}\| \leq \mathfrak{v}_3) \geq 1 - o(N^{-l})$ for any l > 0, then

$$\mathbb{P}(\|Q(z)\| \le \text{dist}(z, [-\max(v_d, \zeta), \max(v_d, \zeta)])^{-1} \le \eta_0^{-1}) \ge 1 - o(N^{-l}). \tag{C.19}$$

Thus, without further specifications, we assume $\|Q(z)\| \leq \eta_0^{-1}$ for any $z \in \mathcal{S}_{\eta_0}$ in the following contexts.

C.3 Singularity of the limiting spectral distribution

Recall that we assume $\mathfrak{c}_1 = \max_{1 \leq l \leq d} \mathfrak{c}_l$, we will prove that

Theorem C.3. ν defined in (C.16) has a unique point mass at 0 if and only if $\mathfrak{c}_1 \geq 1/2$.

By (C.16), we know that ν has a point mass at $E \in \mathbb{R}$ if and only if $\lim_{\eta \to 0^+} \Im(g(E + i\eta)) = \infty$. Thus, let's show that

Lemma C.3. For any $z = E + i\eta \in \mathbb{C}^+$ and $E \neq 0$, then

$$\lim_{\eta \to 0^+} \Im(g(E + i\eta)) < \infty,$$

where $g(z) = \sum_{j=1}^{d} g_j(z)$ defined in (C.16).

Proof. Taking the imaginary and real part of (B.1) respectively, we have

$$\frac{\mathfrak{c} \circ \Im(\boldsymbol{g}(z))}{|\boldsymbol{g}|^2} = \eta + \boldsymbol{S}_d \Im(\boldsymbol{g}(z)) \quad \text{and} \quad -\frac{\mathfrak{c} \circ \Re(\boldsymbol{g}(z))}{|\boldsymbol{g}(z)|^2} = E + \boldsymbol{S}_d \Re(\boldsymbol{g}(z)). \tag{C.20}$$

Suppose there exists an $E \neq 0$ such that $\lim_{\eta \to 0^+} \Im(g(E + i\eta)) = \infty$, without loss of generality, assume $\lim_{\eta \to 0^+} \Im(g_1(E + i\eta)) = \infty$, which implies that $\lim_{\eta \to 0^+} |g_1(E + i\eta)| = \infty$. By the second equation in (C.20), we have

$$|g_1(E + i\eta)| = \frac{-\mathfrak{c}_1 \cos \theta_1}{E + \sum_{i \neq 1}^d \Re(g_i(E + i\eta))},$$

where $\cos \theta_j := \Re(g_j(z))/|g_j(z)|$ and $\sin \theta_j := \Im(g_j(z))/|g_j(z)|$, so we obtain $\lim_{\eta \to 0^+} \sum_{i \neq 1}^d \Re(g_i(E + i\eta)) = -E$. On the other hand, notice that for $j \neq 1$

$$|g_j(E+\mathrm{i}\eta)| = \frac{\mathfrak{c}_j \sin \theta_j}{\eta + \sum_{i \neq j}^d \Im(g_i(E+\mathrm{i}\eta))} < \frac{1}{\Im(g_1(E+\mathrm{i}\eta))},$$

it yields that $\lim_{\eta\to 0^+} |g_j(E+i\eta)| = 0$ and $\lim_{\eta\to 0^+} \Re(g_j(E+i\eta)) = 0$. But it is a contradiction since

$$\lim_{\eta \to 0^+} \sum_{i \neq 1}^d \Re(g_i(z)) = -E \neq 0,$$

which completes our claim.

By the above lemma, we only need to focus on the limiting behaviors of $g(i\eta)$ as $\eta \to 0^+$. If we replace z by $-\bar{z}$ in (B.1) and take the imaginary part on the both sides of (B.1) respectively, i.e.

$$-\frac{\mathfrak{c}}{\boldsymbol{g}(-\bar{z})} = -\bar{z} + \boldsymbol{S}_d \boldsymbol{g}(-\bar{z}) \quad \Longleftrightarrow \quad -\frac{\mathfrak{c}}{-\overline{\boldsymbol{g}(z)}} = (-\bar{z}) + \boldsymbol{S}_d(-\overline{\boldsymbol{g}(z)})$$

it implies that $g(-\bar{z}) = -\overline{g(z)}$ by Theorem B.1. Hence, $\Re(g_i(i\eta)) = 0$ for $\eta > 0, i = 1, \dots, d$ and denote $g_i(i\eta) := i\tilde{g}_i(\eta)$, then (B.1) can be rewritten as

$$\frac{\mathbf{c}}{\tilde{\mathbf{g}}(\eta)} = \eta + \mathbf{S}_d \tilde{\mathbf{g}}(\eta). \tag{C.21}$$

Before giving the proof of Theorem C.3, we need the following results:

Lemma C.4. Let $c > 0, z = E + i\eta \in \mathbb{C}^+, E \ge 0$ and $x_{1,2} = r_{1,2} \exp(i\theta_{1,2})$ be the solutions of $x^2 - zx - c = 0$, where $\theta_{1,2} \in [0, 2\pi)$. Without loss of generality, let $r_1 \ge r_2$, then we have

- $r_2 \le \sqrt{c} \le r_1 \text{ and } \theta_1, \theta_2 \in [0, \pi], \theta_1 + \theta_2 = \pi.$
- $sign(\Re(x_1)) = -sign(\Re(x_2))$ and $\Im(x_1), \Im(x_2) > 0$.
- Let $\theta(E, \eta, c) := \min\{\theta_1, \theta_2\}$ and $r_1 := r_1(E, \eta, c)$, then $\partial_E \theta < 0$, $\partial_\eta \theta > 0$ and $\partial_E r_1, \partial_\eta r_1 > 0$.

Proof. Since $x_1x_2 = -c$, it implies that $r_2 \leq \sqrt{c} \leq r_1$ and $\theta_1 + \theta_2 = \pi$ or 3π . Notice that $x_1 + x_2 = E + i\eta$ and $E \geq 0, \eta > 0$, we further conclude that $\theta_1 + \theta_2 = \pi$ and

$$(r_1 - r_2)\cos\theta = E, \quad (r_1 + r_2)\sin\theta = \eta,$$

where $\theta := \min\{\theta_1, \theta_2\} = \theta_1$. Then we can solve that

$$\sin^2 \theta = \frac{E^2 + \eta^2 + 4c - \sqrt{(E^2 + \eta^2 + 4c)^2 - 16c\eta^2}}{8c} := s(E, \eta, c) = \frac{E}{4c} \left(1 - \frac{E^2 + \eta^2 + 4c}{\sqrt{(E^2 + \eta^2 + 4c)^2 - 16c\eta^2}} \right) < 0,$$

$$\partial_{\eta} s(E, \eta, c) = \frac{\eta}{4c} \left(1 - \frac{E^2 + \eta^2 - 4c}{\sqrt{(E^2 + \eta^2 - 4c)^2 + 16cE^2}} \right) > 0.$$

Notice that $\theta = \min\{\theta_1, \theta_2\} \in [0, \pi/2]$ and the monotonicity of $\sin^2 \theta$ and θ are the same when $\theta \in [0, \pi/2]$, which implies that $\partial_E \theta < 0, \partial_{\eta} \theta > 0$. Besides, we also have

$$r_1 = \frac{1}{2} \left(\frac{E}{\cos \theta} + \frac{\eta}{\sin \theta} \right) = \frac{1}{2} \left(\frac{E}{\sqrt{1 - s}} + \frac{\eta}{\sqrt{s}} \right) = \frac{1}{2\sqrt{2}} \left(\sqrt{M + \sqrt{M^2 - 16c\eta^2}} + \sqrt{N + \sqrt{N^2 + 16cE^2}} \right),$$

where $M := E^2 + \eta^2 + 4c$, $N := E^2 + \eta^2 - 4c$ and $M^2 - 16c\eta^2 = N^2 + 16cE^2$. Therefore, it implies that

$$\partial_{E}r_{1} = \frac{E}{2\sqrt{2}} \left(1 + \frac{M}{\sqrt{M^{2} - 16c\eta^{2}}} \right) \left[\left(M + \sqrt{M^{2} - 16c\eta^{2}} \right)^{-1/2} + \left(N + \sqrt{N^{2} + 16cE^{2}} \right)^{-1/2} \right] > 0,$$

$$\partial_{\eta}r_{1} = \frac{\eta}{2\sqrt{2}} \left(1 + \frac{N}{\sqrt{N^{2} + 16cE^{2}}} \right) \left[\left(M + \sqrt{M^{2} - 16c\eta^{2}} \right)^{-1/2} + \left(N + \sqrt{N^{2} + 16cE^{2}} \right)^{-1/2} \right] > 0,$$
which completes our proof.

As a consequence of above lemma, we have that

Lemma C.5. Recall that $\mathfrak{c}_1 = \max_{1 \leq i \leq d} \mathfrak{c}_i$, when $\eta \geq \max_{1 \leq i \leq d} \mathfrak{c}_i^{-1/2}$, we have

$$\mathfrak{c}_1^{-1/2}|g_1(\mathrm{i}\eta)| = \arg\max_{1 \le i \le d} \mathfrak{c}_i^{-1/2}|g_i(\mathrm{i}\eta)|$$

and

$$\max_{1 \le i \le d} |g_i(\mathrm{i}\eta)| \le \frac{d}{2(d-1)} \sqrt{\eta^2 + 4(d-1)\mathfrak{c}_1} - \frac{\eta}{d-1}.$$

Proof. Since $g(-\bar{z}) = -\overline{g(z)}$, we assume $\Re(z) \geq 0$ without loss of generality. Since $g_i(z)$ is the solution of $\mathfrak{c}_i + g_i(z)(z + g(z) - g_i(z)) = 0$ by (B.1) and $|g_i(z)| \leq \Im(z)^{-1} \leq \min_{1 \leq i \leq d} \mathfrak{c}_i^{1/2}$, it concludes that $g_i(z) = r_2(z) \exp(\mathrm{i}\theta_2(z))$ when $\Im(z) \geq \max_{1 \leq i \leq d} \mathfrak{c}_i^{-1/2}$ by Lemma C.4. Let

$$h(z) := z + g(z)$$
 and $\mathfrak{g}_i(z) := g_i(z)/\sqrt{\mathfrak{c}_i},$ (C.22)

then

$$\mathfrak{g}_{i}^{2}(z) - \mathfrak{c}_{i}^{-1/2}h(z)\mathfrak{g}_{i}(z) - 1 = 0 \text{ and } |\mathfrak{g}_{i}(z)|^{-1} = r_{1}(\Re(h(z))/\sqrt{\mathfrak{c}_{i}}, \Im(h(z))/\sqrt{\mathfrak{c}_{i}}, 1).$$

Since r_1 is increasing function of the real and imaginary part of $h(z)/\sqrt{c_i}$ by Lemma C.4, then

$$\arg \max_{1 \le i \le d} \mathfrak{c}_i^{-1/2} |g_i(z)| = \arg \min_{1 \le i \le d} |\mathfrak{g}_i(z)|^{-1} = \arg \max_{1 \le i \le d} \mathfrak{c}_i,$$

which implies that

$$\mathfrak{c}_1^{-1/2}|g_1(z)| = \arg\max_{1 \le i \le d} \mathfrak{c}_i^{-1/2}|g_i(z)|.$$

Next, since h(z) = z + g(z) and $z = i\eta \in \mathbb{C}^+$, then $\Re(h(i\eta)) = 0$. Hence, let

$$h(i\eta) = i\mathfrak{h}(\eta), \text{ where } \mathfrak{h}(\eta) > 0,$$
 (C.23)

and the two solutions of $\mathfrak{c}_i + g_i(z)(z + g(z) - g_i(z)) = 0$ are denoted as

$$g_i^{\pm}(\mathrm{i}\eta) = \mathrm{i}\tilde{g}_i^{\pm}(\eta) := \frac{h(\mathrm{i}\eta) \pm \sqrt{h^2(\mathrm{i}\eta) + 4\mathfrak{c}_i}}{2} = \frac{\mathrm{i}\mathfrak{h}(\eta) \pm \sqrt{4\mathfrak{c}_i - \mathfrak{h}^2(\eta)}}{2},\tag{C.24}$$

where $|\tilde{g}_i^+(\eta)| \geq \sqrt{\mathfrak{c}_i} \geq |\tilde{g}_i^-(\eta)|$ and $|\tilde{g}_i^+(\eta)\tilde{g}_i^-(\eta)| = \mathfrak{c}_i$ by Lemma C.4. Recall that $\Re(g_i(\mathrm{i}\eta)) = 0$, it implies that $\mathfrak{h}(\eta) \geq 2 \max_{1 \leq i \leq d} \sqrt{\mathfrak{c}_i} = 2\sqrt{\mathfrak{c}_1}$ whatever $g_i(\mathrm{i}\eta) = \mathrm{i}\tilde{g}_i^+(\eta)$ or $g_i(\mathrm{i}\eta) = \mathrm{i}\tilde{g}_i^-(\eta)$. Furthermore, when $\eta \geq \max_{1 \leq i \leq d} \mathfrak{c}_i^{-1/2}$, $|g_i(\mathrm{i}\eta)| \leq \eta^{-1} \leq \sqrt{\mathfrak{c}_i}$, hence

$$g_i(i\eta) = i\tilde{g}_i^-(\eta) = i\frac{\mathfrak{h}(\eta) - \sqrt{\mathfrak{h}^2(\eta) - 4\mathfrak{c}_i}}{2}, \text{ for } i = 1, \dots, d,$$
(C.25)

by Lemma C.4. Summing above equations for $i = 1, \dots, d$, it has

$$2\mathrm{i}(\mathfrak{h}(\eta) - \eta) = 2\sum_{i=1}^{d} g_i(\mathrm{i}\eta) = \mathrm{i}\left(d\mathfrak{h}(\eta) - \sum_{i=1}^{d} \sqrt{\mathfrak{h}^2(\eta) - 4\mathfrak{c}_i}\right)$$

$$\Longrightarrow 2\eta + (d-2)\mathfrak{h}(\eta) = \sum_{i=1}^{d} \sqrt{\mathfrak{h}^2(\eta) - 4\mathfrak{c}_i} > d\sqrt{\mathfrak{h}^2(\eta) - 4\max_{1 \le i \le d} \mathfrak{c}_i},$$
(C.26)

which implies that

$$2\max_{1\leq i\leq d}\sqrt{\mathfrak{c}_i}\leq \mathfrak{h}(\eta)<\frac{d}{2(d-1)}\sqrt{\eta^2+4(d-1)\max_{1\leq i\leq d}\mathfrak{c}_i}+\frac{\eta(d-2)}{d-1}.$$

Finally, since $|g_i(i\eta)| = \tilde{g}_i(\eta)$ and $\mathfrak{h}(\eta) = \eta + \sum_{i=1}^d \tilde{g}_i(\eta)$, it implies that

$$|g_i(\mathrm{i}\eta)| \le \mathfrak{h}(\eta) - \eta < \frac{d}{2(d-1)}\sqrt{\eta^2 + 4(d-1)\mathfrak{c}_1} - \frac{\eta}{d-1},$$

which completes our proof.

Based on proofs of above lemma, if $g_i(i\eta) = g_i^-(i\eta)$ for all $\eta > 0$ and $1 \le i \le d$, we have

$$\max_{1\leq i\leq d}|g_i(\mathrm{i}\eta)|<\min\left\{\frac{d}{2(d-1)}\sqrt{\eta^2+4(d-1)\mathfrak{c}_1}-\frac{\eta}{d-1},\eta^{-1}\right\},$$

In other words, $g(z) = \sum_{i=1}^{d} g_i(z)$ will not have a singularity at z = 0. However, $g_i(i\eta) = g_i^-(i\eta)$ will not hold under some certain conditions. Here, let $\Pi_0 := \{ \mathfrak{c} \in \mathbb{R}^d : \sum_{l=1}^d \mathfrak{c}_l = 1, \mathfrak{c}_l \geq 0 \}$ be the d-dimensional affine hyperplane, then we define the *invariant branch region* as follows:

$$\Pi_1 := \left\{ \mathfrak{c} \in \Pi_0 : \sum_{i=1}^d \sqrt{\mathfrak{c}_1 - \mathfrak{c}_i} \le (d-2)\sqrt{\mathfrak{c}_1} \right\},\tag{C.27}$$

then we provide the following result.

Proposition C.1. For any $\mathfrak{c} \in \Pi_0 \setminus \Pi_1$ in (C.27), let $\eta_1 := \sum_{i=1}^d \sqrt{\mathfrak{c}_1 - \mathfrak{c}_i} - (d-2)\sqrt{\mathfrak{c}_1} > 0$, then

$$g_{j}(i\eta) = \begin{cases} i\tilde{g}_{j}^{-}(\eta) & \eta \in (\eta_{1}, +\infty), 1 \leq j \leq d, \\ i\tilde{g}_{j}^{-}(\eta) & \eta \in (0, \eta_{1}], 2 \leq j \leq d, \\ i\tilde{g}_{j}^{+}(\eta) & \eta \in (0, \eta_{1}], j = 1, \end{cases}$$

where $g_j^{\pm}(\eta)$ are defined in (C.24). On the other hand, for any $\mathfrak{c} \in \Pi_1$, $g_j(i\eta) = i\tilde{g}_j^-(\eta)$ for any $\eta > 0$ and $j = 1, \dots, d$.

Proof. First, taking the derivative of η in (C.21), we obtain

$$(\mathbf{I}_d + \operatorname{diag}(\mathbf{c}^{-1} \circ \tilde{\mathbf{g}}^{\circ 2}) \mathbf{S}_d) \tilde{\mathbf{g}}' = -\mathbf{c}^{-1} \circ \tilde{\mathbf{g}}^{\circ 2}. \tag{C.28}$$

In fact, since

$$\frac{\mathfrak{c}_i}{\tilde{g}_i} = \eta + \sum_{j \neq i} \tilde{g}_j \quad \Rightarrow \quad -\tilde{g}_i' \frac{\mathfrak{c}_i}{\tilde{g}_i^2} = 1 + \sum_{j \neq i} \tilde{g}_j' \quad \Leftrightarrow \quad \tilde{g}_i' + \mathfrak{c}_i^{-1} \tilde{g}_i^2 \sum_{j \neq i} \tilde{g}_j' = -\mathfrak{c}_i^{-1} \tilde{g}_i^2,$$

then we obtain (C.28) and

$$\tilde{g}_{i}' + \mathfrak{c}_{i}^{-1} \tilde{g}_{i}^{2} \sum_{j \neq i} \tilde{g}_{j}' = -\mathfrak{c}_{i}^{-1} \tilde{g}_{i}^{2} \quad \Rightarrow \quad (\mathfrak{c}_{i}/\tilde{g}_{i}^{2}) \tilde{g}_{i}' + (\tilde{g}' - \tilde{g}_{i}') = -1 \quad \Rightarrow \quad (1 - \mathfrak{c}_{i}/\tilde{g}_{i}^{2}(\eta)) \tilde{g}_{i}'(\eta) = \mathfrak{h}'(\eta), \tag{C.29}$$

where $\mathfrak{h}(\eta) = \eta + \tilde{g}(\eta)$ in (C.23). Here, we claim that $\mathfrak{h}'(\eta) > 0$ when $\eta > \max_{1 \leq i \leq d} \mathfrak{c}_i^{-1/2}$. Actually, if $\eta > \max_{1 \leq i \leq d} \mathfrak{c}_i^{-1/2}$, $\tilde{g}_i(\eta) < \sqrt{\mathfrak{c}_i}$ for all $i = 1, \dots, d$. Suppose $\mathfrak{h}(\eta) \leq 0$, due to $\tilde{g}_i(\eta) > \sqrt{\mathfrak{c}_i}$, we know that $1 - \mathfrak{c}_i/\tilde{g}_i^2(\eta) < 0$, so it implies that $\tilde{g}_i'(\eta) \geq 0$ by (C.29) and $\mathfrak{h}'(\eta) = 1 + \sum_{i=1}^d \tilde{g}_i'(\eta) > 0$, which is a contradiction. Next, let's consider two scenarios.

Case 1: $\mathfrak{h}'(\eta) > 0$ for all $\eta > 0$. It is easy to see that

$$\tilde{g}(0) \le \mathfrak{h}(0) \le \mathfrak{h}\left(\max_{1 \le i \le d} \mathfrak{c}_i^{-1/2}\right) \le \max_{1 \le i \le d} \mathfrak{c}_i^{-1/2} + \sum_{i=1}^d \sqrt{\mathfrak{c}_i},$$

where $g(0) = i\tilde{g}(0)$ is defined in (C.21), it implies that g(z) in (C.16) is nonsingular at 0. Moreover, all $\tilde{g}_i(\eta) = \tilde{g}_i^-(\eta)$ in (C.24) for $\eta > 0$. Otherwise, suppose one $\tilde{g}_i(\eta) = \tilde{g}_i^+(\eta)$, by Lemma C.4, we know that $\tilde{g}_i^+(\eta) \ge \sqrt{\mathfrak{c}_i}$, since $\tilde{g}_i(\eta)$ is continuous and $\tilde{g}_i(\eta) < \sqrt{\mathfrak{c}_i}$ when $\eta > \max_{1 \le i \le d} \mathfrak{c}_i^{-1/2}$, then there exists a $\eta_0 > 0$ such that $\tilde{g}_i^+(\eta_0) = \sqrt{\mathfrak{c}_i}$, so (C.29) deduces that $\mathfrak{h}'(\eta_0) = 0$, which is a contradiction.

Case 2: there exists an $\eta_1 \in (0, \max_{1 \le i \le d} \mathfrak{c}_i^{-1/2}]$ such that $\mathfrak{h}'(\eta) \le 0$. Without loss of generality, let

$$\eta_1 := \max \Big\{ \eta \in \Big(0, \max_{1 \leq i \leq d} \mathfrak{c}_i^{-1/2} \Big] : \mathfrak{h}'(\eta) = 0 \Big\},$$

by Remark B.1 and Lemma C.4, we know that $\tilde{g}_i(\eta) < \sqrt{\mathfrak{c}_i}$ and $\tilde{g}_i(\eta) = \tilde{g}_i^-(\eta)$ in (C.24) for $i = 2, \dots, d$ and $\eta > 0$, combining with (C.29), we obtain that

$$\tilde{g}'_i(\eta_1) = 0$$
, for $i = 2, \dots, d$, $\tilde{g}'_1(\eta_1) = \mathfrak{h}'(\eta_1) - 1 - \sum_{i=2}^d \tilde{g}'_i(\eta_1) = -1$, (C.30)

which further implies that $\tilde{g}_1(\eta_1) = \sqrt{\mathfrak{c}_1}$ by (C.29) and $\mathfrak{h}(\eta_1) = \tilde{g}_1(\eta_1) + \mathfrak{c}_1/\tilde{g}_1(\eta_1) = 2\sqrt{\mathfrak{c}_1}$. Let $\mathfrak{h}(\eta_1) = 2\sqrt{\mathfrak{c}_1}$ in (C.26), we deduce that

$$\eta_1 = \sum_{i=1}^d \sqrt{\mathfrak{c}_1 - \mathfrak{c}_i} - (d-2)\sqrt{\mathfrak{c}_1}.$$

Therefore, the case 2 is valid if and only if the above $\eta_1 > 0$, i.e. $\mathfrak{c} \in \Pi_1$ in (C.27). Moreover, we claim that $\mathfrak{h}'(\eta) = 0$ has a unique solution in $\eta \in (0, \max_{1 \le i \le d} \mathfrak{c}_i^{-1/2}]$. Suppose there exists another $\eta_2 \in (0, \eta_1]$ such that $\mathfrak{h}'(\eta_2) = 0$, we can still obtain that $\tilde{g}_1(\eta_2) = \sqrt{\mathfrak{c}_1}$ and $\mathfrak{h}(\eta_2) = 2\sqrt{\mathfrak{c}_1}$ by previous arguments, so (C.26) further implies that

$$\eta_2 = \sum_{i=1}^d \sqrt{\mathfrak{c}_1 - \mathfrak{c}_i} - (d-2)\sqrt{\mathfrak{c}_1} = \eta_1,$$

i.e. η_1 is unique. Thus, suppose $\eta_1 > 0$, $\mathfrak{h}'(\eta)$ is either positive or negative in $(0, \eta_1)$. Next, we will claim that

$$\mathfrak{h}'(\eta) < 0 \quad \text{for } \eta \in (0, \eta_1).$$
 (C.31)

In fact, recall that $\tilde{g}'_1(\eta_1) = -1$ in (C.30), there exists an $\epsilon > 0$ such that $\tilde{g}'_1(\eta) < 0$ for $\eta \in (\eta_1 - \epsilon, \eta_1)$. Hence, $\tilde{g}_1(\eta) > \sqrt{\mathfrak{c}_1}$ in $(\eta_1 - \epsilon, \eta_1)$ due to $\tilde{g}_1(\eta_1) = \sqrt{\mathfrak{c}_1}$. By (C.29), we have

$$\mathfrak{h}'(\eta) = (1 - \mathfrak{c}_1/\tilde{g}_1^2(\eta))\tilde{g}_1'(\eta) < 0 \text{ for } \eta \in (\eta_1 - \epsilon, \eta_1),$$

which confirms our claim (C.31). Finally, by Remark B.1 and Lemma C.4, we have $\tilde{g}_i(\eta) < \sqrt{\mathfrak{c}_i}$ and $\tilde{g}_i(\eta) = \tilde{g}_i^-(\eta)$ in (C.24) for $i = 2, \dots, d$ and $\eta > 0$, so (C.29) implies that $g_i'(i\eta) > 0$ for $i = 2, \dots, d$, then

$$\tilde{g}'_1(\eta) = \mathfrak{h}'(\eta) - 1 - \sum_{i=2}^d \tilde{g}'_i(\eta) < 0 \text{ for } \eta \in (0, \eta_1),$$

which further implies that $\tilde{g}_1(\eta) > \sqrt{\mathfrak{c}_1}$ in $(0, \eta_1)$. Thus, by Lemma C.4, we conclude that $\tilde{g}_1(\eta) = \tilde{g}_1^+(\eta)$ in $(0, \eta_1)$.

As a consequence of above proposition, we know that $\tilde{g}_1(\eta)$ will have a branch change at η_1 if $\mathfrak{c} \in \Pi_0 \backslash \Pi_1$. Under this situation, $\tilde{g}_1(\eta)$ will increase as $\eta \to 0^+$. Therefore, to determine whether g(z) (C.16) is singular or not at 0, it is enough to show that whether $\lim_{\eta \downarrow 0} \tilde{g}_1(\eta)$ is infinite or not. Here, let's define a new function

$$F_d(x) = \sum_{i=2}^d \sqrt{x^2 - 4\mathfrak{c}_i} - \sqrt{x^2 - 4\mathfrak{c}_1} - (d-2)x, \text{ for } x \ge 2\sqrt{\mathfrak{c}_1},$$

then we can provide a sufficient and necessary condition for the limiting behaviors of $\tilde{g}_1(\eta)$ as $\eta \downarrow 0$ based on the number of solutions of $F_d(x) = 0$.

Proposition C.2. Suppose η_1 in Proposition C.1 is strictly positive, then the solutions $F_d(x) = 0$ on $[2\sqrt{\mathfrak{c}_1}, \infty)$ are bounded $\iff \mathfrak{c}_1 < 0.5$.

Proof. Note that $F_d(2\sqrt{\mathfrak{c}_1}) = 2\eta_1 > 0$, then $F_d(x) = 0$ has no bounded solution on $[2\sqrt{\mathfrak{c}_1}, \infty)$ is equivalent to $F_d(x) > 0$ for all $x \in [2\sqrt{\mathfrak{c}_1}, \infty)$. Now, suppose $\mathfrak{c}_1 \geq 0.5$, we can obtain that

$$\sum_{i=2}^{d} \sqrt{x^2 - 4\mathfrak{c}_i} > (d-2)x + \sqrt{x^2 - 4(1-\mathfrak{c}_1)}, \text{ for } x \ge 2\sqrt{\mathfrak{c}_1}.$$
 (C.32)

In fact, since

$$\sqrt{x^2 - 4\mathfrak{c}_2} + \sqrt{x^2 - 4\mathfrak{c}_3} > x + \sqrt{x^2 - 4(\mathfrak{c}_2 + \mathfrak{c}_3)} \iff \mathfrak{c}_2\mathfrak{c}_3 > 0,$$

we can easily conclude (C.32). Therefore, if $\mathfrak{c}_1 \geq 0.5$, it implies that

$$F_d(x) > \sqrt{x^2 - 4(1 - \mathfrak{c}_1)} - \sqrt{x^2 - 4\mathfrak{c}_1} \ge 0,$$

i.e. $F_d(x) = 0$ has no bounded solution. On the other hand, suppose $\mathfrak{c}_1 < 0.5$, since

$$F_d(x) \leq (d-1)\sqrt{x^2 - \frac{4(1-\mathfrak{c}_1)}{(d-1)}} - \sqrt{x^2 - 4\mathfrak{c}_1} - (d-2)x := \widetilde{F}_d(x),$$

by the method of Lagrange multipliers. We only need to show that there exists a bounded $x \in [2\sqrt{\mathfrak{c}_1}, \infty)$ such that $\widetilde{F}_d(x) \leq 0$. Notice that

$$\widetilde{F}_d(x) \le 0 \iff x^2 - x\sqrt{x^2 - 4\mathfrak{c}_1} \le 2\frac{(d-1)(1-\mathfrak{c}_1) - \mathfrak{c}_1}{d-2},$$

and

$$\mathfrak{c}_1 < 0.5 \iff 2\mathfrak{c}_1 < 2\frac{(d-1)(1-\mathfrak{c}_1)-\mathfrak{c}_1}{d-2}$$

so we can choose a sufficiently small $\epsilon > 0$ such that

$$2\mathfrak{c}_1 + \epsilon < 2\frac{(d-1)(1-\mathfrak{c}_1) - \mathfrak{c}_1}{d-2}.$$

On the other hand, we can also choose a sufficiently large $x = x(\epsilon) > 0$ such that

$$x^{2} - x\sqrt{x^{2} - 4\mathfrak{c}_{1}} = \frac{4\mathfrak{c}_{1}x}{x + \sqrt{x^{2} - 4\mathfrak{c}_{1}}} < 2\mathfrak{c}_{1} + \epsilon,$$

it implies that $F_d(y) \leq \widetilde{F}_d(y) \leq 0$ for all $y \in [x(\epsilon), \infty)$, i.e. the solutions of $F_d(x) = 0$ are bounded if and only if $\mathfrak{c}_1 < 0.5$.

Finally, let's prove Theorem C.3 as follows:

Proof of Theorem C.3. Recall that $\mathfrak{c}_1 = \max_{1 \leq i \leq d} \mathfrak{c}_i$ and $\Pi_0 := \{\mathfrak{c} \in \mathbb{R}^d : \sum_{i=1}^d \mathfrak{c}_i = 1, \mathfrak{c}_i > 0\}$ be the d-dimensional affine hyperplane, then we will show that the invariant branch region Π_1 is a subset of nonsingular region Π_2 , i.e.

$$\Pi_1 = \left\{ \mathfrak{c} \in \Pi_0 : \sum_{i=1}^d \sqrt{\mathfrak{c}_1 - \mathfrak{c}_i} \le (d-2)\sqrt{\mathfrak{c}_1} \right\} \subset \Pi_2 = \{ \mathfrak{c} \in \Pi_0 : \mathfrak{c}_1 < 0.5 \}.$$

Suppose there is a $\mathfrak{c} \in \Pi_1$ such that $\mathfrak{c} \notin \Pi_2$, i.e. $\mathfrak{c}_1 \geq 0.5$, then according to (C.32), we have

$$(d-2)\sqrt{\mathfrak{c}_1} \ge \sum_{i=1}^d \sqrt{\mathfrak{c}_1 - \mathfrak{c}_i} > (d-2)\sqrt{\mathfrak{c}_1} + \sqrt{2\mathfrak{c}_1 - 1},$$

it implies that $0 \leq (2\mathfrak{c}_1 - 1)^{1/2} < 0$, which is a contradiction. Finally, according to (C.26), if $\eta \leq \eta_1$, $\mathfrak{h}(\eta)$ is the solution of $2\eta = F_d(\mathfrak{h}(\eta))$. By Proposition C.2, if $\mathfrak{c}_1 \geq 0.5$, $F_d(x) = 0$ has no finite solution. Notice that $\lim_{x\to\infty} F_d(x) = 0$, then $\mathfrak{h}(\eta) \to +\infty$ as $\eta \to 0^+$, i.e. $\tilde{g}_1(\eta) \to \infty$. Therefore, (C.16) is singular at z=0. On the other hand, if $\mathfrak{c}_1 < 0.5$, there exist a bounded x_0 such that $F_d(x) < 0$ for all $x > x_0$. Since $F_d(\mathfrak{h}(\eta_1)) = 2\eta_1$, then $\mathfrak{h}(\eta) \leq x_0$ for all $\eta \in (0, \eta_1]$, which suggests $\tilde{g}_i(\eta)$ are all bounded for $i=1,\cdots,d$. Now, we complete our proof.

D Entrywise law when d = 3

In this section, we will establish the entrywise law for Q(z) as follows:

Theorem D.1. Under Assumptions A.1 and A.2, for any $z \in S_{\eta_0}$ in (C.18) and $\omega \in (1/2-\delta, 1/2)$, where $\delta > 0$ is a sufficiently small number, let

$$\mathbf{W}^{(3)}(z) = -((z+g(z))\mathbf{I}_3 - \operatorname{diag}(\mathbf{g}(z)) + g(z)\mathbf{S}_3 - \operatorname{diag}(\mathbf{g}(z))\mathbf{S}_3 - \mathbf{S}_3\operatorname{diag}(\mathbf{g}(z)))^{-1}.$$
 (D.1)

For $s, t \in \{1, 2, 3\}$, we have

$$\left| Q_{i_s i_t}^{st}(z) - \mathfrak{c}_s^{-1} g_s(z) \left[\delta_{st} \delta_{i_s i_t} + (a_{i_s}^{(s)})^2 \sum_{k \neq s}^3 (g(z) - g_s(z) - g_k(z)) W_{sk}^{(3)}(z) \right] \right| \prec \mathcal{O}(\eta_0^{-21} N^{-\omega}),$$

where $Q_{i_si_t}^{st}(z)$ is the (i_s,i_t) -th entry of \mathbf{Q}^{st} and $a_{i_s}^{(s)}$ is the i_s -th entry of $\mathbf{a}^{(s)}$, so does $W_{sk}^{(3)}(z)$.

The existence of $W^{(3)}(z)$ on S_{η_0} is proven in Lemma G.5 later. For simplicity, we rewrite the three deterministic unit vectors as follows:

$$a := a^{(1)} \in \mathbb{S}^{m-1}, \quad b := a^{(2)} \in \mathbb{S}^{n-1}, \quad c := a^{(3)} \in \mathbb{S}^{p-1},$$
 (D.2)

and

$$m{M} = rac{1}{\sqrt{N}} m{\Phi}_3(m{X}, m{a}, m{b}, m{c}), \quad m{Q}(z) = (m{M} - z m{I}_N)^{-1} = \left(egin{array}{ccc} m{Q}^{11}(z) & m{Q}^{12}(z) & m{Q}^{13}(z) \ m{Q}^{12}(z)' & m{Q}^{22}(z) & m{Q}^{23}(z) \ m{Q}^{13}(z)' & m{Q}^{23}(z)' & m{Q}^{33}(z) \end{array}
ight),$$

where $z \in \mathbb{C}^+$ and N = m + n + p. Besides, the following lemmas are necessary:

Lemma D.1 ([31]). Let $\Omega \subset \mathbb{R}$ and $f: \Omega^n \to \mathbb{C}$ such that

$$\sup_{x_1,\dots,x_n,x_i'\in\Omega}|f(\dots,x_i,\dots)-f(\dots,x_i',\dots)|\leq M_i.$$

where M_i are bounded positive constants. Then

$$\mathbb{P}(|f(X_1,\dots,X_n)^c| \ge t) \le 4 \exp\left(-\frac{t^2}{\sum_{i=1}^n M_i^2}\right).$$
 (D.3)

Lemma D.2 ([24]). For any real-valued random variable ξ with $\mathbb{E}[|\xi|^{K+2}] < \infty$ and complex valued function g(z) with continuous and bounded K+1 derivatives, then

$$\mathbb{E}\left[\xi g(\xi)\right] = \sum_{l=0}^{K} \frac{\kappa_{l+1}}{l!} \mathbb{E}\left[g^{(l)}(\xi)\right] + \epsilon_{(K+1)},\tag{D.4}$$

where κ_l is the l-th cumulant of ξ , and

$$|\epsilon_{(K+1)}| \le C_K \sup_{z \in \mathbb{C}} |g^{(K+1)}(z)| \mathbb{E}[|\xi|^{K+2}].$$

Here, the l-th cumulant of ξ is defined via

$$\log \mathbb{E}[e^{\mathrm{i}x\xi}] = \sum_{l=1}^{\infty} \kappa_l \frac{(\mathrm{i}x)^l}{l!}, \quad x \in \mathbb{R}.$$

D.1 Preliminary Lemmas

To prove Theorem D.1, we need to deal with quadratic forms of Q(z) and $\operatorname{diag}(Q(z))$. Actually, the (s,t)-th entry of Q(z) is itself a special case of such quadratic forms. So we propose several lemmas in this section to deal with such quadratic forms. Here, we use a simple example to illustrate the main purpose of lemmas in §D.1. Note that the $N^{-1}\operatorname{Tr}(Q(z)) = N^{-1}\mathbf{1}'_N\operatorname{diag}(Q(z))\mathbf{1}_N$ is a quadratic form of $\operatorname{diag}(Q(z))$, and general procedures of calculating $N^{-1}\operatorname{Tr}(Q(z))$ have two steps:

- 1. Show that $N^{-1}\operatorname{Tr}(\boldsymbol{Q}(z)) \xrightarrow{a.s.} N^{-1}\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}(z))];$
- 2. Compute $N^{-1}\mathbb{E}[\text{Tr}(\boldsymbol{Q}(z))]$.

For the first step, we need Lemma D.3 in §D.1.1. This lemma establishes the convergence rate of quadratic forms of $\mathbf{Q}(z)$ and $\operatorname{diag}(\mathbf{Q}(z))$ to their mean, where $N^{-1}\operatorname{Tr}(\mathbf{Q}(z))=N^{-1}\mathbf{1}'_N\operatorname{diag}(\mathbf{Q}(z))\mathbf{1}_N$ is a quadratic form of $\operatorname{diag}(\mathbf{Q}(z))$. For the second step, by the definition of $\mathbf{Q}(z)$ in (A.10), we know that $\mathbf{M}\mathbf{Q}(z)-z\mathbf{Q}(z)=\mathbf{I}_N$, i.e. $\mathbf{Q}(z)=z^{-1}(\mathbf{M}\mathbf{Q}(z)-\mathbf{I}_N)$, so we obtain (e.g.)

$$\frac{1}{N}\mathbb{E}[\text{Tr}(\boldsymbol{Q}^{11}(z))] = \frac{1}{N}\sum_{i=1}^{m}\mathbb{E}[Q_{ii}^{11}(z)] = \frac{z^{-1}}{N^{3/2}}\sum_{i,j,k=1}^{m,n,p}\mathbb{E}[X_{ijk}(c_kQ_{ij}^{12}(z) + b_jQ_{ik}^{13}(z))] - z^{-1}\mathfrak{c}_1.$$

To compute $\mathbb{E}[X_{ijk}(c_kQ_{ij}^{12}(z) + b_jQ_{ik}^{13}(z))]$, we will use the cumulant expansion (D.4). In precise, the definition of $Q_{st}(z)$ allows us to treat it as a smooth function of X. Consequently, we can compute its expectation using the cumulant expansion (D.4). Next, define

$$\partial_{ijk}^{(l)} := \frac{\partial^l}{\partial X_{ijk}^l} \quad l \in \mathbb{N}^+, \tag{D.5}$$

then we have

$$\left(\partial_{ijk}^{(1)}\boldsymbol{M}\right)\boldsymbol{Q}(z) + (\boldsymbol{M} - z\boldsymbol{I}_N)\partial_{ijk}^{(1)}\boldsymbol{Q}(z) = 0 \quad \Rightarrow \quad \partial_{ijk}^{(1)}\boldsymbol{Q}(z) = -\boldsymbol{Q}(z)\left(\partial_{ijk}^{(1)}\boldsymbol{M}\right)\boldsymbol{Q}(z).$$

By the notations in (D.2), we rewrite (A.6) as follows:

$$\mathcal{A}_{ijk}^{(j_1,j_2)} = \begin{cases}
 a_i, & (j_1,j_2) = (1,2) \text{ or } (2,1) \\
 b_j, & (j_1,j_2) = (1,3) \text{ or } (3,1) \\
 c_k, & (j_1,j_2) = (2,3) \text{ or } (3,2)
\end{cases}$$

$$\tilde{t}_{\alpha} = \begin{cases}
 i, & t_{\alpha} = 1 \\
 j, & t_{\alpha} = 2 \\
 k, & t_{\alpha} = 3
\end{cases}$$
(D.6)

so we obtain that

$$\partial_{ijk}^{(1)} Q_{i_1 i_2}^{j_1 j_2}(z) = -N^{-1/2} \sum_{\substack{t_1, t_2 \\ t_1 \neq t_2}} Q_{i_1 \bar{t}_1}^{j_1 t_1}(z) \mathcal{A}_{ijk}^{(t_1, t_2)} Q_{\bar{t}_2 i_2}^{t_2 j_2}(z), \tag{D.7}$$

where the summations of t_1 and t_2 are over $\{1, 2, 3\}$. For notational simplicity and clarity, we will henceforth denote $\mathbf{Q}(z)$ as \mathbf{Q} and refer to its entries without the explicit dependency on z, unless otherwise specified. By the cumulant expansion (D.4) and (D.7), we have

$$\frac{1}{N} \sum_{i=1}^{m} \mathbb{E}[Q_{ii}^{11}] = \frac{z^{-1}}{N^{3/2}} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}[\partial_{ijk}^{(1)}(c_k Q_{ij}^{12} + b_j Q_{ik}^{13})] + \frac{z^{-1}}{N^{3/2}} \sum_{i,j,k=1}^{m,n,p} \epsilon_{ijk}^{(2)} - z^{-1} \mathfrak{c}_1 \qquad (D.8)$$

$$= -z^{-1} \mathfrak{c}_1 - \frac{z^{-1}}{N^2} \mathbb{E}\left[\operatorname{Tr}(\boldsymbol{Q}^{11}) \operatorname{Tr}(\boldsymbol{Q}^{22} + \boldsymbol{Q}^{33}) + \operatorname{Tr}(\boldsymbol{Q}^{12} \boldsymbol{Q}^{21} + \boldsymbol{Q}^{13} \boldsymbol{Q}^{31}) + \boldsymbol{a}' \boldsymbol{Q}^{12} \boldsymbol{Q}^{23} \boldsymbol{c} + \boldsymbol{a}' \boldsymbol{Q}^{13} \boldsymbol{Q}^{32} \boldsymbol{b} + 2\boldsymbol{b}' \boldsymbol{Q}^{23} \boldsymbol{c} \operatorname{Tr}(\boldsymbol{Q}^{11}) + \boldsymbol{a}' \boldsymbol{Q}^{13} \boldsymbol{c} \operatorname{Tr}(\boldsymbol{Q}^{22}) + \boldsymbol{a}' \boldsymbol{Q}^{12} \boldsymbol{b} \operatorname{Tr}(\boldsymbol{Q}^{33})\right] + \frac{z^{-1}}{N^{3/2}} \sum_{i,j,k=1}^{m,n,p} \epsilon_{ijk}^{(2)},$$

to further compute the above equations, Lemmas in §D.1.1 and §D.1.2 can solve the following dilemmas.

1. Lemma D.3 in §D.1.1 establishes the convergence rate of quadratic forms of Q and diag(Q) to their mean, e.g. $b'Q^{23}c$ and $N^{-1}\operatorname{Tr}(Q^{11})=N^{-1}\mathbf{1}'_m\operatorname{diag}(Q^{11})\mathbf{1}_m$, so we can conclude that

$$\lim_{N \to \infty} \left| \mathbb{E}[N^{-1} \operatorname{Tr}(\boldsymbol{Q}^{11}) N^{-1} \operatorname{Tr}(\boldsymbol{Q}^{22})] - \mathbb{E}[N^{-1} \operatorname{Tr}(\boldsymbol{Q}^{11})] \mathbb{E}[N^{-1} \operatorname{Tr}(\boldsymbol{Q}^{22})] \right| = 0$$

and

in (D.8).

$$\lim_{N \to \infty} \left| \mathbb{E}[N^{-1} \operatorname{Tr}(\boldsymbol{Q}^{11}) \boldsymbol{b}' \boldsymbol{Q}^{23} \boldsymbol{c}] - \mathbb{E}[N^{-1} \operatorname{Tr}(\boldsymbol{Q}^{11})] \mathbb{E}[\boldsymbol{b}' \boldsymbol{Q}^{23} \boldsymbol{c}] \right| = 0$$

2. To prove the remainder $N^{-3/2} \sum_{i,j,k=1}^{m,n,p} \epsilon_{ijk}^{(2)}$ in (D.8) vanishes to zero as $N \to \infty$, we need lemmas in §D.1.2. Actually, for later calculations of the asymptotic mean and variance of the LSS of the matrix M, see §E, we need to compute $\sum_{i,j,k=1}^{m,n,p} \mathbb{E}[\partial_{ijk}^{(l)}(c_kQ_{ij}^{12} + b_jQ_{ik}^{13})]$ for l=2,3,4, and there will appear lots of different complicate terms as those in (D.8). The lemmas in §D.1.2 assist us in determining which terms in $\sum_{i,j,k=1}^{m,n,p} \mathbb{E}[\partial_{ijk}^{(l)}(c_kQ_{ij}^{12} + b_jQ_{ik}^{13})]$ vanish to 0 as $N \to \infty$. We refer to these terms as minor terms. By distinguishing between major and minor terms, we can concentrate on the terms that significantly contribute to the asymptotic mean and variance of the LSS of the matrix M.

Consequently, Lemmas in §D.1.1 and §D.1.2 will simplify calculations of (D.8) as follows:

$$N^{-1}\mathbb{E}[\mathrm{Tr}(\boldsymbol{Q}^{11})](z+N^{-1}\mathbb{E}[\mathrm{Tr}(\boldsymbol{Q}^{22}+\boldsymbol{Q}^{33})])+\mathfrak{c}_1=\mathrm{o}(1),$$

i.e. $-\frac{\mathfrak{c}_1}{\mathfrak{m}_1(z)} = z + \mathfrak{m}_2(z) + \mathfrak{m}_3(z) + \mathrm{o}(1)$, and the limiting form of this equation is just the vector Dyson equation (B.1). For more details, readers can refer to §D.2 later.

D.1.1 Almost surely convergence of quadratic forms

Lemma D.3. When d=3, for any $K \in \mathbb{N}^+, z_1, \dots, z_K \in \mathbb{C}_{\eta}^+$ and $\omega \in (1/2-\delta, 1/2)$, where $\delta > 0$ is a sufficiently small number, let $s_i \in \{1, 2, 3\}$ for $i=1, \dots, K$ such that $s_{2j} = s_{2j+1}$, then for any two deterministic vectors $\boldsymbol{x} \in \mathbb{C}^{n_{s_1}}, \boldsymbol{y} \in \mathbb{C}^{n_{s_{K+1}}}$ with bounded L^2 norms, we have

$$\left| \boldsymbol{x}' \prod_{i=1}^{K} \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \boldsymbol{y} - \mathbb{E} \left[\boldsymbol{x}' \prod_{i=1}^{K} \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \boldsymbol{y} \right] \right| \prec C_K \eta^{-(K+4)} N^{-\omega}. \tag{D.9}$$

Moreover, if $s_1 = s_{K+1}$, we have

$$\left| \boldsymbol{x}' \operatorname{diag} \left(\prod_{i=1}^{K} \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \right) \boldsymbol{y} - \mathbb{E} \left[\boldsymbol{x}' \operatorname{diag} \left(\prod_{i=1}^{K} \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \right) \boldsymbol{y} \right] \right| \prec C_K \eta^{-(K+4)} N^{-\omega}.$$
 (D.10)

Lemma D.3 implies that $a'Q^{12}(z)b \xrightarrow{a.s.} \mathbb{E}[a'Q^{12}(z)b]$ and

$$\frac{1}{N}\operatorname{Tr}(\boldsymbol{Q}(z)) \xrightarrow{a.s.} \frac{1}{N}\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}(z))], \quad \frac{1}{N}\operatorname{Tr}(\boldsymbol{Q}^{12}(z_1)\boldsymbol{Q}^{21}(z_2)) \xrightarrow{a.s.} \frac{1}{N}\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{12}(z_1)\boldsymbol{Q}^{21}(z_2))].$$

and all above quadratic forms will appear in the asymptotic covariance and mean functions of $\text{Tr}(\boldsymbol{Q}(z)) - Ng(z)$.

Moreover, we have given the formula of $\partial_{ijk}^{(1)} Q$ in (D.7). For higher derivatives, we can show that $\partial_{ijk}^{(l)} Q = (-1)^l l! (Q \partial_{ijk}^{(1)} M)^l Q$ for $l \geq 2$ and

$$\partial_{ijk}^{(l)} Q_{i_1 i_2}^{j_1 j_2} = (-N^{-1/2})^l l! \sum_{t_1 \cdots t_{2l}} Q_{i_1 \tilde{t}_1}^{j_1 t_1} \left(\prod_{\alpha=1}^{l-1} \mathcal{A}_{ijk}^{(t_{2\alpha-1}, t_{2\alpha})} Q_{\tilde{t}_{2\alpha} \tilde{t}_{2\alpha+1}}^{t_{2\alpha} t_{2\alpha+1}} \right) \mathcal{A}_{ijk}^{(t_{2l-1}, t_{2l})} Q_{\tilde{t}_{2l} i_2}^{t_{2l} j_2}, \tag{D.11}$$

where the summations of all t_{α} are over $\{1,2,3\}$ such that $t_{2\alpha-1} \neq t_{2\alpha}$ for all $\alpha = 1, \dots, l$.

Remark D.1. Let's use a simple example to show the formulation of (D.11), since

$$\partial_{ijk}^{(1)} M = \frac{1}{\sqrt{N}} \begin{pmatrix} \mathbf{0}_{m \times m} & c_k \mathbf{e}_i^m (\mathbf{e}_j^n)' & b_j \mathbf{e}_i^m (\mathbf{e}_k^p)' \\ c_k \mathbf{e}_j^n (\mathbf{e}_i^m)' & \mathbf{0}_{n \times m} & a_i \mathbf{e}_j^n (\mathbf{e}_k^p)' \\ b_j \mathbf{e}_k^p (\mathbf{e}_i^m)' & a_i \mathbf{e}_k^p (\mathbf{e}_j^n)' & \mathbf{0}_{p \times p} \end{pmatrix},$$
(D.12)

where e_i^m is a m dimensional vector whose i-th entry is 1 and others are 0, so does e_j^n, e_k^p . Consider $\partial_{ijk}^{(1)}Q_{11}^{(1)}$, which is indeed the (1,1) entry in the (1,1) block of $\partial_{ijk}^{(1)}Q = -Q(\partial_{ijk}^{(1)}M)Q$, so we first consider $\partial_{ijk}^{(1)}Q^{11}$, i.e.

$$\partial_{ijk}^{(1)} \boldsymbol{Q}^{11} = -\sum_{t_2,t_3} \boldsymbol{Q}^{1t_2} (\partial_{ijk}^{(1)} \boldsymbol{M}^{t_2t_3}) \boldsymbol{Q}^{t_31},$$

notice that the diagonal blocks of $\partial_{ijk}^{(1)} M$ are zero, then it deduces that $t_2 \neq t_3$. Besides, for each $\partial_{ijk}^{(1)} M^{t_2t_3}$, $t_2 \neq t_3$, it only has one nonzero entry with value of $\mathcal{A}_{ijk}^{t_2t_3}$. Hence, we show that for any two adjacent $Q_{\tilde{t}_{2\alpha-1}\tilde{t}_{2\alpha}}^{t_{2\alpha-1}t_{2\alpha}}$, i.e. $Q_{\tilde{t}_{2\alpha-1}\tilde{t}_{2\alpha}}^{t_{2\alpha-1}t_{2\alpha}} \mathcal{A}_{ijk}^{(t_{2\alpha},t_{2\alpha+1})} Q_{\tilde{t}_{2\alpha+1}\tilde{t}_{2\alpha+2}}^{t_{2\alpha+1}t_{2\alpha+2}}$, it has $t_{2\alpha} \neq t_{2\alpha+1}$.

We say $Q_{\tilde{t}_{2\alpha-1}\tilde{t}_{2\alpha}}^{t_{2\alpha-1}t_{2\alpha}}$ comes from **diagonal** blocks if $t_{2\alpha-1}=t_{2\alpha}$, otherwise from **off-diagonal** blocks. Since we will apply the bounded difference inequality (D.3) to prove Lemma D.3, we need the upper bound for the summation of higher order derivatives over all i, j, k. Hence, we propose the following lemma.

Lemma D.4. When d=3, for any $K \in \mathbb{N}^+$ and $z \in \mathbb{C}^+_{\eta}$, let $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{C}^N$ be two deterministic vectors with bounded L^2 norms, then we have

$$\sum_{i,j,k=1}^{m,n,p} |\mathbf{x}' \partial_{ijk}^{(l)} \Big(\prod_{k=1}^K \mathbf{Q}(z) \Big) \mathbf{y} |^2 < \begin{cases} C_{l,K} || \mathbf{Q}(z) ||^{2(l+K)} N^{-1} & l = 1, 2, \\ C_{l,K} || \mathbf{Q}(z) ||^{2(l+K)} N^{-2} & l = 3. \end{cases}$$

Proof. Recall the notations in (D.2), assume that $\boldsymbol{x}=(\boldsymbol{x}^1,\boldsymbol{x}^2,\boldsymbol{x}^3)'$ such that $\boldsymbol{x}^1\in\mathbb{C}^m,\boldsymbol{x}^2\in\mathbb{C}^n,\boldsymbol{x}^3\in\mathbb{C}^p$ and $\|\boldsymbol{x}^1\|_2=\|\boldsymbol{x}^2\|_2=\|\boldsymbol{x}^3\|_2=1$, so does $\boldsymbol{y}=(\boldsymbol{y}^1,\boldsymbol{y}^2,\boldsymbol{y}^3)'$. It's enough to show that for given $s_1,\cdots,s_{K+1}\in\{1,2,3\}$ and l=1,2,3, we have

$$\sum_{i,j,k=1}^{m,n,p} \left| (\boldsymbol{x}^{s_1})' \partial_{ijk}^{(l)} \left(\prod_{l=1}^K \boldsymbol{Q}^{s_l s_{l+1}} \right) \boldsymbol{y}^{s_{K+1}} \right|^2 < C_l \eta^{-2(l+1)} N^{-1}.$$
 (D.13)

For simplicity, let

$$\boldsymbol{x}^{(i_0)} = \begin{cases} \prod_{i=1}^{i_0-1} \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \boldsymbol{x}^{s_1} & i_0 > 1, \\ \boldsymbol{x} & i_0 = 1. \end{cases} \quad \boldsymbol{y}^{(i_0)} = \begin{cases} \prod_{i=i_0+1}^{K} \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \boldsymbol{y}^{s_{K+1}} & i_0 < K, \\ \boldsymbol{y} & i_0 = K. \end{cases}$$
(D.14)

According to (D.7) and (D.11), we have

$$(\mathbf{x}^{j_1})'\partial_{ijk}^{(l)}\mathbf{Q}^{j_1j_2}\mathbf{y}^{j_2}$$
 (D.15)

$$= \left\{ \begin{array}{ll} (-N^{-1/2})^l l! \sum_{t_1 \cdots t_{2l}} (\boldsymbol{x}^{j_1})' Q_{\cdot \tilde{t}_1}^{j_1 t_1} \left(\prod_{\alpha=1}^{l-1} \mathcal{A}_{ijk}^{(t_{2\alpha-1},t_{2\alpha})} Q_{\tilde{t}_{2\alpha}\tilde{t}_{2\alpha+1}}^{t_{2\alpha t_{2\alpha+1}}} \right) \mathcal{A}_{ijk}^{(t_{2l-1},t_{2l})} Q_{\tilde{t}_{2l}}^{t_{2l} j_2} \boldsymbol{y}^{j_2} & l \geq 2 \\ -N^{-1/2} \sum_{t_1,t_2} (\boldsymbol{x}^{j_1})' Q_{\cdot \tilde{t}_2}^{j_1 t_1} \mathcal{A}_{ijk}^{(t_1,t_2)} Q_{\tilde{t}_2}^{t_2 j_2} \boldsymbol{y}^{j_2} & l = 1 \end{array} \right.$$

where $t_1, \dots, t_{2l} \in \{1, 2, 3\}$ such that $t_{2\alpha-1} \neq t_{2\alpha}$ for $\alpha = 1, \dots, l$ and \tilde{t}_{α} is defined in (D.6).

First derivatives: When l = 1, since

$$\begin{split} &\sum_{i,j,k=1}^{m,n,p} \left| (\boldsymbol{x}^{s_1})' \partial_{ijk}^{(1)} \Big(\prod_{l=1}^K \boldsymbol{Q}^{s_l s_{l+1}} \Big) \boldsymbol{y}^{s_{K+1}} \right|^2 \leq \sum_{l_0=1}^K \sum_{i,j,k=1}^{m,n,p} \left| (\boldsymbol{x}^{(l_0)})' \partial_{ijk}^{(1)} \boldsymbol{Q}^{s_{l_0} s_{l_0+1}} \boldsymbol{y}^{(l_0)} \right|^2 \\ &= \sum_{l_0=1}^K \sum_{i,j,k=1}^{m,n,p} \left| \sum_{t_1 \neq t_2} N^{-1/2} (\boldsymbol{x}^{(l_0)})' Q_{\cdot \tilde{t}_1}^{s_{l_0} t_1} \mathcal{A}_{ijk}^{(t_1,t_2)} Q_{\tilde{t}_2}^{t_2 s_{l_0+1}} \boldsymbol{y}^{(l_0)} \right|^2 \\ &\leq 6 \sum_{l_0=1}^K \sum_{t_1 \neq t_2} \sum_{i,j,k=1}^{m,n,p} N^{-1} \left| (\boldsymbol{x}^{(l_0)})' Q_{\cdot \tilde{t}_1}^{s_{l_0} t_1} \mathcal{A}_{ijk}^{(t_1,t_2)} Q_{\tilde{t}_2}^{t_2 s_{l_0+1}} \boldsymbol{y}^{(l_0)} \right|^2 := 6 \sum_{l_0=1}^K \sum_{t_1 \neq t_2} \mathcal{P}_{t_1 t_2}, \end{split}$$

where we use the Cauchy's inequality in the third step and $t_1, t_2 \in \{1, 2, 3\}$. To conclude Lemma D.4 for l = 1, it is enough to show that each $\mathcal{P}_{t_1t_2} < N^{-1} \|\mathbf{Q}\|^{2(K+1)}$. For example,

$$\mathcal{P}_{t_1t_2} = \sum_{i,j,k=1}^{m,n,p} |(\boldsymbol{x}^{(l_0)})'Q_{.j}^{s_{l_0}2} a_i Q_{k.}^{3s_{l_0+1}} \boldsymbol{y}^{(l_0)}|^2 = N^{-1} \|\boldsymbol{Q}^{t_1s_{l_0}} \boldsymbol{x}^{(l_0)}\|_2^2 \times \|\boldsymbol{Q}^{t_2s_{l_0+1}} \boldsymbol{y}^{(l_0)}\|_2^2 \leq N^{-1} \|\boldsymbol{Q}\|^{2(K+1)},$$

where we use the fact that $\|\boldsymbol{Q}^{t_1s_{l_0}}\boldsymbol{x}^{(l_0)}\|_2 \leq \|\boldsymbol{Q}^{t_1s_{l_0}}\| \cdot \|\boldsymbol{x}^{(l_0)}\|_2 \leq \|\boldsymbol{Q}\|^{l_0}$ and $\|\boldsymbol{Q}^{t_2s_{l_0+1}}\boldsymbol{y}^{(l_0)}\|_2 \leq \|\boldsymbol{Q}\|^{K-l_0+1}$. The arguments for others are the same, we omit details here.

Second derivatives: For the second derivatives, i.e.

$$(\boldsymbol{x}^{s_1})'\partial_{ijk}^{(2)} \Big(\prod_{l=1}^K \boldsymbol{Q}^{s_l s_{l+1}} \Big) \boldsymbol{y}^{s_{K+1}} = \sum_{l_0=1}^K (\boldsymbol{x}^{(l_0)})'\partial_{ijk}^{(2)} \boldsymbol{Q}^{s_{l_0} s_{l_0+1}} \boldsymbol{y}^{(l_0)}$$
(D.16)

$$+2\sum_{l_0< l_1}^{K} (\boldsymbol{x}^{(l_0)})' \partial_{ijk}^{(1)} \boldsymbol{Q}^{s_{l_0}s_{l_0+1}} \boldsymbol{P}^{l_0l_1} \partial_{ijk}^{(1)} \boldsymbol{Q}^{s_{l_1}s_{l_1+1}} \boldsymbol{y}^{(l_1)},$$
(D.17)

where $\boldsymbol{x}^{(l_0)}, \boldsymbol{y}^{(l_0)}$ are defined in (D.14) and

$$\boldsymbol{P}^{l_0 l_1} := \begin{cases} \prod_{i=l_0+1}^{l_1} \boldsymbol{Q}^{s_i s_{i+1}} & l_0 + 1 < l_0 \\ \boldsymbol{I}_{n_{s_{l_0+1}}} & l_0 + 1 = l_1 \end{cases} . \tag{D.18}$$

Let's consider the following two possible scenarios.

Case 1 (D.16): by the Cauchy's inequality and (D.15), for any $l_0 \in \{1, \dots, K\}$, consider

$$\begin{split} &\mathcal{R}_{(2,2)}^{(l_0)} := \sum_{i,j,k=1}^{m,n,p} \left| (\boldsymbol{x}^{(l_0)})' \partial_{ijk}^{(2)} \boldsymbol{Q}^{s_{l_0} s_{l_0+1}} \boldsymbol{y}^{(l_0)} \right|^2 \\ &= \sum_{i,j,k=1}^{m,n,p} \left| 2N^{-1} \sum_{t_1 \neq t_2} \sum_{t_3 \neq t_4} (\boldsymbol{x}^{(l_0)})' Q_{.\tilde{t}_1}^{s_{l_0} t_1} \mathcal{A}_{ijk}^{(t_1,t_2)} Q_{\tilde{t}_2 \tilde{t}_3}^{t_2 t_3} \mathcal{A}_{ijk}^{(t_3,t_4)} Q_{\tilde{t}_4}^{t_4 s_{l_0+1}} \boldsymbol{y}^{(l_0)} \right|^2 \\ &\leq C \sum_{t_1 \neq t_2} \sum_{t_3 \neq t_4} \sum_{i,j,k=1}^{m,n,p} N^{-2} \left| (\boldsymbol{x}^{(l_0)})' Q_{.\tilde{t}_1}^{s_{l_0} t_1} \mathcal{A}_{ijk}^{(t_1,t_2)} Q_{\tilde{t}_2 \tilde{t}_3}^{t_2 t_3} \mathcal{A}_{ijk}^{(t_3,t_4)} Q_{\tilde{t}_4}^{t_4 s_{l_0+1}} \boldsymbol{y}^{(l_0)} \right|^2 \\ &:= C \sum_{t_1 \neq t_2} \sum_{t_3 \neq t_4} \mathcal{P}_{t_1 \cdots t_4}, \end{split}$$

where $t_1, \dots, t_4 \in \{1, 2, 3\}$. Therefore, it is enough to show that each $\mathcal{P}_{t_1 \dots t_4} \leq N^{-1} \|\boldsymbol{Q}\|^{2(K+2)}$. First, consider the case where $Q_{t_2 t_3}^{t_2 t_3}$ is an element of the off-diagonal blocks, which implies that $t_2 \neq t_3$. In this scenario, there are two possible subcases:

• Both $\mathcal{A}_{ijk}^{(t_1,t_2)}$ and $\mathcal{A}_{ijk}^{(t_3,t_4)}$ do not contain $a_{it_2}^{(t_2)}$ and $a_{it_3}^{(t_3)}$, it implies that $t_1 = t_3$ and $t_2 = t_4$,

$$\begin{split} \mathcal{P}_{t_{1}\cdots t_{4}} &= \sum_{i,j,k=1}^{m,n,p} N^{-2} \Big| (\boldsymbol{x}^{(l_{0})})' Q_{.\tilde{t}_{1}}^{s_{l_{0}}t_{1}} \mathcal{A}_{ijk}^{(t_{1},t_{2})} Q_{\tilde{t}_{2}\tilde{t}_{1}}^{t_{2}t_{1}} \mathcal{A}_{ijk}^{(t_{1},t_{2})} Q_{\tilde{t}_{2}}^{t_{2}s_{l_{0}+1}} \boldsymbol{y}^{(l_{0})} \Big|^{2} \\ &\leq N^{-2} (|\boldsymbol{x}^{(l_{0})}|^{\circ 2})' |\boldsymbol{Q}^{s_{l_{0}}t_{1}}|^{\circ 2} |\boldsymbol{Q}^{t_{1}t_{2}}|^{\circ 2} |\boldsymbol{Q}^{t_{2}s_{l_{0}+1}}|^{\circ 2} |\boldsymbol{y}^{(l_{0})}|^{\circ 2} \leq N^{-2} \|\boldsymbol{Q}\|^{2(K+2)}, \end{split}$$

where we use the fact that $\||Q|^{\circ 2}\| = \|Q \circ \overline{Q}\| \le \|Q\|^2$ and all $a^{(i)}$ are unit vectors.

• Otherwise, at least one of $\mathcal{A}_{ijk}^{(t_1,t_2)}$ and $\mathcal{A}_{ijk}^{(t_3,t_4)}$ contains $a_{i_2}^{(t_2)}$ or $a_{i_3}^{(t_3)}$. Without loss of generality, assume $a_{i_2}^{(t_2)}$ exists, then

$$\mathcal{P}_{t_1\cdots t_4} \leq N^{-2} \|\boldsymbol{Q}^{t_1s_{l_0}}\boldsymbol{x}^{(l_0)}\|_2^2 \times \|\boldsymbol{Q}^{t_4s_{l_0+1}}\boldsymbol{y}^{(l_0)}\|_2^2 \times \|\boldsymbol{Q}^{t_3t_2}\boldsymbol{a}^{(t_2)}\|_2^2 \leq N^{-2} \|\boldsymbol{Q}\|^{2(K+2)}.$$

Second, suppose $Q_{\tilde{t}_2\tilde{t}_3}^{t_2t_3}$ comes from the diagonal blocks, i.e. $t_2=t_3$. Similarly to the previous case, this scenario can be further divided into two subcases:

• If $t_1 = t_4$, we have

$$\mathcal{P}_{t_{1}\cdots t_{4}} = \sum_{i,j,k=1}^{m,n,p} N^{-2} \left| (\boldsymbol{x}^{(l_{0})})' Q_{.\tilde{t}_{1}}^{s_{l_{0}}t_{1}} \mathcal{A}_{ijk}^{(t_{1},t_{2})} Q_{\tilde{t}_{2}\tilde{t}_{2}}^{t_{2}t_{2}} \mathcal{A}_{ijk}^{(t_{2},t_{1})} Q_{\tilde{t}_{1}}^{t_{1}s_{l_{0}+1}} \boldsymbol{y}^{(l_{0})} \right|^{2} \\
\leq N^{-2} \operatorname{Tr}(|\boldsymbol{Q}^{t_{2}t_{2}}|^{2\circ}) \cdot (|\boldsymbol{x}^{(l_{0})}|^{\circ 2})' |\boldsymbol{Q}^{s_{l_{0}}t_{1}}|^{\circ 2} |\boldsymbol{Q}^{t_{1}s_{l_{0}+1}}|^{\circ 2} |\boldsymbol{y}^{(l_{0})}|^{\circ 2} \leq N^{-1} \|\boldsymbol{Q}\|^{2(K+2)},$$

• if $t_1 \neq t_4$, we have

$$\mathcal{P}_{t_{1}\cdots t_{4}} = \sum_{i,j,k=1}^{m,n,p} N^{-2} \left| (\boldsymbol{x}^{(l_{0})})' Q_{.\bar{t}_{1}}^{s_{l_{0}}t_{1}} \mathcal{A}_{ijk}^{(t_{1},t_{2})} Q_{\bar{t}_{2}\bar{t}_{2}}^{t_{2}t_{2}} \mathcal{A}_{ijk}^{(t_{2},t_{4})} Q_{\bar{t}_{4}}^{t_{4}s_{l_{0}+1}} \boldsymbol{y}^{(l_{0})} \right|^{2} \\
\leq N^{-2} \operatorname{Tr}(|\boldsymbol{Q}^{t_{2}t_{2}}|^{2\circ}) \cdot (|\boldsymbol{x}^{(l_{0})}|^{\circ 2})' |\boldsymbol{Q}^{s_{l_{0}}t_{1}}|^{\circ 2} |\boldsymbol{a}^{(t_{1})}|^{\circ 2} \cdot (|\boldsymbol{a}^{(t_{4})}|^{\circ 2})' |\boldsymbol{Q}^{t_{1}s_{l_{0}+1}}|^{\circ 2} |\boldsymbol{y}^{(l_{0})}|^{\circ 2} \leq N^{-1} \|\boldsymbol{Q}\|^{2(K+2)}.$$

Case 2 (D.17): for any $l_0, l_1 \in \{1, \dots, K\}$ such that $l_0 < l_1$, consider

$$\begin{split} &\mathcal{R}_{(2,1)}^{(l_0,l_1)} := \sum_{i,j,k=1}^{m,n,p} \left| (\boldsymbol{x}^{(l_0)})' \partial_{ijk}^{(1)} \boldsymbol{Q}^{s_{l_0}s_{l_0+1}} \boldsymbol{P}^{l_0l_1} \partial_{ijk}^{(1)} \boldsymbol{Q}^{s_{l_1}s_{l_1+1}} \boldsymbol{y}^{(l_0)} \right|^2 \\ &\leq C \sum_{t_1 \neq t_2} \sum_{t_3 \neq t_4} \sum_{i,j,k=1}^{m,n,p} N^{-2} \left| (\boldsymbol{x}^{(l_0)})' Q_{\cdot \tilde{t}_1}^{s_{l_0}t_1} \mathcal{A}_{ijk}^{(t_1,t_2)} Q_{\tilde{t}_2}^{t_2s_{l_0+1}} \boldsymbol{P}^{l_0l_1} Q_{\cdot \tilde{t}_3}^{s_{l_1}t_3} \mathcal{A}_{ijk}^{(t_3,t_4)} Q_{\tilde{t}_4}^{t_4s_{l_0+1}} \boldsymbol{y}^{(l_0)} \right|^2 \\ &:= C \sum_{t_1 \neq t_2} \sum_{t_3 \neq t_4} \mathcal{P}_{t_1 \cdots t_4}, \end{split}$$

where we use (D.15) and Cauchy's inequality again. In this situation, we can also show that each $\mathcal{P}_{t_1\cdots t_4} \leq N^{-1} \|\mathbf{Q}\|^{2(K+2)}$ by the same method as in Case 1, so we omit the details here. Now, notice that

$$\sum_{i,j,k=1}^{m,n,p} \left| (\boldsymbol{x}^{s_1})' \partial_{ijk}^{(2)} \Big(\prod_{l=1}^K \boldsymbol{Q}^{s_l s_{l+1}} \Big) \boldsymbol{y}^{s_{K+1}} \right|^2 \leq \sum_{l_0=1}^K \mathcal{R}_{(2,2)}^{(l_0)} + \sum_{l_0 \neq l_1}^K \mathcal{R}_{(2,1)}^{(l_0,l_1)},$$

then we can conclude Lemma D.4 for l=2.

Third derivatives: Similar as (D.16) and (D.17), for the third derivatives, we have

$$(\boldsymbol{x}^{(l_0)})'\partial_{ijk}^{(3)}\boldsymbol{Q}^{s_{l_0}s_{l_0+1}}\boldsymbol{y}^{(l_0)} = \sum_{l_0=1}^{K} (\boldsymbol{x}^{(l_0)})'\partial_{ijk}^{(3)}\boldsymbol{Q}^{s_{l_0}s_{l_0+1}}\boldsymbol{y}^{(l_0)}$$

$$+ 3\sum_{l_0< l_1}^{K} (\boldsymbol{x}^{(l_0)})'\partial_{ijk}^{(2)}\boldsymbol{Q}^{s_{l_0}s_{l_0+1}}\boldsymbol{P}^{l_0l_1}\partial_{ijk}^{(1)}\boldsymbol{Q}^{s_{l_1}s_{l_1+1}}\boldsymbol{y}^{(l_1)} + 3\sum_{l_0< l_1}^{K} (\boldsymbol{x}^{(l_0)})'\partial_{ijk}^{(1)}\boldsymbol{Q}^{s_{l_0}s_{l_0+1}}\boldsymbol{P}^{l_0l_1}\partial_{ijk}^{(2)}\boldsymbol{Q}^{s_{l_1}s_{l_1+1}}\boldsymbol{y}^{(l_1)}$$

$$+ 6\sum_{l_0< l_1< l_2}^{K} (\boldsymbol{x}^{(l_0)})'\partial_{ijk}^{(1)}\boldsymbol{Q}^{s_{l_0}s_{l_0+1}}\boldsymbol{P}^{l_0l_1}\partial_{ijk}^{(1)}\boldsymbol{Q}^{s_{l_1}s_{l_1+1}}\boldsymbol{P}^{l_1l_2}\partial_{ijk}^{(1)}\boldsymbol{Q}^{s_{l_2}s_{l_2+1}}\boldsymbol{y}^{(l_2)}. \tag{D.19}$$

Here, we only present the detailed calculation procedures for $(\boldsymbol{x}^{(l_0)})'\partial_{ijk}^{(3)}\boldsymbol{Q}^{s_{l_0}s_{l_0+1}}\boldsymbol{y}^{(l_0)}$, since others

are the same. By the Cauchy's inequality and (D.15), for any $l_0 \in \{1, \dots, K\}$, we have

$$\mathcal{R}_{(3,3)}^{(l_0)} := \sum_{i,j,k=1}^{m,n,p} \left| (\boldsymbol{x}^{(l_0)})' \partial_{ijk}^{(3)} \boldsymbol{Q}^{s_{l_0} s_{l_0+1}} \boldsymbol{y}^{(l_0)} \right|^2$$

$$\leq C \sum_{t_1 \neq t_2} \sum_{t_3 \neq t_4} \sum_{t_5 \neq t_6} \sum_{i,j,k=1}^{m,n,p} N^{-3} \left| (\boldsymbol{x}^{(l_0)})' Q_{.\tilde{t}_1}^{s_{l_0} t_1} \mathcal{A}_{ijk}^{(t_1,t_2)} Q_{\tilde{t}_2 \tilde{t}_3}^{t_2 t_3} \mathcal{A}_{ijk}^{(t_3,t_4)} Q_{\tilde{t}_4 \tilde{t}_5}^{t_4 t_5} \mathcal{A}_{ijk}^{(t_5,t_6)} Q_{\tilde{t}_6}^{t_6 s_{l_0+1}} \boldsymbol{y}^{(l_0)} \right|^2$$

$$:= C \sum_{t_1 \neq t_2} \sum_{t_3 \neq t_4} \sum_{t_5 \neq t_6} \mathcal{P}_{t_1 \cdots t_6},$$
(D.20)

where $t_1, \dots, t_6 \in \{1, 2, 3\}$. First, if both $Q_{\tilde{t}_2\tilde{t}_3}^{t_2t_3}, Q_{\tilde{t}_4\tilde{t}_5}^{t_4t_5}$ come from the off-diagonal blocks, i.e. $t_2 \neq t_3, t_4 \neq t_5$, we claim that $\mathcal{P}_{t_1 \dots t_6} \leq N^{-3} \|\boldsymbol{Q}\|^{2(K+3)}$. Let's consider the following two subcases.

• If there is no $a_{i_{t_2}}^{(t_2)}$ and $a_{i_{t_3}}^{(t_3)}$ associating with $Q_{\bar{t}_2\bar{t}_3}^{t_2t_3}$ or $a_{i_{t_4}}^{(t_4)}$ and $a_{i_{t_5}}^{(t_5)}$ associating with $Q_{\bar{t}_4\bar{t}_5}^{t_4t_5}$. Without loss of generality, assume there is no $a_{i_{t_2}}^{(t_2)}$ and $a_{i_{t_3}}^{(t_3)}$ in all $A_{ijk}^{(t_1,t_2)}$, $A_{ijk}^{(t_3,t_4)}$, $A_{ijk}^{(t_5,t_6)}$, then $A_{ijk}^{(t_1,t_2)} = A_{ijk}^{(t_3,t_4)} = A_{ijk}^{(t_5,t_6)}$, i.e. $t_1 = t_3 = t_5$, $t_2 = t_4 = t_6$ while $t_1 \neq t_2$, then it implies that

$$\mathcal{P}_{t_1\cdots t_6} = N^{-3}(|\boldsymbol{x}^{(l_0)}|^{\circ 2})'|\boldsymbol{Q}^{s_{l_0}t_1}|^{\circ 2}|\boldsymbol{Q}^{t_1t_2}|^{\circ 2}|\boldsymbol{Q}^{t_2t_3}|^{\circ 2}|\boldsymbol{Q}^{t_3s_{s_{l_0+1}}}|^{\circ 2}|\boldsymbol{y}^{(l_0)}|^{\circ 2} \leq N^{-3}\|\boldsymbol{Q}\|^{2(K+3)}.$$

• Otherwise, both $Q_{t_2t_3}^{t_2t_3}$ and $Q_{t_4t_5}^{t_4t_5}$ have at least one of $a_{it_2}^{(t_2)}, a_{it_3}^{(t_3)}$ and $a_{it_4}^{(t_4)}, a_{it_5}^{(t_5)}$ associating with itself, respectively. Since the case when $(t_2, t_3) = (t_4, t_5)$ is solved previously, let's consider the situation when there is one common t_i in (t_2, t_3) and (t_4, t_5) , i.e. $t_2 = t_5$ while $t_3 \neq t_4$, then we have $t_2 \neq t_3$ and $t_2 \neq t_4$ due to both $Q_{t_2t_3}^{t_2t_3}$ and $Q_{t_4t_5}^{t_4t_5}$ come from the off-diagonal blocks, so $A_{ijk}^{(t_3,t_4)}$ must contain $a_{it_2}^{(t_2)}$. In this case, if $A_{ijk}^{(t_1,t_2)}$ or $A_{ijk}^{(t_2,t_6)}$ contains $a_{it_3}^{(t_3)}$ or $a_{it_4}^{(t_4)}$, without loss of generality, assume there exists $a_{it_3}^{(t_3)}$, then

$$\begin{split} & \mathcal{P}_{t_1 \cdots t_6} = N^{-3} \sum_{i,j,k=1}^{m,n,p} \left| (\boldsymbol{x}^{(l_0)})' Q_{.\tilde{t}_1}^{s_{l_0}t_1} \mathcal{A}_{ijk}^{(t_1,t_2)} Q_{\tilde{t}_2\tilde{t}_3}^{t_2t_3} \mathcal{A}_{ijk}^{(t_3,t_4)} Q_{\tilde{t}_4\tilde{t}_2}^{t_4t_2} \mathcal{A}_{ijk}^{(t_2,t_6)} Q_{\tilde{t}_6}^{t_6s_{l_0+1}} \boldsymbol{y}^{(l_0)} \right|^2 \\ & \leq N^{-3} \| \boldsymbol{Q}^{t_1s_{l_0}} \boldsymbol{x}^{(l_0)} \|_2^2 \times \| \boldsymbol{Q}^{t_6s_{l_0+1}} \boldsymbol{y}^{(l_0)} \|_2^2 \times \| \boldsymbol{Q}^{t_2t_3} \boldsymbol{a}^{(t_3)} \|_2^2 \times \| \boldsymbol{Q}^{t_4t_2} \boldsymbol{a}^{(t_2)} \|_2^2 \leq N^{-3} \| \boldsymbol{Q} \|^{2(K+3)}. \end{split}$$

If not, then $t_1 = t_3 \neq t_4 = t_6$ or $t_1 = t_6 \neq t_3 = t_4$, so we have (e.g.)

$$\begin{split} & \mathcal{P}_{t_1 \cdots t_6} = N^{-3} \sum_{i,j,k=1}^{m,n,p} \left| (\boldsymbol{x}^{(l_0)})' Q_{.\tilde{t}_1}^{s_{l_0}t_1} \mathcal{A}_{ijk}^{(t_1,t_2)} Q_{\tilde{t}_2\tilde{t}_1}^{t_2t_1} \mathcal{A}_{ijk}^{(t_1,t_4)} Q_{\tilde{t}_4\tilde{t}_2}^{t_4t_2} \mathcal{A}_{ijk}^{(t_2,t_4)} Q_{\tilde{t}_4}^{t_4s_{l_0+1}} \boldsymbol{y}^{(l_0)} \right|^2 \\ & \leq N^{-3} (|\boldsymbol{x}^{(l_0)}|^{\circ 2})' |\boldsymbol{Q}^{s_{l_0}t_1}|^{\circ 2} |\boldsymbol{Q}^{t_1t_2}|^{\circ 2} |\boldsymbol{Q}^{t_2t_4}|^{\circ 2} |\boldsymbol{Q}^{t_4s_{s_{l_0+1}}}|^{\circ 2} |\boldsymbol{y}^{(l_0)}|^{\circ 2} \leq N^{-3} \|\boldsymbol{Q}\|^{2(K+3)} \end{split}$$

Finally, when there is no common t_i in (t_2, t_3) and (t_4, t_5) , since both $Q_{\tilde{t}_2 \tilde{t}_3}^{t_2 t_3}$ and $Q_{\tilde{t}_4 \tilde{t}_5}^{t_4 t_5}$ have at least one of $a_{i_{t_2}}^{(t_2)}, a_{i_{t_3}}^{(t_3)}$ and $a_{i_{t_4}}^{(t_4)}, a_{i_{t_5}}^{(t_5)}$ associating with itself, respectively, we have (e.g.)

$$\begin{split} & \mathcal{P}_{t_1 \cdots t_6} = N^{-3} \sum_{i,j,k=1}^{m,n,p} \left| (\boldsymbol{x}^{(l_0)})' Q_{.\tilde{t}_1}^{s_{l_0}t_1} \mathcal{A}_{ijk}^{(t_1,t_2)} Q_{\tilde{t}_2\tilde{t}_3}^{t_2t_3} \mathcal{A}_{ijk}^{(t_3,t_4)} Q_{\tilde{t}_4\tilde{t}_5}^{t_4t_5} \mathcal{A}_{ijk}^{(t_5,t_6)} Q_{\tilde{t}_6}^{t_6s_{l_0+1}} \boldsymbol{y}^{(l_0)} \right|^2 \\ & \leq N^{-3} \| \boldsymbol{Q}^{t_1s_{l_0}} \boldsymbol{x}^{(l_0)} \|_2^2 \times \| \boldsymbol{Q}^{t_6s_{l_0+1}} \boldsymbol{y}^{(l_0)} \|_2^2 \times \| \boldsymbol{Q}^{t_2t_3} \boldsymbol{a}^{(t_3)} \|_2^2 \times \| \boldsymbol{Q}^{t_4t_5} \boldsymbol{a}^{(t_5)} \|_2^2 \leq N^{-3} \| \boldsymbol{Q} \|^{2(K+3)}. \end{split}$$

Next, if one of $Q_{\tilde{t}_2\tilde{t}_3}^{t_2t_3}, Q_{\tilde{t}_4\tilde{t}_5}^{t_4t_5}$ comes from the diagonal blocks, e.g. $t_2 = t_3$ without loss of generality, let's consider the following two subcases.

• First, if $\mathcal{A}_{ijk}^{(t_5,t_6)}$ does not contain $a_{i_2}^{(t_2)}$, then $t_5=t_2$ or $t_6=t_2$. Suppose $t_6=t_2$, it implies that $t_4 \neq t_2$ and $t_5 \neq t_2$, since $t_4 \neq t_5$, $\mathcal{A}_{ijk}^{(t_1,t_2)}$ must contains $a_{i_{t_4}}^{(t_4)}$ or $a_{i_{t_5}}^{(t_5)}$, then we have (e.g.)

$$\mathcal{P}_{t_{1}\cdots t_{6}} = \sum_{i,j,k=1}^{m,n,p} N^{-3} \left| (\boldsymbol{x}^{(l_{0})})' Q_{.\tilde{t}_{1}}^{s_{l_{0}}t_{1}} \mathcal{A}_{ijk}^{(t_{1},t_{2})} Q_{\tilde{t}_{2}\tilde{t}_{2}}^{t_{2}t_{2}} \mathcal{A}_{ijk}^{(t_{2},t_{4})} Q_{\tilde{t}_{4}\tilde{t}_{5}}^{t_{4}t_{5}} \mathcal{A}_{ijk}^{(t_{5},t_{2})} Q_{\tilde{t}_{2}}^{t_{2}s_{l_{0}+1}} \boldsymbol{y}^{(l_{0})} \right|^{2} \\ \leq N^{-3} \|\boldsymbol{Q}^{t_{1}s_{l_{0}}} \boldsymbol{x}^{(l_{0})}\|_{2}^{2} \cdot \|\boldsymbol{Q}^{t_{5}t_{4}} \boldsymbol{a}^{(t_{4})}\|_{2}^{2} \cdot \mathbf{1}' \operatorname{diag}(|\boldsymbol{Q}^{t_{2}t_{2}}|^{\circ 2}) |\boldsymbol{Q}^{t_{2}s_{l_{0}+1}}|^{\circ 2} |\boldsymbol{y}^{(l_{0})}|^{\circ 2} \leq N^{-2} \|\boldsymbol{Q}\|^{2(K+3)}.$$

Otherwise, $t_5 = t_2$, if $\mathcal{A}_{ijk}^{(t_1,t_2)}$ and $\mathcal{A}_{ijk}^{(t_2,t_6)}$ do not contain $a_{i_{t_4}}^{(t_4)}$, then $t_1 = t_4 = t_6$ and

$$\mathcal{P}_{t_1\cdots t_6} = \sum_{i,j,k=1}^{m,n,p} N^{-3} \Big| (\boldsymbol{x}^{(l_0)})' Q_{.\tilde{t}_1}^{s_{l_0}t_1} \mathcal{A}_{ijk}^{(t_1,t_2)} Q_{\tilde{t}_2\tilde{t}_2}^{t_2t_2} \mathcal{A}_{ijk}^{(t_2,t_1)} Q_{\tilde{t}_1\tilde{t}_2}^{t_1t_2} \mathcal{A}_{ijk}^{(t_2,t_1)} Q_{\tilde{t}_1}^{t_1s_{l_0+1}} \boldsymbol{y}^{(l_0)} \Big|^2$$

$$\leq N^{-3}(|\boldsymbol{x}^{(l_0)}|^{\circ 2})'|\boldsymbol{Q}^{s_{l_0}t_1}|^{\circ 2}\operatorname{diag}(\boldsymbol{1}'\operatorname{diag}(|\boldsymbol{Q}^{t_2t_2}|^{\circ 2})|\boldsymbol{Q}^{t_2t_1}|^{\circ 2})|\boldsymbol{Q}^{t_1s_{l_0+1}}|^{\circ 2}|\boldsymbol{y}^{(l_0)}|^{\circ 2}\leq N^{-2}\|\boldsymbol{Q}\|^{2(K+3)}.$$

Finally, if $\mathcal{A}_{ijk}^{(t_1,t_2)}$ or $\mathcal{A}_{ijk}^{(t_2,t_6)}$ contains $a_{i_{t_4}}^{(t_4)}$, then

$$\mathcal{P}_{t_1 \cdots t_6} \leq N^{-3} \|\boldsymbol{Q}^{t_1 s_{l_0}} \boldsymbol{x}^{(l_0)}\|_2^2 \cdot \|\boldsymbol{Q}^{t_2 s_{l_0+1}} \boldsymbol{y}^{(l_0)}\|_2^2 \cdot \|\operatorname{diag}(\boldsymbol{Q}^{t_2 t_2}) \boldsymbol{Q}^{t_2 t_4} \boldsymbol{a}^{(t_4)}\|_2^2 \leq N^{-3} \|\boldsymbol{Q}\|^{2(K+3)} \cdot \|\boldsymbol{Q}\|^{2(K+3)}$$

• Next, if $\mathcal{A}_{ijk}^{(t_5,t_6)}$ contains $a_{i_{t_2}}^{(t_2)}$, i.e. $t_5 \neq t_2$ and $t_6 \neq t_2$. Notice that $t_4 \neq t_2$ and $t_4 \neq t_5$ due to $Q_{\tilde{t}_4\tilde{t}_5}^{t_4t_5}$ comes from off-diagonal blocks, then $\mathcal{A}_{ijk}^{(t_1,t_2)}$ must contain $a_{i_{t_4}}^{(t_4)}$ or $a_{i_{t_5}}^{(t_5)}$, so

$$\begin{split} \mathcal{P}_{t_{1}\cdots t_{6}} &= \sum_{i,j,k=1}^{m,n,p} N^{-3} \Big| (\boldsymbol{x}^{(l_{0})})' Q_{.\tilde{t}_{1}}^{s_{l_{0}}t_{1}} \mathcal{A}_{ijk}^{(t_{1},t_{2})} Q_{\tilde{t}_{2}\tilde{t}_{2}}^{t_{2}t_{2}} \mathcal{A}_{ijk}^{(t_{2},t_{4})} Q_{\tilde{t}_{4}\tilde{t}_{5}}^{t_{4}t_{5}} \mathcal{A}_{ijk}^{(t_{5},t_{6})} Q_{\tilde{t}_{6}}^{t_{6}s_{l_{0}+1}} \boldsymbol{y}^{(l_{0})} \Big|^{2} \\ &\leq N^{-3} \|\boldsymbol{Q}^{t_{1}s_{l_{0}}} \boldsymbol{x}^{(l_{0})}\|_{2}^{2} \cdot \|\boldsymbol{Q}^{t_{2}s_{l_{0}+1}} \boldsymbol{y}^{(l_{0})}\|_{2}^{2} \cdot \|\boldsymbol{Q}^{t_{5}t_{4}} \boldsymbol{a}^{(t_{4})}\|_{2}^{2} \cdot \mathbf{1}' \operatorname{diag}(|\boldsymbol{Q}^{t_{2}t_{2}}|^{\circ 2}) |\boldsymbol{a}^{(t_{2})}|^{\circ 2} \leq N^{-2} \|\boldsymbol{Q}\|^{2(K+3)}. \end{split}$$

Finally, if both of $Q_{\tilde{t}_2\tilde{t}_3}^{t_2t_3}, Q_{\tilde{t}_4\tilde{t}_5}^{t_4t_5}$ comes from the diagonal blocks, i.e. $t_2=t_3, t_4=t_5$. We have three subcases.

• Since $t_2 \neq t_4$, if both $\mathcal{A}^{(t_1,t_2)}_{ijk}$ and $\mathcal{A}^{(t_5,t_6)}_{ijk} = \mathcal{A}^{(t_4,t_6)}_{ijk}$ does not contain $a^{(t_2)}_{i_2}$ and $a^{(t_4)}_{i_{t_4}}$, then $\mathcal{A}^{(t_1,t_2)}_{ijk} = \mathcal{A}^{(t_3,t_4)}_{ijk} = \mathcal{A}^{(t_2,t_4)}_{ijk} = \mathcal{A}^{(t_5,t_6)}_{ijk} = \mathcal{A}^{(t_4,t_6)}_{ijk}$ and

$$\mathcal{P}_{t_{1}\cdots t_{6}} = \sum_{i,j,k=1}^{m,n,p} N^{-3} \left| (\boldsymbol{x}^{(l_{0})})' Q_{.\tilde{t}_{4}}^{s_{l_{0}}t_{4}} \mathcal{A}_{ijk}^{(t_{4},t_{2})} Q_{\tilde{t}_{2}\tilde{t}_{2}}^{t_{2}t_{2}} \mathcal{A}_{ijk}^{(t_{2},t_{4})} Q_{\tilde{t}_{4}\tilde{t}_{4}}^{t_{4}t_{4}} \mathcal{A}_{ijk}^{(t_{4},t_{2})} Q_{\tilde{t}_{2}}^{t_{2}s_{l_{0}+1}} \boldsymbol{y}^{(l_{0})} \right|^{2} \\
\leq N^{-3} (|\boldsymbol{x}^{(l_{0})}|^{\circ 2})' |\boldsymbol{Q}^{s_{l_{0}}t_{4}}|^{\circ 2} \operatorname{diag}(|\boldsymbol{Q}^{t_{4}t_{4}}|^{\circ 2}) \mathbf{1} \cdot \mathbf{1}' \operatorname{diag}(|\boldsymbol{Q}^{t_{2}t_{2}}|^{\circ 2}) |\boldsymbol{Q}^{t_{2}s_{l_{0}+1}}|^{\circ 2} |\boldsymbol{y}^{(l_{0})}|^{\circ 2} \leq N^{-2} \|\boldsymbol{Q}\|^{2(K+3)}.$$

• Otherwise, if there exists one of $a_{i_{t_2}}^{(t_2)}$ and $a_{i_{t_4}}^{(t_4)}$, without loss generality, assume $a_{i_{t_2}}^{(t_2)}$ exists, then $t_6 \neq t_2$ and $t_1 = t_4$. Since $t_6 \neq t_4$, then $\mathcal{A}_{ijk}^{(t_2,t_4)}$ must contain $a_{i_{t_6}}^{(t_6)}$ and we have

$$\mathcal{P}_{t_{1}\cdots t_{6}} = \sum_{i,j,k=1}^{m,n,p} N^{-3} \Big| (\boldsymbol{x}^{(l_{0})})' Q_{.\tilde{t}_{4}}^{s_{l_{0}}t_{4}} \mathcal{A}_{ijk}^{(t_{4},t_{2})} Q_{\tilde{t}_{2}\tilde{t}_{2}}^{t_{2}t_{2}} \mathcal{A}_{ijk}^{(t_{2},t_{4})} Q_{\tilde{t}_{4}\tilde{t}_{4}}^{t_{4}t_{4}} \mathcal{A}_{ijk}^{(t_{4},t_{6})} Q_{\tilde{t}_{6}}^{t_{6}s_{l_{0}+1}} \boldsymbol{y}^{(l_{0})} \Big|^{2} \\
\leq N^{-3} \mathbf{1} \operatorname{diag}(|\boldsymbol{Q}^{t_{2}t_{2}}|^{\circ 2}) |\boldsymbol{a}^{(t_{2})}|^{\circ 2} \cdot (|\boldsymbol{x}^{(l_{0})}|^{\circ 2})' |\boldsymbol{Q}^{s_{l_{0}}t_{4}}|^{\circ 2} \operatorname{diag}(|\boldsymbol{Q}^{t_{4}t_{4}}|^{\circ 2}) \mathbf{1} \cdot (|\boldsymbol{a}^{(t_{6})}|^{\circ 2})' |\boldsymbol{Q}^{t_{6}s_{l_{0}+1}}|^{\circ 2} |\boldsymbol{y}^{(l_{0})}|^{\circ 2} \\
\leq N^{-2} \|\boldsymbol{Q}\|^{2(K+3)}.$$

• Finally, when both $a_{i_{t_2}}^{(t_2)}$ and $a_{i_{t_4}}^{(t_4)}$ exists, we have

$$\mathcal{P}_{t_1 \cdots t_6} \leq N^{-3} \| \boldsymbol{Q}^{t_1 s_{l_0}} \boldsymbol{x}^{(l_0)} \|_2^2 \cdot \| \boldsymbol{Q}^{t_2 s_{l_0 + 1}} \boldsymbol{y}^{(l_0)} \|_2^2 \cdot \mathbf{1} \operatorname{diag}(|\boldsymbol{Q}^{t_2 t_2}|^{\circ 2}) |\boldsymbol{a}^{(t_2)}|^{\circ 2}$$
$$\cdot \mathbf{1} \operatorname{diag}(|\boldsymbol{Q}^{t_4 t_4}|^{\circ 2}) |\boldsymbol{a}^{(t_4)}|^{\circ 2} \leq N^{-2} \|\boldsymbol{Q}\|^{2(K+3)}.$$

Now, we have shown that each $\mathcal{P}_{t_1\cdots t_6}$ in (D.20) is bounded by $N^{-2}\|\boldsymbol{Q}\|^{2(K+3)}$. Similar as the previous arguments, for any $l_0, l_1 \in \{1, \cdots, K\}$ such that $l_0 < l_1$ or $l_0, l_1, l_2 \in \{1, \cdots, K\}$ such that $l_0 < l_1 < l_2$, we can show that

$$\mathcal{R}_{(3,2)}^{(l_0,l_1)} = \sum_{i,j,k=1}^{m,n,p} \left| (\boldsymbol{x}^{(l_0)})' \partial_{ijk}^{(2)} \boldsymbol{Q}^{s_{l_0}s_{l_0+1}} \boldsymbol{P}^{l_0l_1} \partial_{ijk}^{(1)} \boldsymbol{Q}^{s_{l_1}s_{l_1+1}} \boldsymbol{y}^{(l_1)} \right|^2 \le N^{-2} \|\boldsymbol{Q}\|^{2(K+3)}, \quad (D.21)$$

and

$$\mathcal{R}_{(3,1)}^{(l_0,l_1,l_2)} := \sum_{i,j,k=1}^{m,n,p} \left| (\boldsymbol{x}^{(l_0)})' \partial_{ijk}^{(1)} \boldsymbol{Q}^{s_{l_0}s_{l_0+1}} \boldsymbol{P}^{l_0l_1} \partial_{ijk}^{(1)} \boldsymbol{Q}^{s_{l_1}s_{l_1+1}} \boldsymbol{P}^{l_1l_2} \partial_{ijk}^{(1)} \boldsymbol{Q}^{s_{l_2}s_{l_2+1}} \boldsymbol{y}^{(l_2)} \right|^2 \le N^{-2} \|\boldsymbol{Q}\|^{2(K+3)},$$
(D.22)

here we omit the details to save space. Finally, combining (D.19), (D.20), (D.21) and (D.22), we have

$$\begin{split} &\sum_{i,j,k=1}^{m,n,p} \Big| (\boldsymbol{x}^{s_1})' \partial_{ijk}^{(3)} \Big(\prod_{l=1}^K \boldsymbol{Q}^{s_l s_{l+1}} \Big) \boldsymbol{y}^{s_{K+1}} \Big|^2 \leq \sum_{l_0=1}^K \mathcal{R}_{(3,3)}^{(l_0)} + \sum_{l_0 \neq l_2}^K \mathcal{R}_{(3,2)}^{(l_0,l_1)} + \sum_{l_0 \neq l_1 \neq l_2}^K \mathcal{R}_{(3,1)}^{(l_0,l_1,l_2)} \leq \mathcal{O}(N^{-2} \| \boldsymbol{Q} \|^{2(K+3)}), \end{split}$$
 we complete the proofs of Lemma D.4 for $l=3$.

Now, we provide the proof of Lemma D.3 as follows:

Proof of Lemma D.3. We will demonstrate the proof for equation (D.9), as the approach for proving (D.10) follows an identical strategy. Without loss of generality, we assume that $\|\boldsymbol{x}\|_2 = \|\boldsymbol{y}\|_2 = 1$. Notice that

$$m{x}'\prod_{i=1}^Km{Q}(z_i)m{y} = \sum_{s_1\cdots s_{K+1}}m{x}^{s_1}\prod_{i=1}^Km{Q}^{s_is_{i+1}}(z_i)m{y}^{s_{K+1}},$$

where $s_i \in \{1, 2, 3\}$ for $i = 1, \dots, K + 1$. Hence, we only need to show that for each given (s_1, \dots, s_{K+1}) , it has that

$$\left| (\boldsymbol{x}^{s_1})' \prod_{i=1}^K \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \boldsymbol{y}^{s_{K+1}} - \mathbb{E} \Big[(\boldsymbol{x}^{s_1})' \prod_{i=1}^K \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \boldsymbol{y}^{s_{K+1}} \Big] \right| \prec C_K \eta_0^{-(K+4)} N^{-\omega}.$$

For a sufficiently small $\delta > 0$, we split the following probability into two parts:

$$\mathbb{P}\left(\left|\boldsymbol{x}^{s_{1}}\prod_{i=1}^{K}\boldsymbol{Q}^{s_{i}s_{i+1}}(z_{i})\boldsymbol{y}^{s_{K+1}} - \mathbb{E}\left[\boldsymbol{x}^{s_{1}}\prod_{i=1}^{K}\boldsymbol{Q}^{s_{i}s_{i+1}}(z_{i})\boldsymbol{y}^{s_{K+1}}\right]\right| \geq t\right)$$

$$\leq \mathbb{P}\left(\left|\boldsymbol{x}^{s_{1}}\prod_{i=1}^{K}\boldsymbol{Q}^{s_{i}s_{i+1}}(z_{i})\boldsymbol{y}^{s_{K+1}} - \mathbb{E}\left[\boldsymbol{x}^{s_{1}}\prod_{i=1}^{K}\boldsymbol{Q}^{s_{i}s_{i+1}}(z_{i})\boldsymbol{y}^{s_{K+1}}\right]\right| \geq t, \forall X_{ijk} \leq N^{\delta}\right) \qquad (D.23)$$

$$+ \mathbb{P}\left(\left|\boldsymbol{x}^{s_{1}}\prod_{i=1}^{K}\boldsymbol{Q}^{s_{i}s_{i+1}}(z_{i})\boldsymbol{y}^{s_{K+1}} - \mathbb{E}\left[\boldsymbol{x}^{s_{1}}\prod_{i=1}^{K}\boldsymbol{Q}^{s_{i}s_{i+1}}(z_{i})\boldsymbol{y}^{s_{K+1}}\right]\right| \geq t, \exists X_{ijk} > N^{\delta}\right). \qquad (D.24)$$

For the second part (D.24), by Assumption A.1, the tail probability satisfies that

$$(D.24) \le \sum_{i,j,k=1}^{m,n,p} \mathbb{P}(|X_{ijk}| > N^{\delta}) \le N^3 \exp(-N^{\delta\theta}).$$
(D.25)

For the first part (D.23), since all X_{ijk} are bounded by N^{δ} , then we will apply the bounded differences inequality (D.3) to compute (D.23). Note that $Q^{s_i s_{i+1}}(z)$ is a differentiable function of X, denoted as $Q^{s_i s_{i+1}}(z, X)$, let X and $X^{(ijk)}$ be two random tensors that are identical for all elements except at position (i, j, k), where X_{ijk} and $X^{(ijk)}_{ijk}$ are independent and identically distributed (one can refer to Lemma D.1). By the bounded difference inequality (D.3), we have

$$(D.23) \le 4 \exp\left(-\frac{t^2}{\sum_{i,j,k=1}^{m,n,p} \Delta_{ijk}^2}\right),$$

where

$$\Delta_{ijk} := \sup_{|X_{ijk}|, |X_{ijk}^{(ijk)}| \le N^{\delta}} \left| (\boldsymbol{x}^{s_1})' \prod_{i=1}^{K} \boldsymbol{Q}^{s_i s_{i+1}}(z_i, \boldsymbol{X}^{(ijk)}) \boldsymbol{y}^{s_{K+1}} - (\boldsymbol{x}^{s_1})' \prod_{i=1}^{K} \boldsymbol{Q}^{s_i s_{i+1}}(z_i, \boldsymbol{X}) \boldsymbol{y}^{s_{K+1}} \right|.$$

By the Taylor expansion, we have

$$\Delta_{ijk} = \sup_{|X_{ijk}|, |X_{ijk}^{(ijk)}| \le N^{\delta}} \left| \sum_{l=1}^{\infty} (l!)^{-1} (\boldsymbol{x}^{s_1})' \partial_{ijk}^{(l)} \left\{ \prod_{i=1}^{K} \boldsymbol{Q}^{s_i s_{i+1}} (z_i, \boldsymbol{X}) \right\} \boldsymbol{y}^{s_{K+1}} (X_{ijk}^{(ijk)} - X_{ijk})^{l} \right| \\
\leq \sup_{|X_{ijk}|, |X_{ijk}^{(ijk)}| \le N^{\delta}} \sum_{l=1}^{\infty} (l!)^{-1} \left| (\boldsymbol{x}^{s_1})' \partial_{ijk}^{(l)} \left\{ \prod_{i=1}^{K} \boldsymbol{Q}^{s_i s_{i+1}} (z_i, \boldsymbol{X}) \right\} \boldsymbol{y}^{s_{K+1}} (X_{ijk}^{(ijk)} - X_{ijk})^{l} \right| \\
\leq \sup_{|X_{ijk}| \le N^{\delta}} \sum_{l=1}^{\infty} (l!)^{-1} 2^{l} N^{\delta l} \left| (\boldsymbol{x}^{s_1})' \partial_{ijk}^{(l)} \left\{ \prod_{i=1}^{K} \boldsymbol{Q}^{s_i s_{i+1}} (z_i, \boldsymbol{X}) \right\} \boldsymbol{y}^{s_{K+1}} \right|, \tag{D.26}$$

where we use the fact that all $|X_{ijk}|, |X_{ijk}^{(ijk)}| \leq N^{\delta}$ in (D.26). Notice that $\partial_{ijk}^{(l)} \{ \prod_{i=1}^{K} \boldsymbol{Q}^{s_i s_{i+1}}(z_i, \boldsymbol{X}) \}$ in (D.26) does not involve $\boldsymbol{X}^{(ijk)}$, we simplify $\boldsymbol{Q}^{s_i s_{i+1}}(z, \boldsymbol{X})$ by $\boldsymbol{Q}^{s_i s_{i+1}}(z)$, so does their entries. Next, we separate above Taylor expansion (D.26) into following two cases, higher derivatives $(l \geq 4)$ and lower derivatives (l = 1, 2, 3).

Case 1: When $l \geq 4$, recall that $\partial_{ijk}^{(l)} \boldsymbol{Q}(z) = (-1)^l l! (\boldsymbol{Q}(z) \partial_{ijk}^{(1)} \boldsymbol{M})^l \boldsymbol{Q}(z)$ and $\partial_{ijk}^{(1)} \boldsymbol{M}$ is defined in (D.12), which implies that $\|\partial_{ijk}^{(1)} \boldsymbol{M}\| \leq 3N^{-1/2}$ and

$$\|\partial_{ijk}^{(l)} \mathbf{Q}(z)\| \le l! \|\mathbf{Q}(z)\|^{l+1} (3N^{-1/2})^l \le l! \eta_0^{-1} (3\eta_0^{-1} N^{-1/2})^l.$$
 (D.27)

by (D.27), we have

$$\begin{aligned} &(l!)^{-1} \bigg| (\boldsymbol{x}^{s_1})' \partial_{ijk}^{(l)} \Big\{ \prod_{i=1}^K \boldsymbol{Q}^{s_i s_{i+1}}(z_i, \boldsymbol{X}) \Big\} \boldsymbol{y}^{s_{K+1}} \bigg| \leq (l!)^{-1} \bigg\| \partial_{ijk}^{(l)} \Big\{ \prod_{i=1}^K \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \Big\} \bigg\| \\ &\leq (l!)^{-1} \sum_{l_1 + \dots + l_K = l} \binom{l}{l_1, \dots, l_K} \prod_{i=1}^K \| \partial_{ijk}^{(l_i)} \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \| \leq \eta_0^{-K} \binom{l+K-1}{K-1} (3N^{-1/2} \eta_0^{-1})^l, \end{aligned}$$

where l_1, \dots, l_K such that $l_1 + \dots + l_K = l$ and $l_i \ge 0$ for $i = 1, \dots, K$, so it gives that

$$(l!)^{-1}2^{l}N^{\delta l}\Big|(\boldsymbol{x}^{s_{1}})'\partial_{ijk}^{(l)}\Big\{\prod_{i=1}^{K}\boldsymbol{Q}^{s_{i}s_{i+1}}(z_{i})\Big\}\boldsymbol{y}^{s_{d+1}}\Big| \leq \eta_{0}^{-K}\binom{l+K-1}{K-1}(6N^{-1/2+\delta}\eta_{0}^{-1})^{l}.$$

Let $q := 6N^{-1/2+\delta}\eta_0^{-1}$, it implies that

$$\sum_{l=4}^{\infty} {l+K-1 \choose K-1} q^l = \frac{1}{(K-1)!} \sum_{l=4}^{\infty} \frac{\partial^{K-1}}{\partial q^{K-1}} q^{l+K-1} = \frac{1}{(K-1)!} \frac{\partial^{K-1}}{\partial q^{K-1}} [q^{3+K} (1-q)^{-1}]$$

$$= \sum_{r=0}^{K-1} [r!(K-1-r)!]^{-1} \frac{\partial^r q^{3+K}}{\partial q^r} \frac{\partial^{(K-r-1)} (1-q)^{-1}}{\partial q^{(K-r-1)}} \le C_K q^4,$$

so we conclude that

$$\sup_{|X_{ijk}| \le N^{\delta}} \Big| \sum_{l=4}^{\infty} (l!)^{-1} 2^{l} N^{\delta l}(\boldsymbol{x}^{s_1})' \partial_{ijk}^{(l)} \Big\{ \prod_{i=1}^{K} \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \Big\} \boldsymbol{y}^{s_{K+1}} \Big| \le C_K N^{-2+4\delta} \eta_0^{-4-K},$$

and

$$\sum_{i,j,k=1}^{m,n,p} \sup_{|X_{ijk}| \le N^{\delta}} \left| \sum_{l=4}^{\infty} (l!)^{-1} (\boldsymbol{x}^{s_1})' \partial_{ijk}^{(l)} \left\{ \prod_{i=1}^{K} \boldsymbol{Q}^{s_i s_{i+1}} (z_i) \right\} \boldsymbol{y}^{s_{K+1}} \right|^2 \le C_K \eta_0^{-2(K+4)} N^{-1+8\delta}. \quad (D.28)$$

Case 2: When l = 3, by Lemma D.4, we have shown that

$$\sum_{i \ i \ k=1}^{m,n,p} \big| (\boldsymbol{x}^{s_1})' \partial_{ijk}^{(3)} \Big\{ \prod_{i=1}^K \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \Big\} \boldsymbol{y}^{s_{K+1}} \big|^2 < C_l \eta_0^{-2(l+K)} N^{-2},$$

so

$$\sum_{i,j,k=1}^{m,n,p} \left| (\boldsymbol{x}^{s_1})' \partial_{ijk}^{(3)} \left\{ \prod_{i=1}^K \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \right\} \boldsymbol{y}^{s_{K+1}} (X_{ijk}^{(ijk)} - X_{ijk})^3 \right|^2 \le C_K \eta_0^{-2(K+3)} N^{-2+6\delta}. \tag{D.29}$$

Similarly, for l = 1, 2, we have

$$\sum_{i,j,k=1}^{m,n,p} \left| (\boldsymbol{x}^{s_1})' \partial_{ijk}^{(l)} \left\{ \prod_{i=1}^K \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \right\} \boldsymbol{y}^{s_{K+1}} (X_{ijk}^{(ijk)} - X_{ijk})^l \right|^2 \le C_K \eta_0^{-2(K+l)} N^{-1+2l\delta}. \tag{D.30}$$

Finally, by the Cauchy's inequality and (D.30), (D.29) and (D.28), we have

$$\sum_{i,j,k=1}^{m,n,p} \Delta_{ijk}^{2} \leq 4 \sum_{l=1}^{3} \sum_{i,j,k=1}^{m,n,p} \sup_{|X_{ijk}| \leq N^{\delta}} \left| (l!)^{-1} 2^{l} N^{\delta l} (\boldsymbol{x}^{s_{1}})' \partial_{ijk}^{(l)} \left\{ \prod_{i=1}^{K} \boldsymbol{Q}^{s_{i}s_{i+1}} (z_{i}, \boldsymbol{X}) \right\} \boldsymbol{y}^{s_{K+1}} \right|^{2} \\
+ 4 \sum_{i,j,k=1}^{m,n,p} \sup_{|X_{ijk}| \leq N^{\delta}} \left| \sum_{l=4}^{\infty} (l!)^{-1} 2^{l} N^{\delta l} (\boldsymbol{x}^{s_{1}})' \partial_{ijk}^{(l)} \left\{ \prod_{i=1}^{K} \boldsymbol{Q}^{s_{i}s_{i+1}} (z_{i}, \boldsymbol{X}) \right\} \boldsymbol{y}^{s_{K+1}} \right|^{2} \\
\leq C_{K} \eta_{0}^{-2(K+4)} N^{-1+8\delta}.$$

Thus, we have

$$(D.23) \le 4 \exp\left(-\frac{t^2}{\sum_{i,j,k=1}^{m,n,p} \Delta_{ijk}^2}\right) \le 4 \exp\left(-C_K \eta_0^{2(K+4)} N^{1-8\delta} t^2\right),$$

combining with (D.23), (D.24) and (D.25), we conclude that

$$\mathbb{P}\left(\left|\boldsymbol{x}^{s_{1}}\prod_{i=1}^{K}\boldsymbol{Q}^{s_{i}s_{i+1}}(z_{i})\boldsymbol{y}^{s_{K+1}} - \mathbb{E}\left[\boldsymbol{x}^{s_{1}}\prod_{i=1}^{K}\boldsymbol{Q}^{s_{i}s_{i+1}}(z_{i})\boldsymbol{y}^{s_{K+1}}\right]\right| \geq t\right) \\
\leq 4\exp\left(-C_{K}\eta_{0}^{2(K+4)}N^{1-8\delta}t^{2}\right) + N^{3}\exp(-N^{\delta\theta}),$$

then choose any $t = \eta_0^{-(K+4)} N^{-1/2+4\delta+\epsilon}$, where $\epsilon \in (0, 1/2 - 4\delta)$ is a sufficiently small positive number, we can show the almost surly convergence for (D.9) by the BorelâĂŞCantelli lemma. Furthermore, for (D.10), since

$$\boldsymbol{x}' \operatorname{diag} \Big\{ \prod_{i=1}^K \boldsymbol{Q}(z_i) \Big\} \boldsymbol{y} = \sum_{s_1 \cdots s_K} \boldsymbol{x}^{s_1} \operatorname{diag} \Big\{ \prod_{i=1}^K \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \Big\} \boldsymbol{y}^{s_{K+1}},$$

where $s_1 = s_{K+1}, s_i \in \{1, 2, 3\}$ for $i = 1, \dots, K$. We only need to show

$$\left| (\boldsymbol{x}^{s_1})' \operatorname{diag} \left\{ \prod_{i=1}^K \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \right\} \boldsymbol{y}^{s_{K+1}} - \mathbb{E} \left[(\boldsymbol{x}^{s_1})' \operatorname{diag} \left\{ \prod_{i=1}^K \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \right\} \boldsymbol{y}^{s_{K+1}} \right] \right| \prec C_K \eta_0^{-(4+K)} N^{-\omega}.$$

Actually, the proof arguments are totally the same as those for (D.9), i.e. separate the following Taylor expansion

$$(\boldsymbol{x}^{s_1})' \operatorname{diag} \Big\{ \prod_{i=1}^K \boldsymbol{Q}^{s_i s_{i+1}}(z_i, \boldsymbol{X}^{ijk}) \Big\} \boldsymbol{y}^{s_{K+1}} - (\boldsymbol{x}^{s_1})' \operatorname{diag} \Big\{ \prod_{i=1}^K \boldsymbol{Q}^{s_i s_{i+1}}(z_i, \boldsymbol{X}) \Big\} \boldsymbol{y}^{s_{K+1}}$$

$$= \sum_{l=1}^{\infty} (l!)^{-1} (\boldsymbol{x}^{s_1})' \operatorname{diag} \Big\{ \partial_{ijk}^{(l)} \prod_{i=1}^K \boldsymbol{Q}^{s_i s_{i+1}}(z_i, \boldsymbol{X}) \Big\} \boldsymbol{y}^{s_{K+1}} (X_{ijk}^{ijk} - X_{ijk})^l$$

into $l \ge 4$ and l = 1, 2, 3, and we can obtain the same conclusion as (D.9), so we omit the details here.

D.1.2 Systematic treatment for minor terms in cumulant expansions

As we have mentioned before, to derive the asymptotic mean of the LSS of the matrix M, we need to compute $N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}[\partial_{ijk}^{(l)}(c_k Q_{ij}^{12} + b_j Q_{ik}^{13})]$ for l = 2, 3, 4. By (D.11), we know that

$$c_k \partial_{ijk}^{(l)} Q_{ij}^{12} = (-N^{-1/2})^l l! c_k \sum_{t_1 \cdots t_{2l}} Q_{i\tilde{t}_1}^{1t_1} \left(\prod_{\alpha=1}^{l-1} \mathcal{A}_{ijk}^{(t_{2\alpha-1}, t_{2\alpha})} Q_{\tilde{t}_{2\alpha}\tilde{t}_{2\alpha+1}}^{t_{2\alpha}t_{2\alpha+1}} \right) \mathcal{A}_{ijk}^{(t_{2l-1}, t_{2l})} Q_{\tilde{t}_{2l}j}^{t_{2l}2},$$

where $t_1 \cdots t_{2l} \in \{1, 2, 3\}$ such that $t_{2\alpha-1} \neq t_{2\alpha}$ for $\alpha = 1, \cdots, l$. To compute $\sum_{i,j,k=1}^{m,n,p} c_k \partial_{ijk}^{(l)} Q_{ij}^{12}$, it is essential to determine which terms in above equation vanish to 0 as $N \to \infty$. The following lemma will provide a criterion for distinguishing major and minor terms.

Lemma D.5. For any $z \in \mathbb{C}^+$ and $l \in \mathbb{N}^+$, let $s_1, \dots, s_{2(l+1)} \in \{1, 2, 3\}$ such that $s_{2\alpha} \neq s_{2\alpha+1}$ and $s_1 \neq s_{2(l+1)}$ for $1 \leq \alpha \leq l$, consider the following two equations:

$$\begin{cases}
\sum_{i,j,k=1}^{m,n,p} \mathcal{A}_{ijk}^{(s_1,s_{2l+2})} Q_{\tilde{s}_1\tilde{s}_2}^{s_1s_2}(z) \left(\prod_{\alpha=1}^{l} \mathcal{A}_{ijk}^{(s_{2\alpha},s_{2\alpha+1})} Q_{\tilde{s}_{2\alpha+1}\tilde{s}_{2\alpha+2}}^{s_{2\alpha+1}s_{2\alpha+2}}(z) \right), \\
\sum_{i,j,k=1}^{m,n,p} \mathcal{A}_{ijk}^{(s_{2l},s_{2l+1})} Q_{\tilde{s}_{2l+1}}^{s_{2l+1}s_1}(z) Q_{\tilde{s}_2}^{s_1s_2}(z) \left(\prod_{\alpha=1}^{l-1} \mathcal{A}_{ijk}^{(s_{2\alpha},s_{2\alpha+1})} Q_{\tilde{s}_{2\alpha+1}\tilde{s}_{2\alpha+2}}^{s_{2\alpha+1}s_{2\alpha+2}}(z) \right),
\end{cases} (D.31)$$

where $Q_{i\cdot}, Q_{\cdot i}$ means the *i*-th row and column of \mathbf{Q} , $\mathcal{A}_{ijk}^{(s_{2l}, s_{2l+1})}$ is defined in (D.6). If there is at least one terms in

$$\left\{Q_{\tilde{s}_{2\alpha-1}\tilde{s}_{2\alpha}}^{s_{2\alpha-1}s_{2\alpha}}:\alpha=1,\cdots,l+1\right\} \text{ or } \left\{Q_{\tilde{s}_{2\alpha-1}\tilde{s}_{2\alpha}}^{s_{2\alpha-1}s_{2\alpha}},Q_{\tilde{s}_{2l+1}}^{s_{2l+1}s_1}Q_{\tilde{s}_2}^{s_1s_2}:\alpha=2,\cdots,l\right\}$$

coming from the off-diagonal block, then the norms of (D.31) are bounded by $O(\|Q\|^{l+1}N)$.

In particular, we say $Q_{\tilde{s}_{2l+1}}^{s_{2l+1}s_1}Q_{\tilde{s}_2}^{s_1s_2}$ in the second equation of (D.31) comes from the off-diagonal blocks if $s_{2l+1} \neq s_2$; otherwise, it comes from the diagonal block. For the second equation in (D.31), it appears in $\partial_{ijk}^{(l)} \operatorname{Tr}(\boldsymbol{Q})$. For example,

$$\partial_{ijk}^{(1)}\operatorname{Tr}(\boldsymbol{Q}^{11}) = \sum_{i=1}^{m} \partial_{ijk}^{(1)}Q_{ii}^{11} = -N^{-1/2}\sum_{i=1}^{m} \sum_{t_1,t_2} Q_{i\tilde{t}_1}^{1t_1} \mathcal{A}_{ijk}^{(t_1,t_2)}Q_{\tilde{t}_2i}^{t_21} = -N^{-1/2}\sum_{t_1,t_2} \mathcal{A}_{ijk}^{(t_1,t_2)}Q_{\tilde{t}_2}^{t_21}Q_{\tilde{t}_1}^{1t_1},$$

where $t_1, t_2 \in \{1, 2, 3\}$ and $t_1 \neq t_2$.

Proof of Lemma D.5. In fact, the two cases in (D.31) are indeed coincide. Since $Q_{\tilde{s}_{2l+1}}^{s_{2l+1}s_1}Q_{\tilde{s}_2}^{s_1s_2}$ is just the $(\tilde{s}_{2l+1}, \tilde{s}_2)$ -th entry of $Q^{s_{2l+1}s_1}Q^{s_1s_2}$, whose spectral norm is bounded by $\|Q\|^2$. Therefore, we only consider the first case in (D.31) and rewrite it into the following form

$$\sum_{i,j,k=1}^{m,n,p} (a_i)^{n_a} (b_j)^{n_b} (c_k)^{n_c} (Q_{ii}^{11})^{n_{11}} (Q_{jj}^{22})^{n_{22}} (Q_{kk}^{33})^{n_{33}} (Q_{ij}^{12})^{n_{12}} (Q_{ik}^{13})^{n_{13}} (Q_{jk}^{23})^{n_{23}}, \tag{D.32}$$

where n_a is the number of a_i appearing in $\{\mathcal{A}_{ijk}^{(s_2,s_3)}, \cdots, \mathcal{A}_{ijk}^{(s_{2l},s_{2l+1})}, \mathcal{A}_{ijk}^{(s_{2l+2},s_1)}\}$, so does n_b and n_c . Similarly, n_{12} is the number of Q_{ij}^{12} appearing in $\{Q_{\bar{s}_{2\alpha-1}\bar{s}_{2\alpha}}^{s_{2\alpha-1}\bar{s}_{2\alpha}}: \alpha=1,\cdots,l+1\}$, so does n_{ij} for $1 \leq i \leq j \leq 3$. By definitions, we have $n_a+n_b+n_c=l+1$ and $\sum_{1\leq i\leq j\leq 3}n_{ij}=l+1$. Next, based on the number of nonzero terms in $\{n_{12},n_{13},n_{23}\}$, let's consider the following three situations.

Case 1: Suppose all n_{12}, n_{13}, n_{23} are nonzero, then we claim that at least two of n_a, n_b, n_c are nonzero. Otherwise, if $n_a = n_b = 0$ without loss of generality, then all $Q_{\tilde{s}_{2\alpha-1}\tilde{s}_{2\alpha}}^{s_{2\alpha-1}\tilde{s}_{2\alpha}}$ come from block Q^{12} , Q^{11} or Q^{22} , which is contradiction. Therefore, suppose $n_a, n_b \geq 1$ without loss of generality, then the norm of (D.32) is bounded by

$$(|\boldsymbol{a}|^{\circ n_a})' \mathrm{diag} \left(|\boldsymbol{Q}^{11}|^{\circ n_{11}} \right) \left(|\boldsymbol{Q}^{12}|^{\circ n_{12}} \circ \left(|\boldsymbol{Q}^{13}|^{\circ n_{13}} \mathrm{diag} \left(|\boldsymbol{Q}^{33}|^{\circ n_{33}} \right) |\boldsymbol{Q}^{32}|^{\circ n_{23}} \right) \right) \mathrm{diag} \left(|\boldsymbol{Q}^{22}|^{\circ n_{22}} \right) |\boldsymbol{b}|^{\circ n_b},$$
 which is smaller than $\|\boldsymbol{Q}\|^{l+1}$.

Case 2: If there are only two terms in $\{n_{12}, n_{13}, n_{23}\}$ are nonzero, without loss of generality, suppose $n_{23} = 0$ and $n_{12}, n_{13} > 0$, then at least two of n_a, n_b, n_c are nonzero; otherwise, as the arguments in Case 1, there will only be one type off-diagonal block. So we assume $n_a, n_b > 0$, and the norm of (D.31) is bounded by

$$(|\boldsymbol{b}|^{\circ n_b})' \mathrm{diag}(|\boldsymbol{Q}^{22}|^{\circ n_{22}}) |\boldsymbol{Q}^{21}|^{\circ n_{12}} \mathrm{diag}(|\boldsymbol{a}|^{\circ n_a}) \mathrm{diag}(|\boldsymbol{Q}^{11}|^{\circ n_{11}}) |\boldsymbol{Q}^{13}|^{\circ n_{13}} \mathrm{diag}(|\boldsymbol{Q}^{33}|^{\circ n_{33}}) \mathbf{1}_k,$$

which is smaller than $\|\boldsymbol{Q}\|^{l+1}N^{1/2}$.

Case 3: If there is only one term in (D.31) coming from the off-diagonal block, suppose $n_{12} > 0$, $n_{13} = n_{23} = 0$, then if $n_a, n_c > 0$ or $n_b, n_c > 0$, the norm of (D.31) is bounded by (e.g. $n_a, n_c > 0$)

$$(|\boldsymbol{a}|^{\circ n_a})' \mathrm{diag}(|\boldsymbol{Q}^{11}|^{\circ n_{11}}) |\boldsymbol{Q}^{12}|^{\circ n_{12}} \mathrm{diag}(|\boldsymbol{Q}^{22}|^{\circ n_{22}}) \mathbf{1}_n \times \mathbf{1}_p' |\boldsymbol{Q}^{33}|^{\circ n_{33}} |\boldsymbol{c}|^{\circ n_c},$$

which is smaller than $\|\mathbf{Q}\|^{l+1}N$. Otherwise, if $n_c = 0$, i.e. $n_a, n_b > 0$; the norm of (D.31) is bounded by

$$(|\boldsymbol{a}|^{\circ n_a})' \mathrm{diag}(|\boldsymbol{Q}^{11}|^{\circ n_{11}}) |\boldsymbol{Q}^{12}|^{\circ n_{12}} \mathrm{diag}(|\boldsymbol{Q}^{22}|^{\circ n_{22}}) |\boldsymbol{b}| \times \mathrm{Tr} |\boldsymbol{Q}^{33}|^{\circ n_{33}},$$

which is smaller than $\|\mathbf{Q}\|^{l+1}N$. Finally, if only one of $\{n_a, n_b, n_c\}$ is nonzero, the only possible case is that $n_c > 0, n_a = n_b = 0$. Otherwise, if $n_a > 0, n_b = n_c = 0$, then all $\mathcal{A}^{(t_{2\alpha}, t_{2\alpha+1})}, \mathcal{A}^{(s_{2\gamma}, s_{2\gamma+1})} = a_i$, it implies that $(t_{2\alpha}, t_{2\alpha+1}) = (2, 3)$ or (3, 2), so does $(s_{2\gamma}, s_{2\gamma+1})$. Hence, the only possible off-diagonal block is Q_{jk}^{23} , i.e. $n_{23} > 0$, which is a contradiction. Now, since $n_c > 0, n_a = n_b = 0$, then $n_{11}, n_{22} \geq 0$ and $n_{33} = 0$. If $n_{11}, n_{22} > 0$, (D.31) is bounded by

$$\mathbf{1}'_m \operatorname{diag}(|Q^{11}|^{\circ n_{11}})|Q^{12}|^{\circ n_{12}} \operatorname{diag}(|Q^{22}|^{\circ n_{22}})\mathbf{1}_n \le ||Q||^{l+1}N.$$

Now, we complete the proof of Lemma D.5.

For simplicity, we define two operators \mathcal{D}, \mathcal{O} as follows:

$$\mathscr{D}\left(\partial_{ijk}^{(l)}Q_{i_1i_2}^{j_1j_2}\right) := (-1)^l l! N^{-l/2} \sum_{\substack{t_1 \cdots t_l \\ t_{l+1} = j_2}} Q_{i_1i_2}^{j_1j_1} \mathcal{A}_{ijk}^{(j_1,t_1)} \left(\prod_{\alpha=1}^{l-1} Q_{i_t_{\alpha}i_t_{\alpha}}^{t_{\alpha}t_{\alpha}} \mathcal{A}_{ijk}^{(t_{\alpha},t_{\alpha+1})}\right) Q_{i_j_2i_2}^{j_2j_2}, \tag{D.33}$$

$$\mathscr{O}\left(\partial_{ijk}^{(l)}Q_{i_1i_2}^{j_1j_2}\right) := \partial_{ijk}^{(l)}Q_{i_1i_2}^{j_1j_2} - \mathscr{D}\left(\partial_{ijk}^{(l)}Q_{i_1i_2}^{j_1j_2}\right),\tag{D.34}$$

The operator \mathscr{D} is to select the summation terms in $\partial_{ijk}^{(l)}Q_{i_1i_2}^{j_1j_2}$ which only contains diagonal terms. According to Lemma D.5, when $l \geq 2$, for any $z \in \mathbb{C}^+_{\eta_0}$, we can conclude that

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \left| \mathbb{E} \left[\mathscr{O} \left(c_k Q_{ij}^{12} + b_j Q_{ik}^{13} \right) \right] \right| \le \mathcal{O}(\eta_0^{-(l+1)} N^{-(l-1)/2}),$$

thus, the major terms will only appear in $N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\mathscr{D} \left(c_k Q_{ij}^{12} + b_j Q_{ik}^{13} \right) \right]$.

Finally, when calculating the asymptotic variance of the LSS of the matrix M, we need to compute

$$\sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\partial_{ijk}^{(\alpha)}(c_k Q_{ij}^{12} + b_j Q_{ik}^{13})\partial_{ijk}^{(l-\alpha)} \{\text{Tr}(\boldsymbol{Q}^{11})\}\right], \quad l = 2, 3, 4; \alpha = 0, 1, \dots, l,$$

see (E.6) later for an example. To further determine the major terms in above equation, we need the following result.

Lemma D.6. For any $z \in \mathbb{C}_{\eta}^{+}$ and $l_{1}, l_{2} \in \mathbb{N}$ such that $l_{1} + l_{2} \geq 2$, let $t_{\alpha}, s_{\gamma} \in \{1, 2, 3\}$ such that $t_{2\alpha} \neq t_{2\alpha+1}, s_{2\gamma} \neq s_{2\gamma+1}$ for $1 \leq \alpha \leq l_{1}, 1 \leq \gamma \leq l_{2}$ and $t_{1} \neq t_{2l_{1}+2}, s_{1} \neq s_{2l_{2}+2}$, then define

$$\begin{cases} P_1(z) := \mathcal{A}_{ijk}^{(t_1,t_{2l_1+2})} Q_{it_1i_2}^{t_1t_2}(z) \left(\prod_{\alpha=1}^{l_1} \mathcal{A}_{ijk}^{(t_{2\alpha},t_{2\alpha+1})} Q_{it_{2\alpha+1}i_{2\alpha+2}}^{t_{2\alpha+1}t_{2\alpha+2}}(z) \right) \\ P_2(z) := \mathcal{A}_{ijk}^{(s_1,s_{2l_2+2})} Q_{is_1i_2}^{s_1s_2}(z) \left(\prod_{\gamma=1}^{l_2} \mathcal{A}_{ijk}^{(s_{2\gamma},s_{2\gamma+1})} Q_{is_{2\gamma+1}i_{2\gamma+2}}^{s_{2\gamma+1}s_{2\gamma+2}}(z) \right) \end{cases}$$

If there are at least one terms in

$$\left\{Q_{i_{t_{2\alpha+1}}i_{t_{2\alpha+2}}}^{t_{2\alpha+1}t_{2\alpha+2}}(z):\alpha=1,\cdots,l_{1}+1\right\}\quad\text{or}\quad \left\{Q_{i_{s_{2\gamma+1}}i_{s_{2\gamma+2}}}^{s_{2\gamma+1}s_{2\gamma+2}}(z):\gamma=1,\cdots,l_{2}+1\right\}$$

coming from the off-diagonal block, then the norm of $\sum_{i,j,k=1}^{m,n,p} P_1(z)P_2(z)$ is bounded by $O(\|Q\|^{l_1+l_2+2}N)$.

Before proving the above lemma, we need one preliminary result. By Lemma D.5, if there exists at least one off-diagonal term in (D.31), then

$$\begin{cases}
\sum_{i,j,k=1}^{m,n,p} \left| \mathcal{A}_{ijk}^{(s_{1},s_{2l+2})} Q_{\tilde{s}_{1}\tilde{s}_{2}}^{s_{1}s_{2}}(z) \left(\prod_{\alpha=1}^{l} \mathcal{A}_{ijk}^{(s_{2\alpha},s_{2\alpha+1})} Q_{\tilde{s}_{2\alpha+1}\tilde{s}_{2\alpha+2}}^{s_{2\alpha+1}s_{2\alpha+2}}(z) \right) \right|^{2} \leq \|\boldsymbol{Q}\|^{2(l+1)} N, & l \geq 1, \\
\sum_{i,j,k=1}^{m,n,p} \left| \mathcal{A}_{ijk}^{(s_{2l},s_{2l+1})} Q_{\tilde{s}_{2l+1}}^{s_{2l+1}s_{1}}(z) Q_{\cdot\tilde{s}_{2}}^{s_{1}s_{2}}(z) \left(\prod_{\alpha=1}^{l-1} \mathcal{A}_{ijk}^{(s_{2\alpha},s_{2\alpha+1})} Q_{\tilde{s}_{2\alpha+1}\tilde{s}_{2\alpha+2}}^{s_{2\alpha+1}s_{2\alpha+2}}(z) \right) \right|^{2} \leq \|\boldsymbol{Q}\|^{2(l+1)} N, & l \geq 2. \\
(D.35)
\end{cases}$$

The proofs for above two inequalities are the same as those in Lemma D.5, since we can rewrite them into the following forms:

$$\sum_{i,j,k=1}^{m,n,p} (a_i)^{2n_a} (b_j)^{2n_b} (c_k)^{2n_c} |Q_{ii}^{11}|^{2n_{11}} |Q_{jj}^{22}|^{2n_{22}} |Q_{kk}^{33}|^{2n_{33}} |Q_{ij}^{12}|^{2n_{12}} |Q_{ik}^{13}|^{2n_{13}} |Q_{jk}^{23}|^{2n_{23}}.$$

For example, when $n_{12} > 0$, $n_{13} = n_{23} = 0$ and $n_c > 0$, $n_a = n_b = 0$, we can show that the above term equals to

$$\mathbf{1}_n'|\boldsymbol{Q}^{21}|^{\circ n_{12}}\mathrm{diag}(|\boldsymbol{Q}^{11}|^{\circ 2n_{11}})|\boldsymbol{Q}^{12}|^{\circ n_{12}}\mathbf{1}_n \leq \|\boldsymbol{Q}\|^{2(l+1)}N.$$

Here, we omit details to save space.

Proof of Lemma D.6. First, if both $P_1(z)$ and $P_2(z)$ contain off-diagonal terms, by the Cauchy's inequality and (D.35), we have

$$\Big|\sum_{i,j,k=1}^{m,n,p} P_1(z)P_2(z)\Big|^2 \le \sum_{i,j,k=1}^{m,n,p} |P_1(z)|^2 \times \sum_{i,j,k=1}^{m,n,p} |P_1(z)|^2 \le C\|Q\|^{2(l_1+l_2+2)}N^2.$$

Therefore, we only need to consider the case only $P_1(z)$ contains off-diagonal terms. Similar as Lemma D.5, we can rewrite $P_1(z)P_2(z)$ as the following form:

$$\sum_{i,j,k=1}^{m,n,p} (a_i)^{n_a} (b_j)^{n_b} (c_k)^{n_c} (Q_{ii}^{11})^{n_{11}} (Q_{jj}^{22})^{n_{22}} (Q_{kk}^{33})^{n_{33}} (Q_{ij}^{12})^{n_{12}} (Q_{ik}^{13})^{n_{13}} (Q_{jk}^{23})^{n_{23}},$$

where $n_a, n_b, n_c, n_{ij} \in \mathbb{N}$, $n_a + n_b + n_c = \sum_{1 \le i \le j \le 3} n_{ij} = l_1 + l_2 + 2$. Similar as proofs of Lemma D.5, let's consider three situations based on the number of nonzero terms in $\{n_{12}, n_{23}, n_{13}\}$. Actually, we can repeat the proofs of Lemma D.5 for Case 1, 2 and 3 to derive the same conclusion, so we omit details here.

D.2 Proof of Theorem D.1

In this section, we will prove the entrywise law. For the first step, let's show that $\lim_{N\to\infty} |N^{-1}\mathbb{E}[\text{Tr}(\mathbf{Q}(z))] - g(z)| = 0$, where g(z) is defined in (C.16).

Theorem D.2. Under Assumptions A.1 and A.2, for any $z \in S_{\eta_0}$ in (C.18) and $\omega \in (1/2-\delta, 1/2)$, where $\delta > 0$ is a sufficiently small number, let

$$\boldsymbol{\varepsilon}(z) = \frac{\mathbf{c}}{\boldsymbol{m}(z)} + z + \boldsymbol{S}_3 \boldsymbol{m}(z),$$

where S_d and $\mathfrak{m}_i(z)$ are defined in (B.2) and (A.11), then we have

$$\sup_{z \in \mathcal{S}_{n_0}} \| \boldsymbol{\varepsilon}(z) \|_{\infty} = \mathcal{O}(\eta_0^{-11} N^{-2\omega}).$$

Consequently, by Theorem B.2, we obtain

$$\sup_{z \in \mathcal{S}_{\eta_0}} \| \boldsymbol{g}(z) - \boldsymbol{m}(z) \|_{\infty} = O(\eta_0^{-15} N^{-2\omega}).$$

Proof. Without loss of generality, we only prove

$$-\frac{\mathfrak{c}_1}{\mathfrak{m}_1(z)} = z + \mathfrak{m}_2(z) + \mathfrak{m}_3(z) + \mathcal{O}(\eta_0^{-11} N^{-2\omega}), \tag{D.36}$$

since the proof arguments for others are totally the same. By $MQ(z) - zQ(z) = I_N$ and the cumulant expansion (D.4), we have

$$zN^{-1}\mathbb{E}[\text{Tr}(\boldsymbol{Q}^{11}(z))] = N^{-3/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}[X_{ijk}(c_k Q_{ij}^{12}(z) + b_j Q_{ik}^{13}(z))] - \mathfrak{c}_1$$

$$= N^{-3/2} \sum_{i,j,k=1}^{m,n,p} \left(\mathbb{E}\left[\partial_{ijk}^{(1)}(c_k Q_{ij}^{12}(z) + b_j Q_{ik}^{13}(z))\right] + \epsilon_{ijk}^{(2)} \right) - \mathfrak{c}_1,$$

where the remainder $\epsilon^{(2)}_{ijk}$ satisfies that

$$|\epsilon_{ijk}^{(2)}| \le C_{\kappa_3} \sup_{z \in \mathcal{S}_{\eta_0}} |\partial_{ijk}^{(2)}(c_k Q_{ij}^{12}(z) + b_j Q_{ik}^{13}(z))|.$$

Let's first show that $\sum_{i,j,k=1}^{m,n,p} |\epsilon_{ijk}^{(2)}|$ is minor. By the definition of \mathscr{O} in (D.34) and Lemma D.5, we know that

$$N^{-3/2} \sum_{i,j,k-1}^{m,n,p} \left| c_k \mathscr{O} \left(\partial_{ijk}^{(2)} Q_{ij}^{12}(z) \right) \right| \le \mathcal{O}(\eta_0^{-3} N^{-3/2}).$$

On the other hand, based on the definition of \mathcal{D} , we have

$$N^{-3/2} \sum_{i,j,k=1}^{m,n,p} \left| c_k \mathscr{D} \left(\partial_{ijk}^{(2)} Q_{ij}^{12}(z) \right) \right| = N^{-5/2} \sum_{i,j,k=1}^{m,n,p} \left| a_i b_j c_k Q_{ii}^{11}(z) Q_{jj}^{22}(z) Q_{kk}^{33}(z) \right| \le \mathcal{O}(\eta_0^{-3} N^{-1}).$$

Next, by the direct calculation, we have

$$N^{-3/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\partial_{ijk}^{(1)}(c_k Q_{ij}^{12}(z) + b_j Q_{ik}^{13}(z)) \right] = -N^{-2} \mathbb{E} \left[\text{Tr}(\boldsymbol{Q}^{11}(z)) \, \text{Tr}(\boldsymbol{Q}^{22}(z) + \boldsymbol{Q}^{33}(z)) \right]$$

$$- N^{-2} \mathbb{E} \left[\text{Tr}(\boldsymbol{Q}^{12}(z) \boldsymbol{Q}^{21}(z) + \boldsymbol{Q}^{13}(z) \boldsymbol{Q}^{31}(z)) + 2 \, \text{Tr}(\boldsymbol{Q}^{11}(z)) \boldsymbol{b}' \boldsymbol{Q}^{23}(z) \boldsymbol{c} + 2 \boldsymbol{b}' \boldsymbol{Q}^{21}(z) \boldsymbol{Q}^{13}(z) \boldsymbol{c} \right]$$

$$- N^{-2} \mathbb{E} \left[\boldsymbol{a}' \boldsymbol{Q}^{13}(z) \boldsymbol{c} \, \text{Tr}(\boldsymbol{Q}^{22}(z)) + \boldsymbol{a}' \boldsymbol{Q}^{12}(z) \boldsymbol{b} \, \text{Tr}(\boldsymbol{Q}^{33}(z)) + \boldsymbol{a}' \boldsymbol{Q}^{12}(z) \boldsymbol{Q}^{23}(z) \boldsymbol{c} + \boldsymbol{a}' \boldsymbol{Q}^{13}(z) \boldsymbol{Q}^{32}(z) \boldsymbol{b} \right]$$

$$= - \mathbb{E} \left[\rho_1(z) (\rho_2(z) + \rho_3(z)) \right] + \mathcal{O}(\eta_0^{-2} N^{-1}),$$

where $\rho_i(z) = N^{-1} \operatorname{Tr}(\boldsymbol{Q}^{ii}(z))$. Next, by Lemma D.3, we know that $N^{-1} |\operatorname{Tr}(\boldsymbol{Q}^{ii}(z))^c| \prec \operatorname{O}(\eta_0^{-5} N^{-\omega})$, combining with the fact that $|\rho_i(z)| \leq \eta_0^{-1}$, it yields that

$$|\operatorname{Cov}(\rho_1(z), \rho_2(z))| \le \mathbb{E}[|\rho_1(z)^c||\rho_2(z)^c|] \le \eta_0^{-10} N^{-2\omega} + \eta_0^{-2} \exp(-CN^{1-2\omega}) = O(\eta_0^{-10} N^{-2\omega}),$$

so

$$\mathfrak{c}_1 + \mathfrak{m}_1(z)(z + \mathfrak{m}_2(z) + \mathfrak{m}_3(z)) = \mathcal{O}(\eta_0^{-10} N^{-2\omega}).$$

By the definition of S_{η_0} in (C.18), we know that $|\mathfrak{m}_1(z)| \geq O(\eta_0)$, so we can conclude (D.36) by dividing $\mathfrak{m}_1(z)$.

Finally, let's prove the entrywise law for d=3 as follows:

Proof of Theorem D.1. First, let's focus on the diagonal terms, e.g. $Q_{il}^{11}(z)$, by cumulant expansion (D.4), we have

$$\mathbb{E}[Q_{il}^{11}(z)] = \frac{z^{-1}}{\sqrt{N}} \sum_{j,k=1}^{n,p} \mathbb{E}[X_{ijk} \left(c_k Q_{lj}^{12}(z) + b_j Q_{lk}^{13}(z) \right)] - \delta_{il} z^{-1}$$

$$= \frac{z^{-1}}{\sqrt{N}} \sum_{j,k=1}^{n,p} \left(\mathbb{E}\left[c_k \partial_{ijk}^{(1)} Q_{lj}^{12}(z) + b_j \partial_{ijk}^{(1)} Q_{lk}^{13}(z) \right] + \epsilon_{ijk}^{(2)} \right) - \delta_{il} z^{-1},$$

where $|\epsilon_{ijk}^{(2)}| \leq C_{\kappa_3} \sup_{z \in \mathcal{S}_{\eta_0}} |\partial_{ijk}^{(2)}(c_k Q_{lj}^{12}(z) + b_j Q_{lk}^{13}(z))|$. We will show that

$$N^{-1/2} \left| \sum_{i,k=1}^{n,p} \epsilon_{ijk}^{(2)} \right| = \mathcal{O}(\eta_0^{-3} N^{-1/2} (a_i + N^{-1/2})). \tag{D.37}$$

Since $\partial_{ijk}^{(2)} \mathbf{Q}(z) = 2(\mathbf{Q}(z)\partial_{ijk}\mathbf{M}(z))^2 \mathbf{Q}(z)$, without loss of generality, let's consider

$$N^{-1/2} \sum_{j,k=1}^{n,p} c_k \partial_{ijk}^{(2)} Q_{lj}^{12} = N^{-3/2} \sum_{t_1 \neq t_2, t_3 \neq t_4}^{3} \sum_{j,k=1}^{n,p} c_k Q_{l\tilde{t}_2}^{1t_1} \mathcal{A}_{ijk}^{(t_1,t_2)} Q_{\tilde{t}_2\tilde{t}_3}^{t_2t_3} \mathcal{A}_{ijk}^{(t_3,t_4)} Q_{\tilde{t}_4j}^{t_42}, \tag{D.38}$$

where $\mathcal{A}^{(t_1,t_2)}_{ijk}$ is defined in (D.6). If $\mathcal{A}^{(t_1,t_2)}_{ijk}$, $\mathcal{A}^{(t_3,t_4)}_{ijk} \neq a_i$, suppose $\mathcal{A}^{(t_1,t_2)}_{ijk} = \mathcal{A}^{(t_3,t_4)}_{ijk} = c_k$, then all $Q^{1t_1}_{i\tilde{t}_2}$, $Q^{t_2t_3}_{\tilde{t}_2\tilde{t}_3}$, $Q^{t_42}_{\tilde{t}_4\tilde{t}_3}$ must come from Q^{11} , Q^{22} or Q^{12} and there must exist at least one off-diagonal term, which comes from Q^{12} . Here, we have two possible situations: first, all these three terms come from Q^{12} , then

$$N^{-3/2} \sum_{i,k=1}^{n,p} \left| c_k^3 Q_{ij}^{12} Q_{ij}^{12} Q_{ij}^{12} \right| \le N^{-3/2} |Q_{i\cdot}^{12}|^{\circ 2} |Q_{\cdot l}^{21}| = \mathcal{O}(\eta_0^{-3} N^{-3/2}).$$

Next, three terms come from Q^{11}, Q^{22} and Q^{12} , respectively, then

$$N^{-3/2} \sum_{j,k=1}^{n,p} \left| c_k^3 Q_{li}^{11} Q_{ij}^{12} Q_{jj}^{22} \right| \le N^{-3/2} |Q_{l\cdot}^{11}| |Q^{12}| \operatorname{diag} |Q^{22}| \mathbf{1}_n = \mathrm{O}(\eta_0^{-3} N^{-1}).$$

Otherwise, one of $\mathcal{A}_{ijk}^{(t_1,t_2)}$, $\mathcal{A}_{ijk}^{(t_3,t_4)}$ equals to c_k while the other is b_j . First, if $\mathcal{A}_{ijk}^{(t_1,t_2)} = b_j$, $\mathcal{A}_{ijk}^{(t_3,t_4)} = c_k$, then all possible situations are presented as follows:

$$N^{-3/2} \sum_{j,k=1}^{n,p} \left| c_k^2 b_j Q_{li}^{11} Q_{ki}^{31} Q_{jj}^{22} \right| \leq N^{-3/2} |Q_{l\cdot}^{11}| |Q^{13}| |c|^{\circ 2} \cdot \mathbf{1}_n \operatorname{diag} |Q^{22}| |b| = \mathrm{O}(\eta_0^{-3} N^{-1}).$$

$$N^{-3/2} \sum_{j,k=1}^{n,p} \left| c_k^2 b_j Q_{lk}^{13} Q_{ii}^{11} Q_{jj}^{22} \right| \leq N^{-3/2} |Q_{ii}^{11}| |Q_{l\cdot}^{13}| |c|^{\circ 2} \cdot \mathbf{1}_n \operatorname{diag} |Q^{22}| |b| = \mathrm{O}(\eta_0^{-3} N^{-1}).$$

$$N^{-3/2} \sum_{j,k=1}^{n,p} \left| c_k^2 b_j Q_{lk}^{13} Q_{ij}^{12} Q_{ij}^{12} \right| \leq N^{-3/2} |Q_{l\cdot}^{13}| |c|^{\circ 2} \cdot |Q_{i\cdot}^{12}|^{\circ 2} |b| = \mathrm{O}(\eta_0^{-3} N^{-3/2}).$$

$$N^{-3/2} \sum_{j,k=1}^{n,p} \left| c_k^2 b_j Q_{li}^{11} Q_{kj}^{32} Q_{ij}^{12} \right| \leq N^{-3/2} |Q_{il}^{11}| |Q_{i\cdot}^{12}| \operatorname{diag}(|b|) |Q^{23}| |c| = \mathrm{O}(\eta_0^{-3} N^{-3/2}).$$

Finally, when $\mathcal{A}_{ijk}^{(t_1,t_2)} = \mathcal{A}_{ijk}^{(t_3,t_4)} = b_j$, we can also derive that (D.38) is no more than $O(\eta_0^{-3}N^{-1})$, e.g.

$$N^{-3/2} \sum_{i,k=1}^{n,p} \left| c_k b_j^2 Q_{li}^{11} Q_{kk}^{33} Q_{ij}^{12} \right| \le N^{-3/2} |Q_{il}^{11}| |Q_{i\cdot}^{12}| |\boldsymbol{b}|^{\circ 2} \cdot \mathbf{1}_p' \operatorname{diag}(|\boldsymbol{Q}^{33}|) |\boldsymbol{c}| = \mathrm{O}(\eta_0^{-3} N^{-1}).$$

Here, we omit other situations, we can still verify that their norms are also bounded by $O(\eta_0^{-3}N^{-1})$ by similar calculations as the above equation. Now, suppose at one of $\mathcal{A}_{ijk}^{(t_1,t_2)}, \mathcal{A}_{ijk}^{(t_3,t_4)}$ equal to a_i . First, if $\mathcal{A}_{ijk}^{(t_1,t_2)} = \mathcal{A}_{ijk}^{(t_3,t_4)} = a_i$, we have the following three cases:

$$N^{-3/2} \sum_{j,k=1}^{n,p} \left| c_k a_i^2 Q_{lj}^{12} Q_{kk}^{33} Q_{jj}^{22} \right|, \ N^{-3/2} \sum_{j,k=1}^{n,p} \left| c_k a_i^2 Q_{lj}^{12} Q_{kj}^{32} Q_{kj}^{32} \right| \le \mathcal{O}(a_i^2 \eta_0^{-3} N^{-1/2}),$$

$$N^{-3/2} \sum_{j,k=1}^{n,p} \left| c_k a_i^2 Q_{lk}^{13} Q_{jk}^{23} Q_{jj}^{22} \right| \le \mathcal{O}(a_i^2 \eta_0^{-3} N^{-1}).$$

Next, if $A_{ijk}^{(t_1,t_2)} = a_i, A_{ijk}^{(t_3,t_4)} = c_k$, we have

$$\begin{split} N^{-3/2} \sum_{j,k=1}^{n,p} \left| c_k^2 a_i Q_{lj}^{12} Q_{ki}^{31} Q_{jj}^{22} \right|, \ N^{-3/2} \sum_{j,k=1}^{n,p} \left| c_k^2 a_i Q_{lk}^{13} Q_{ji}^{21} Q_{jj}^{22} \right| &\leq \mathcal{O}(a_i \eta_0^{-3} N^{-1}) \\ N^{-3/2} \sum_{j,k=1}^{n,p} \left| c_k^2 a_i Q_{lj}^{12} Q_{kj}^{32} Q_{ij}^{12} \right| &\leq \mathcal{O}(a_i \eta_0^{-3} N^{-3/2}). \end{split}$$

For other situations as $\mathcal{A}_{ijk}^{(t_1,t_2)} = c_k$, $\mathcal{A}_{ijk}^{(t_3,t_4)} = a_i$ and $\mathcal{A}_{ijk}^{(t_1,t_2)} = a_i$, $\mathcal{A}_{ijk}^{(t_3,t_4)} = b_j$ and $\mathcal{A}_{ijk}^{(t_1,t_2)} = b_j$, $\mathcal{A}_{ijk}^{(t_3,t_4)} = a_i$, we can also show that

$$\sum_{i,k=1}^{n,p} \left| c_k Q_{l\tilde{t}_2}^{1t_1} \mathcal{A}_{ijk}^{(t_1,t_2)} Q_{\tilde{t}_2\tilde{t}_3}^{t_2t_3} \mathcal{A}_{ijk}^{(t_3,t_4)} Q_{\tilde{t}_4j}^{t_42} \right| \le \mathcal{O}(a_i \eta_0^{-3} N^{-1/2}),$$

we omit details to save space. Now, we obtain that

$$N^{-1/2} \sum_{j,k=1}^{n,p} \left| c_k \partial_{ijk}^{(2)} Q_{lj}^{12} \right| \le \mathcal{O}(\eta_0^{-3} N^{-1/2} (a_i + N^{-1/2})).$$

Similarly, we can show the above conclusion is valid for $\partial_{ijk}^{(2)}Q_{lk}^{13}$ by the same argument, so we conclude that (D.37). Notice that

$$N^{-1/2} \sum_{j,k=1}^{n,p} \mathbb{E} \left[c_k \partial_{ijk}^{(1)} Q_{lj}^{12}(z) + b_j \partial_{ijk}^{(1)} Q_{lk}^{13}(z) \right] =$$

$$- N^{-1} \mathbb{E} \left[Q_{li}^{11} \operatorname{Tr} \left(\mathbf{Q}^{22} + \mathbf{Q}^{33} \right) + a_i Q_{l\cdot}^{12} \mathbf{b} \operatorname{Tr} \left(\mathbf{Q}^{33} \right) + a_i Q_{l\cdot}^{13} \mathbf{c} \operatorname{Tr} \left(\mathbf{Q}^{22} \right) \right]$$

$$- N^{-1} \mathbb{E} \left[a_i Q_{l\cdot}^{12} \mathbf{Q}^{23} \mathbf{c} + a_i Q_{l\cdot}^{13} \mathbf{Q}^{32} \mathbf{b} + Q_{i\cdot}^{12} \mathbf{b} Q_{l\cdot}^{13} \mathbf{c} + Q_{i\cdot}^{12} Q_{\cdot l}^{21} + Q_{l\cdot}^{12} \mathbf{b} Q_{i\cdot}^{13} \mathbf{c} + Q_{i\cdot}^{13} Q_{\cdot l}^{31} + 2 Q_{il}^{11} \mathbf{b}' \mathbf{Q}^{23} \mathbf{c} \right]$$

$$= - \mathbb{E} \left[Q_{li}^{11} (\rho_2(z) + \rho_3(z)) + a_i (Q_{l\cdot}^{12} \mathbf{b} \rho_3(z) + Q_{l\cdot}^{13} \mathbf{c} \rho_2(z)) \right] + O(\eta_0^{-2} N^{-1}), \tag{D.39}$$

where $Q_{i\cdot}^{12}$ and $Q_{\cdot l}^{21}$ is the *i*-th row and *l*-th column of \mathbf{Q}^{12} and \mathbf{Q}^{21} , respectively. Besides, we use the fact of

$$|a_l Q_l^{12} Q^{23} c| \le ||Q|| ||Q_l^{12}|| \le ||Q||^2$$
, $|Q_{i\cdot}^{13} c| \le ||Q|^{13} c|| \le ||Q||$, and $||Q_{i\cdot}^{12}||^2 \le ||Q^{12} Q^{21}|| \le ||Q||^2$,

so we obtain that

$$z\mathbb{E}\left[Q_{il}^{11}\right] = -\mathbb{E}\left[Q_{li}^{11}(\rho_2(z) + \rho_3(z)) + a_i(Q_{l\cdot}^{12}\boldsymbol{b}\rho_3(z) + Q_{l\cdot}^{13}\boldsymbol{c}\rho_2(z))\right] - \delta_{il} + \mathcal{O}(\eta_0^{-3}N^{-1/2}(a_i + N^{-1/2})),$$

i.e.

$$\mathbb{E}\left[(z+\rho_2(z)+\rho_3(z))Q_{il}^{11}\right] = -\mathbb{E}\left[a_i(Q_{l\cdot}^{12}\boldsymbol{b}\rho_3(z)+Q_{l\cdot}^{13}\boldsymbol{c}\rho_2(z))\right] - \delta_{il} + \mathcal{O}(\eta_0^{-3}N^{-1/2}(a_i+N^{-1/2})),$$

where $\rho_l(z) = N^{-1} \operatorname{Tr}(\boldsymbol{Q}^{ll}(z))$. Similarly, we also have

$$z\mathbb{E}\left[Q_{jl}^{22}\right] = -\mathbb{E}\left[Q_{lj}^{22}(\rho_1(z) + \rho_3(z)) + b_j(Q_{l\cdot}^{21}\boldsymbol{a}\rho_3(z) + Q_{l\cdot}^{23}\boldsymbol{c}\rho_1(z))\right] - \delta_{il} + \mathcal{O}(\eta_0^{-3}N^{-1/2}(b_j + N^{-1/2})).$$

$$z\mathbb{E}\left[Q_{kl}^{33}\right] = -\mathbb{E}\left[Q_{lk}^{33}(\rho_1(z) + \rho_2(z)) + c_k(Q_{l\cdot}^{31}\boldsymbol{a}\rho_2(z) + Q_{l\cdot}^{32}\boldsymbol{b}\rho_1(z))\right] - \delta_{il} + \mathcal{O}(\eta_0^{-3}N^{-1/2}(c_k + N^{-1/2})).$$

Next, for off-diagonal blocks such as $Q_{il}^{12}(z)$, we can repeat the previous argument to show that

$$\begin{split} z\mathbb{E}\left[Q_{il}^{12}\right] &= -\mathbb{E}\left[Q_{il}^{12}(\rho_2(z) + \rho_3(z)) + a_i(Q_{l\cdot}^{23}\boldsymbol{c}\rho_2(z) + Q_{l\cdot}^{22}\boldsymbol{b}\rho_3(z))\right] + \mathcal{O}(\eta_0^{-3}N^{-1/2}(a_i + N^{-1/2})). \\ z\mathbb{E}\left[Q_{il}^{13}\right] &= -\mathbb{E}\left[Q_{il}^{13}(\rho_2(z) + \rho_3(z)) + a_i(Q_{l\cdot}^{33}\boldsymbol{c}\rho_2(z) + Q_{l\cdot}^{32}\boldsymbol{b}\rho_3(z))\right] + \mathcal{O}(\eta_0^{-3}N^{-1/2}(b_j + N^{-1/2})). \\ z\mathbb{E}\left[Q_{jl}^{23}\right] &= -\mathbb{E}\left[Q_{il}^{23}(\rho_1(z) + \rho_3(z)) + b_j(Q_{l\cdot}^{33}\boldsymbol{c}\rho_1(z) + Q_{l\cdot}^{31}\boldsymbol{a}\rho_3(z))\right] + \mathcal{O}(\eta_0^{-3}N^{-1/2}(c_k + N^{-1/2})). \end{split}$$

Finally, by similar argument again, we have

$$\mathbb{E}\left[(z+\rho_2(z)+\rho_3(z))Q_i^{12}\boldsymbol{b}\right] = -a_i\mathbb{E}\left[\boldsymbol{b}'\boldsymbol{Q}^{23}\boldsymbol{c}\rho_2(z) + \boldsymbol{b}'\boldsymbol{Q}^{22}\boldsymbol{b}\rho_3(z)\right] + \mathcal{O}(\eta_0^{-3}N^{-1/2}(a_i+N^{-1/2})).$$

According to Lemma D.3, we have that $|(Q_{l}^{13}\boldsymbol{c})^{c}|, |(Q_{l}^{12}\boldsymbol{b})^{c}|, |(\boldsymbol{b'Q}^{23}\boldsymbol{c})^{c}|, |(\boldsymbol{b'Q}^{22}\boldsymbol{b})^{c}|, |\rho_{2}(z)^{c}|, |\rho_{3}(z)^{c}| \prec \eta_{0}^{-5}N^{-\omega}$, then

$$|\text{Cov}(\boldsymbol{b}'\boldsymbol{Q}^{22}\boldsymbol{b},\rho_{3}(z))| \leq \mathbb{E}\left[|\rho_{3}(z)^{c}(\boldsymbol{b}'\boldsymbol{Q}^{22}\boldsymbol{b})^{c}|\right] \leq \mathcal{O}(\eta_{0}^{-10}N^{-2\omega} + \|\boldsymbol{Q}\|^{2}\exp(-CN^{1-2\omega})),$$

so does others, hence we obtain that

$$(z + \mathfrak{m}_{2}(z) + \mathfrak{m}_{3}(z))\mathbb{E}[Q_{il}^{11}] = -a_{i}(\mathfrak{m}_{2}(z)\mathbb{E}[Q_{l}^{13}\boldsymbol{c}] + \mathfrak{m}_{3}(z)\mathbb{E}[Q_{l}^{12}\boldsymbol{b}]) - \delta_{il} + O(\eta_{0}^{-10}N^{-2\omega} + \eta_{0}^{-3}N^{-1/2}(a_{i} + N^{-1/2})),$$

$$(z + \mathfrak{m}_{2}(z) + \mathfrak{m}_{3}(z))\mathbb{E}[Q_{i}^{12}\boldsymbol{b}] = -a_{i}(\mathfrak{m}_{2}(z)W_{23,N}^{(3)} + \mathfrak{m}_{3}(z)W_{22,N}^{(3)}) + O(\eta_{0}^{-10}N^{-2\omega} + \eta_{0}^{-3}N^{-1/2}(a_{i} + N^{-1/2})),$$

where

$$W_{st,N}^{(3)}(z) = \mathbb{E}[(\boldsymbol{a}^{(s)})'\boldsymbol{Q}^{st}(z)\boldsymbol{a}^{(t)}], \tag{D.40}$$

for $1 \le s, t \le 3$. By Theorem D.2 and $(z + g_2(z) + g_3(z))^{-1} = -\mathfrak{c}_1^{-1}g_1(z)$, it yields that

$$\mathbb{E}[Q_{il}^{11}] = \mathfrak{c}_{1}^{-1} g_{1}(z) \left(\delta_{il} + a_{i} \left(\mathfrak{m}_{2}(z) \mathbb{E} \left[Q_{l}^{13} \mathbf{c} \right] + \mathfrak{m}_{3}(z) \mathbb{E} \left[Q_{l}^{12} \mathbf{b} \right] \right) \right) + \mathcal{O}(\eta_{0}^{-17} N^{-2\omega} + \eta_{0}^{-5} N^{-1/2} (a_{i} + N^{-1/2})),$$

$$a_{i} \mathbb{E} \left[Q_{i}^{12} \mathbf{b} \right] = a_{i}^{2} \mathfrak{c}_{1}^{-1} g_{1}(z) \left(g_{2}(z) W_{23,N}^{(d)} + g_{3}(z) W_{22,N}^{(d)} \right) + a_{i} \mathcal{O}(\eta_{0}^{-17} N^{-2\omega} + \eta_{0}^{-5} N^{-1/2} (a_{i} + N^{-1/2})).$$
(D.41)

Summing all $1 \leq i \leq n$ for $a_i \mathbb{E}\left[Q_i^{12} \boldsymbol{b}\right]$, it gives that

$$W_{12N}^{(3)} = \mathfrak{c}_1^{-1} g_1(z) \left(g_2(z) W_{23N}^{(d)} + g_3(z) W_{22N}^{(d)} \right) + \mathcal{O}(\eta_0^{-17} N^{-2\omega + 1/2} + \eta_0^{-5} N^{-1/2}), \tag{D.42}$$

since $\omega \in (1/2 - \delta, 1/2)$ and $\delta > 0$ is sufficiently small, then $2\omega - 1/2 \in (1/2 - 2\delta, 1/2)$, combining (D.41) and (D.42), we have

$$\mathbb{E}\left[Q_{i}^{12}\boldsymbol{b}\right] = a_{i}W_{12,N}^{(3)} + a_{i}O(\eta_{0}^{-17}N^{-2\omega+1/2}),$$

and we can derive the same result for $\mathbb{E}\left[Q_i^{13}\boldsymbol{c}\right]$, it concludes that

$$\mathbb{E}\left[Q_{il}^{11}\right] = \mathfrak{c}_{1}^{-1}g_{1}(z)\left[a_{i}\left(g_{3}(z)\mathbb{E}[Q_{i\cdot}^{12}\boldsymbol{b}] + g_{2}(z)\mathbb{E}[Q_{i\cdot}^{13}\boldsymbol{c}]\right) + \delta_{il}\right] + \mathcal{O}(\eta_{0}^{-17}N^{-2\omega} + \eta_{0}^{-5}N^{-1/2}(a_{i} + N^{-1/2}))$$

$$= \mathfrak{c}_{1}^{-1}g_{1}(z)\left[a_{i}^{2}\left(g_{3}(z)W_{12N}^{(3)} + g_{2}(z)W_{13N}^{(3)}\right) + \delta_{il}\right] + \mathcal{O}(\eta_{0}^{-19}N^{-2\omega+1/2}).$$

Finally, by Lemma D.3, i.e. $|(Q_{ii}^{11})^{\circ}| \prec \eta_0^{-5} N^{-\omega}$, and

$$|W_{st,N}^{(3)}(z) - W_{st}^{(3)}(z)| \le O(\eta_0^{-17} N^{-\omega}),$$

the proof of above equation is postponed to (E.38) for the simplicity of presentation, we can conclude Theorem D.1 for Q_{il}^{11} . For other cases, since the proof arguments are the same, we omit them to save space.

E Mean and covariance functions when d = 3

In this section, we will calculate the mean function $\mathbb{E}[\text{Tr}(\boldsymbol{Q}(z))] - Ng(z)$ and variance function $\text{Var}(\text{Tr}(\boldsymbol{Q}(z)))$, respectively, and these two functions will be used to calculate the asymptotic mean and variance of the LSS in §F. Recall that $\omega \in (1/2 - \delta, 1/2)$ in Lemma D.3 is a fixed constant which can be sufficiently close to 1/2, and we will not specially mention its definition frequently in this section. Next, by (D.6), the notations in (A.4) and (A.5) are equivalent to

$$\mathfrak{b}_{1}^{(1)} = \frac{1}{\sqrt{N}} \sum_{i=1}^{m} a_{i}, \quad \mathfrak{b}_{2}^{(1)} = \frac{1}{\sqrt{N}} \sum_{j=1}^{n} b_{j}, \quad \mathfrak{b}_{3}^{(1)} = \frac{1}{\sqrt{N}} \sum_{k=1}^{P} c_{k}, \tag{E.1}$$

and

$$\mathcal{B}_{(4)}^{(2,3)} = \|\boldsymbol{a}\|_{4}^{4}, \quad \mathcal{B}_{(4)}^{(1,3)} = \|\boldsymbol{b}\|_{4}^{4}, \quad \mathcal{B}_{(4)}^{(1,2)} = \|\boldsymbol{c}\|_{4}^{4}, \tag{E.2}$$

where we use the notations in (D.2).

E.1 Covariance function

Theorem E.1. Under Assumptions A.1 and A.2, for any $\eta_0 > 0$, $z_1, z_2 \in \mathcal{S}_{\eta_0}$ in (C.18), let

$$\mathcal{C}_{st,N}^{(3)}(z_1,z_2) := \operatorname{Cov}(\operatorname{Tr}(\boldsymbol{Q}^{ss}(z_1)),\operatorname{Tr}(\boldsymbol{Q}^{tt}(z_2))) \quad \text{and} \quad \boldsymbol{C}_N^{(3)}(z_1,z_2) := [\mathcal{C}_{st,N}^{(3)}(z_1,z_2)]_{3\times 3}, \quad (\text{E}.3)$$

where $s, t \in \{1, 2, 3\}$. Further define

$$\boldsymbol{F}_{N}^{(3)}(z_{1},z_{2}) = [\mathcal{F}_{st\ N}^{(3)}(z_{1},z_{2})]_{3\times3}, \quad \mathcal{F}_{st\ N}^{(3)}(z_{1},z_{2}) := 2\mathcal{V}_{st}^{(3)}(z_{1},z_{2}) + \kappa_{4}\mathcal{U}_{st\ N}^{(3)}(z_{1},z_{2}),$$

where the precise definitions of $\mathcal{V}_{st}^{(3)}(z_1, z_2)$ and $\mathcal{U}_{st,N}^{(3)}(z_1, z_2)$ are postponed to (E.43) and (E.45), respectively. Then we have

$$\lim_{N \to \infty} \|\boldsymbol{C}_N^{(3)}(z_1, z_2) - \boldsymbol{\Pi}^{(3)}(z_1, z_2)^{-1} \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1} \circ \boldsymbol{g}(z_1)) \boldsymbol{F}_N^{(3)}(z_1, z_2) \| = 0,$$
 (E.4)

where $\Pi^{(3)}(z_1, z_2)$ is defined in (B.11). Consequently, $Var(Tr(\mathbf{Q}(z)))$ is bounded by $C_{\eta_0, \mathfrak{c}}$ for any $z \in \mathcal{S}_{\eta_0}$ and

$$\lim_{N \to \infty} \left| \operatorname{Cov} \left(\operatorname{Tr}(\boldsymbol{Q}(z_1), \operatorname{Tr}(\boldsymbol{Q}(z_2)) \right) - \mathcal{C}_N^{(3)}(z_1, z_2) \right| = 0,$$

where

$$C_N^{(3)}(z_1, z_2) := \text{Cov}(\text{Tr}(\mathbf{Q}(z_1)), \text{Tr}(\mathbf{Q}(z_2))) = \mathbf{1}_3' \mathbf{C}_N^{(3)}(z_1, z_2) \mathbf{1}_3$$
 (E.5)

Proof. Without loss of generality, assume $C_{ii,N}^{(3)}(z,z) > 1$ for i = 1,2,3, otherwise $C_{ii,N}^{(3)}(z,z)$ is already bounded. Here, we only present the detailed proofs for $C_{11,N}^{(3)}(z_1,z_2)$, others are totally the same. Note that

$$\mathcal{C}_{11,N}^{(3)}(z,z) = \mathbb{E}\left[\operatorname{Tr}(\boldsymbol{Q}^{11}(z))(\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z})) - \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))])\right],$$

and $\mathbf{Q}(z)(\mathbf{M} - z\mathbf{I}_N) = \mathbf{I}_N$, we have

$$z\mathcal{C}_{11,N}^{(3)}(z,z) = \frac{1}{\sqrt{N}} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[X_{ijk} F_{ijk}^{1}(z) \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c}\right],$$

where the superscript "c" represents the centering operator and $F_{ijk}^1(z) := c_k Q_{ij}^{12}(z) + b_j Q_{ik}^{13}(z)$, then by cumulant expansion (D.4), we have

$$zC_{11,N}^{(3)}(z,z) = \frac{1}{\sqrt{N}} \sum_{i,j,k=1}^{m,n,p} \left(\sum_{l=1}^{3} \frac{\kappa_{l+1}}{l!} \mathbb{E} \left[\partial_{ijk}^{(l)} \left\{ F_{ijk}^{1}(z) \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c} \right\} \right] + \epsilon_{ijk}^{(4)} \right), \quad (E.6)$$

where the remainder term $\epsilon_{ijk}^{(4)}$ satisfies that

$$|\epsilon_{ijk}^{(4)}| \le C_{\kappa_5} \sup_{z \in \mathcal{S}_{\eta_0}} |\partial_{ijk}^{(4)} \left\{ F_{ijk}^1(z) \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^c \right\} |.$$

First derivatives: When l = 1, by direct computations, we obtain

$$\begin{split} N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\partial_{ijk}^{(1)} \left\{ F_{ijk}^{1}(z) \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c} \right\} \right] = \\ - N^{-1} \operatorname{Cov} \left(\operatorname{Tr}(\boldsymbol{Q}^{11}(z)) \operatorname{Tr}(\boldsymbol{Q}^{22}(z) + \boldsymbol{Q}^{33}(z)), \operatorname{Tr}(\boldsymbol{Q}^{11}(z)) \right) \\ - N^{-1} \operatorname{Cov} \left(\operatorname{Tr}(\boldsymbol{Q}^{12}(z) \boldsymbol{Q}^{21}(z) + \boldsymbol{Q}^{13}(z) \boldsymbol{Q}^{31}(z)), \operatorname{Tr}(\boldsymbol{Q}^{11}(z)) \right) \\ - N^{-1} \operatorname{Cov} \left(2\boldsymbol{b}' \boldsymbol{Q}^{23}(z_{1}) \boldsymbol{c} \operatorname{Tr}(\boldsymbol{Q}^{11}(z)) + \boldsymbol{a}' \boldsymbol{Q}^{13}(z) \boldsymbol{c} \operatorname{Tr}(\boldsymbol{Q}^{22}(z)) + \boldsymbol{a}' \boldsymbol{Q}^{12}(z) \boldsymbol{b} \operatorname{Tr}(\boldsymbol{Q}^{33}(z)), \operatorname{Tr}(\boldsymbol{Q}^{11}(z)) \right) \\ - N^{-1} \operatorname{Cov} \left(2\boldsymbol{b}' \boldsymbol{Q}^{21}(z) \boldsymbol{Q}^{13}(z) \boldsymbol{c} + \boldsymbol{a}' \boldsymbol{Q}^{12}(z) \boldsymbol{Q}^{23}(z) \boldsymbol{c} + \boldsymbol{a}' \boldsymbol{Q}^{13}(z) \boldsymbol{Q}^{32}(z) \boldsymbol{b}, \operatorname{Tr}(\boldsymbol{Q}^{11}(z)) \right) \\ - 2N^{-1} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}) \boldsymbol{Q}^{12}(\bar{z}) \boldsymbol{Q}^{21}(z) + \boldsymbol{Q}^{11}(\bar{z}) \boldsymbol{Q}^{13}(\bar{z}) \boldsymbol{Q}^{31}(z) \right) \right] + \operatorname{O}(\eta^{-3} N^{-1}). \end{split}$$

Here, we claim that, except

$$\begin{cases} N^{-1}\operatorname{Cov}\left(\operatorname{Tr}(\boldsymbol{Q}^{11}(z))\operatorname{Tr}(\boldsymbol{Q}^{22}(z)+\boldsymbol{Q}^{33}(z)),\operatorname{Tr}(\boldsymbol{Q}^{11}(z))\right), \\ N^{-1}\mathbb{E}\left[\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z})\boldsymbol{Q}^{12}(\bar{z})\boldsymbol{Q}^{21}(z)+\boldsymbol{Q}^{11}(\bar{z})\boldsymbol{Q}^{13}(\bar{z})\boldsymbol{Q}^{31}(z))\right], \end{cases}$$

all terms in the above equation are bounded by $O(\eta^{-6}N^{-\omega}C_{11,N}^{(3)}(z,z))$. By Lemma D.3, we have

$$N^{-1} |\operatorname{Tr}(\boldsymbol{Q}^{ii}(z))^c| \prec \eta^{-5} N^{-\omega} \text{ and } N^{-1} |\operatorname{Tr}(\boldsymbol{Q}^{ij}(z) \boldsymbol{Q}^{ji}(z))^c| \prec \eta^{-6} N^{-\omega},$$

with probability of $1 - C \exp(-CN^{1-2\omega})$, then we can imply

$$\begin{split} N^{-1} \Big| &\text{Cov} \left(\text{Tr}(\boldsymbol{Q}^{12}(z) \boldsymbol{Q}^{21}(z)), \text{Tr}(\boldsymbol{Q}^{11}(z)) \right) \Big| = N^{-1} \Big| \mathbb{E} \left[\text{Tr}(\boldsymbol{Q}^{12}(z) \boldsymbol{Q}^{21}(z))^c \text{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^c \right] \Big| \\ &= N^{-1} \Big| \mathbb{E} \left[\text{Tr}(\boldsymbol{Q}^{12}(z) \boldsymbol{Q}^{21}(z))^c \text{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^c \left(\mathbf{1}_{N^{-1}|\text{Tr}(\boldsymbol{Q}^{12}(z) \boldsymbol{Q}^{21}(z))^c| < \eta^{-6} N^{-\omega}} + \mathbf{1}_{N^{-1}|\text{Tr}(\boldsymbol{Q}^{12}(z) \boldsymbol{Q}^{21}(z))^c| \ge \eta^{-6} N^{-\omega}} \right) \right] \\ &\leq \eta^{-6} N^{-\omega} \mathcal{C}_{11,N}^{(3)}(z,z)^{1/2} + \eta^{-3} N \mathbb{P}(N^{-1}|\text{Tr}(\boldsymbol{Q}^{12}(z) \boldsymbol{Q}^{21}(z))^c| \ge \eta^{-6} N^{-\omega}) \le \mathcal{O} \left(\eta^{-6} N^{-\omega} \mathcal{C}_{11,N}^{(3)}(z,z) \right), \end{split}$$

where we use the fact that $C_{11,N}^{(3)}(z,z) > 1$. Similarly, we can also show that

$$N^{-1}\mathrm{Cov}(\boldsymbol{b'Q^{21}}(z)\boldsymbol{Q^{13}}(z)\boldsymbol{c},\mathrm{Tr}(\boldsymbol{Q^{11}}(z))),N^{-1}\mathrm{Cov}(\boldsymbol{b'Q^{23}}(z)\boldsymbol{c}\,\mathrm{Tr}(\boldsymbol{Q^{11}}(z)),\mathrm{Tr}(\boldsymbol{Q^{11}}(z))) \leq \mathrm{O}\big(\eta^{-6}N^{-\omega}\mathcal{C}_{11,N}^{(3)}(z,z)\big).$$

Moreover, note that

$$N^{-1}\text{Cov}\left(\text{Tr}(\boldsymbol{Q}^{11}(z))\,\text{Tr}(\boldsymbol{Q}^{22}(z)),\text{Tr}(\boldsymbol{Q}^{11}(z))\right)$$

$$= N^{-1}\mathbb{E}\left[\left(\text{Tr}(\boldsymbol{Q}^{11}(z))\,\text{Tr}(\boldsymbol{Q}^{22}(z)) - \mathbb{E}[\text{Tr}(\boldsymbol{Q}^{11}(z))]\,\text{Tr}(\boldsymbol{Q}^{22}(z))\right.$$

$$+ \mathbb{E}[\text{Tr}(\boldsymbol{Q}^{11}(z))]\,\text{Tr}(\boldsymbol{Q}^{22}(z)) - \mathbb{E}[\text{Tr}(\boldsymbol{Q}^{11}(z))]\mathbb{E}[\text{Tr}(\boldsymbol{Q}^{22}(z))]\right.$$

$$+ \mathbb{E}[\text{Tr}(\boldsymbol{Q}^{11}(z))]\mathbb{E}[\text{Tr}(\boldsymbol{Q}^{22}(z))] - \mathbb{E}[\text{Tr}(\boldsymbol{Q}^{11}(z))\,\text{Tr}(\boldsymbol{Q}^{22}(z))]\right)\,\text{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c}\right]$$

$$= \mathfrak{m}_{1}(z)\text{Cov}\left(\text{Tr}(\boldsymbol{Q}^{22}(z)),\text{Tr}(\boldsymbol{Q}^{11}(z))\right) + N^{-1}\mathbb{E}\left[\text{Tr}(\boldsymbol{Q}^{22}(z))|\,\text{Tr}(\boldsymbol{Q}^{11}(z))^{c}|^{2}\right], \qquad (E.7)$$

where $\mathfrak{m}_i(z) = N^{-1}\mathbb{E}[\text{Tr}(\boldsymbol{Q}^{ii}(z))], \rho_i(z) = N^{-1}\text{Tr}(\boldsymbol{Q}^{ii}(z))$ are defined in (A.11), and $|\rho_2(z)^c| \leq \eta^{-5}N^{-\omega}$ with probability of $1 - C\exp(-CN^{1-2\omega})$ by Lemma D.3, then we have

$$\begin{split} & \left| N^{-1} \mathbb{E} \left[\text{Tr}(\boldsymbol{Q}^{22}(z)) | \text{Tr}(\boldsymbol{Q}^{11}(z))^c |^2 \right] - \mathfrak{m}_2(z) \mathcal{C}_{11,N}^{(3)}(z,z) \right| = \left| \mathbb{E} \left[\rho_2(z)^c | \text{Tr}(\boldsymbol{Q}^{11}(z))^c |^2 \right] \right| \\ & \leq \eta^{-5} N^{-\omega} \mathcal{C}_{11,N}^{(3)}(z,z) + \mathbb{E} \left[\left| \rho_2(z)^c | 1_{|\rho_2(z)^c| \geq \eta_0^{-4} N^{-\omega}} | \text{Tr}(\boldsymbol{Q}^{11}(z))^c |^2 \right] \\ & \leq \eta^{-5} N^{-\omega} \mathcal{C}_{11,N}^{(3)}(z,z) + \eta^{-3} N^2 \exp(-CN^{1-2\omega}) \leq \mathcal{O}(\eta^{-5} N^{-\omega} \mathcal{C}_{11,N}^{(3)}(z,z)). \end{split}$$

In summary, we obtain that

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\partial_{ijk}^{(1)} \left\{ F_{ijk}^{1}(z) \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c} \right\} \right] = -2 \mathcal{V}_{11,N}^{(3)}(z,\bar{z}) + \operatorname{O}(\eta^{-3}N^{-1})$$

$$- \mathfrak{m}_{1}(z) \left[\mathcal{C}_{2,1}(z,z) + \mathcal{C}_{3,1}(z,z) \right] - (\mathfrak{m}_{2}(z) + \mathfrak{m}_{3}(z) + \operatorname{O}(\eta^{-5}N^{-\omega})) \mathcal{C}_{11,N}^{(3)}(z,z),$$
 (E.8)

where

$$\mathcal{V}_{ij,N}^{(3)}(z_1, z_2) := N^{-1} \sum_{l \neq i}^{3} \mathbb{E}[\text{Tr}(\mathbf{Q}^{ij}(z_2) \mathbf{Q}^{jl}(z_2) \mathbf{Q}^{li}(z_1))]$$
 (E.9)

for $i, j \in \{1, 2, 3\}$. Readers can refer to §E.3 for proofs of $\lim_{N\to\infty} \mathcal{V}_{ij,N}^{(3)}(z_1, z_2) = \mathcal{V}_{ij}^{(3)}(z_1, z_2)$ in (E.43).

Second derivatives: When l = 2, since

$$\partial_{ijk}^{(2)} \left\{ F_{ijk}^{1}(z) \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c} \right\} = \sum_{\alpha=0}^{2} {2 \choose \alpha} \partial_{ijk}^{(2-\alpha)} \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c} \partial_{ijk}^{(\alpha)} F_{ijk}^{1}(z),$$

and $\partial^{(l)}_{ijk} \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))$ have the following expression by Lemma D.5:

$$\partial_{ijk}^{(l)}\operatorname{Tr}(\boldsymbol{Q}^{11}) = (-1)^{l} l! N^{-l/2} \mathcal{A}_{ijk}^{(t_{2l}, t_{2l+1})} Q_{\tilde{t}_{2l+1}}^{t_{2l+1}} Q_{\tilde{t}_{2}}^{1t_{2}} \prod_{\alpha=2}^{l} \mathcal{A}_{ijk}^{(t_{2\alpha-2}, t_{2\alpha-1})} Q_{\tilde{t}_{2\alpha-1}\tilde{t}_{2\alpha}}^{t_{2\alpha-1}t_{2\alpha}}, \text{ for } l \geq 2,$$

and

$$\partial_{ijk}^{(1)}\operatorname{Tr}(\boldsymbol{Q}^{11}) = -2N^{-1/2}(a_iQ_{j\cdot}^{21}Q_{\cdot k}^{13} + b_jQ_{i\cdot}^{11}Q_{\cdot k}^{13} + c_kQ_{i\cdot}^{11}Q_{\cdot j}^{12}) := -2N^{-1/2}(a_iP_{jk}^{23} + b_jP_{ik}^{13} + c_kP_{ij}^{12}),$$

where $Q_{\cdot i}$ and Q_i represent the *i*-th column and row of \boldsymbol{Q} and $P_{\tilde{t}_{2l+1}\tilde{t}_2}^{t_{2l+1}t_2} := Q_{\tilde{t}_{2l+1}}^{t_{2l+1}t_2}Q_{\cdot \tilde{t}_2}^{1t_2}$, it implies that $\partial_{ijk}^{(1)}\operatorname{Tr}(\boldsymbol{Q}^{11})$ only contains off-diagonal parts. By the definitions of operators \mathscr{D},\mathscr{O} in (D.33), (D.34) and Lemma D.5, we know that $|F_{ijk}^1(z)| \leq \mathrm{O}(\eta^{-1})$ and

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\left|F_{ijk}^{1}(z)\mathscr{O}\left(\partial_{ijk}^{(2)}\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c}\right)\right|\right]$$

$$\leq \eta^{-1} N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\left|\mathscr{O}\left(\partial_{ijk}^{(2)}\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c}\right)\right|\right] \leq O(\eta^{-4}N^{-1/2}). \tag{E.10}$$

Next, for

$$\begin{split} N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\left|F_{ijk}^{1}(z)\mathscr{D}\left(\partial_{ijk}^{(2)}\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c}\right)\right|\right] \\ &= 6N^{-3/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\left|F_{ijk}^{1}(z)(a_{i}^{2}P_{jj}^{22}(z)Q_{kk}^{33}(z) + b_{j}^{2}P_{ii}^{11}(z)Q_{kk}^{33}(z) + c_{k}^{2}P_{ii}^{11}(z)Q_{jj}^{22}(z))\right|\right], \end{split}$$

we can show that the above equation is bounded by $O(\eta^{-4}N^{-1/2})$. For example, we have

$$N^{-3/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\left|F_{ijk}^{1}(z)b_{j}^{2}P_{ii}^{11}(z)Q_{kk}^{33}(z)\right|\right]$$

$$\leq N^{-3/2} \left(\mathbf{1}'_{m} \operatorname{diag}(|\boldsymbol{P}^{11}|)|\boldsymbol{Q}^{13}|\operatorname{diag}(|\boldsymbol{Q}^{33}|)\mathbf{1}_{k} + \mathbf{1}'_{m} \operatorname{diag}(|\boldsymbol{P}^{11}|)|\boldsymbol{Q}^{12}||\boldsymbol{b}| \times \mathbf{1}_{k} \operatorname{diag}(|\boldsymbol{Q}^{13}|)|\boldsymbol{c}|\right)$$

$$\leq O(\eta^{-4}N^{-1/2}), \tag{E.11}$$

the calculations for other terms are the same, we omit details here. For the $\partial_{ijk}^{(1)} F_{ijk}^1(z) \partial_{ijk}^{(1)} \operatorname{Tr}(\boldsymbol{Q}(\bar{z}))^c$, since we know that $|\partial_{ijk}^{(1)} \operatorname{Tr}(\boldsymbol{Q}(\bar{z}))| = \mathrm{O}(\eta^{-2}N^{-1/2})$, then by Lemma D.5, it implies that

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\left|\partial_{ijk}^{(1)} \operatorname{Tr}(\boldsymbol{Q}(\bar{z}))^{c} \mathcal{O}\left(\partial_{ijk}^{(1)} F_{ijk}^{1}(z)\right)\right|\right]$$

$$\leq \eta^{-2} N^{-1} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\left|\mathcal{O}\left(\partial_{ijk}^{(1)} F_{ijk}^{1}(z)\right)\right|\right] \leq O(\eta^{-4} N^{-1/2}).$$
(E.12)

By the same arguments as those in (E.11), we can derive that

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\left|\partial_{ijk}^{(1)} \operatorname{Tr}(\boldsymbol{Q}(\bar{z}))^{c} \mathscr{D}\left(\partial_{ijk}^{(1)} F_{ijk}^{1}(z)\right)\right|\right] \leq \mathrm{O}(\eta^{-4} N^{-1/2}).$$

Finally, let's consider

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c} \mathcal{D}\left(\partial_{ijk}^{(2)} F_{ijk}^{1}(z)\right)\right]$$

$$= 4N^{-3/2} \mathbb{E}\left[\mathbf{1}'_{m} \operatorname{diag}(\boldsymbol{Q}^{11}(z)) \boldsymbol{a} \mathbf{1}'_{n} \operatorname{diag}(\boldsymbol{Q}^{22}(z)) \boldsymbol{b} \mathbf{1}'_{p} \operatorname{diag}(\boldsymbol{Q}^{33}(z)) \boldsymbol{c} \times \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c}\right]$$

$$= 4N^{-3/2} \mathbb{E}\left[\mathbf{1}'_{m} \operatorname{diag}(\boldsymbol{Q}^{11}(z)) \boldsymbol{a} \mathbf{1}'_{n} \operatorname{diag}(\boldsymbol{Q}^{22}(z)) \boldsymbol{b} \mathbf{1}'_{p} \operatorname{diag}(\boldsymbol{Q}^{33}(z)) \boldsymbol{c}\right]^{c} \times \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c}.$$

$$= 4N^{-3/2} \mathbb{E}\left[\mathbf{1}'_{m} \operatorname{diag}(\boldsymbol{Q}^{11}(z)) \boldsymbol{a} \mathbf{1}'_{n} \operatorname{diag}(\boldsymbol{Q}^{22}(z)) \boldsymbol{b} \mathbf{1}'_{n} \operatorname{diag}(\boldsymbol{Q}^{33}(z)) \boldsymbol{c}\right]^{c} \times \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c}.$$

For simplicity, let $H_N^{(1)}(z) := N^{-1/2}(\mathbf{1}_m' \mathrm{diag}(\mathbf{Q}^{11}(z))\mathbf{a})^c$ and so does $H_N^{(2)}(z), H_N^{(3)}(z)$, then

$$\begin{split} (H_N^{(1)}H_N^{(2)}H_N^{(3)})^c &= (H_N^{(1)})^c H_N^{(2)}H_N^{(3)} + \mathbb{E}[H_N^{(1)}](H_N^{(2)}H_N^{(3)})^c + \mathbb{E}[H_N^{(1)}(H_N^{(2)}H_N^{(3)})^c], \\ (H_N^{(2)}H_N^{(3)})^c &= (H_N^{(2)})^c H_N^{(3)} + \mathbb{E}[H_N^{(2)}](H_N^{(3)})^c + \mathbb{E}[H_N^{(3)}(H_N^{(3)})^c]. \end{split}$$

By Lemma D.3, $H_N^{(1)}(z), H_N^{(2)}(z), H_N^{(3)}(z) \prec \mathcal{O}(\eta^{-5}N^{-\omega})$, so $|(H_N^{(1)}H_N^{(2)}H_N^{(3)})^c| \prec \mathcal{O}(\eta^{-7}N^{-\omega})$ and

$$N^{-1/2} \Big| \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^c \mathscr{D} \left(\partial_{ijk}^{(2)} F_{ijk}^1(z) \right) \right] \Big| \leq \mathcal{O}(\eta^{-7} N^{-\omega} \mathcal{C}_{1,1}(z,z)).$$

Similarly, by the previous arguments, we can also show that

$$N^{-1/2} \Big| \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\text{Tr}(\mathbf{Q}^{11}(\bar{z}))^c \mathscr{O}(\partial_{ijk}^{(2)} F_{ijk}^1(z)) \right] \Big| \le \mathcal{O}(\eta^{-7} N^{-\omega} \mathcal{C}_{1,1}(z,z)),$$

here we omit the detail to save space. As a result, we obtain

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\partial_{ijk}^{(2)} \left\{ F_{ijk}^{1}(z) \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z})) \right\} \right] = O(\eta^{-7} N^{-\omega} C_{11,N}^{(3)}(z,z) + \eta^{-4} N^{-1/2}).$$
 (E.14)

Third derivatives: When l = 3, let's consider

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\partial_{ijk}^{(3-\alpha)} \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^c \partial_{ijk}^{(\alpha)} F_{ijk}^1(z)\right], \text{ where } \alpha = 0, 1, \dots, 3.$$

Here, we claim that the major terms appears only when $\alpha = 1$. First, when $\alpha = 3$, similar as (E.13), we can show that

$$\begin{split} N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[& \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c} \mathscr{D}(\partial_{ijk}^{(3)} F_{ijk}^{1}(z)) \right] \\ &= -N^{-2} \mathbb{E} \left[& \operatorname{Tr}(\boldsymbol{Q}^{11}(z)^{\circ 2}) \left(\|\boldsymbol{c}\|_{4}^{4} \operatorname{Tr}(\boldsymbol{Q}^{22}(z)^{\circ 2}) + \|\boldsymbol{b}\|_{4}^{4} \operatorname{Tr}(\boldsymbol{Q}^{33}(z)^{\circ 2}) \right) \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c} \right] + \operatorname{O}(\eta^{-5} N^{-1/2}) \\ &= \operatorname{O}(\eta^{-8} N^{-\omega} \mathcal{C}_{11,N}^{(3)}(z,z)) + \operatorname{O}(\eta^{-5} N^{-1/2}), \end{split}$$

where $N^{-1}\operatorname{Tr}(\boldsymbol{Q}^{ll}(z)^{\circ 2})^c \prec \eta^{-6}N^{-\omega}$ by Lemma D.3, and so does

$$N^{-1/2} \Big| \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\text{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^c \mathscr{O}(\partial_{ijk}^{(3)} F_{ijk}^1(z)) \right] \Big| \le \mathcal{O}(\eta^{-8} N^{-\omega} \mathcal{C}_{11,N}^{(3)}(z,z)).$$

Besides, when $\alpha = 0$ and $\alpha = 2$, similar as (E.10) and (E.12), we can show that

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\left| F_{ijk}^1(z) \mathscr{O} \left(\partial_{ijk}^{(3)} \operatorname{Tr} (\boldsymbol{Q}^{11}(\bar{z}))^c \right) \right| \right], N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\left| \partial_{ijk}^{(1)} \operatorname{Tr} (\boldsymbol{Q}^{11}(\bar{z}))^c \mathscr{O} \left(\partial_{ijk}^{(2)} F_{ijk}^1(z) \right) \right| \right] \leq \mathcal{O}(\eta^{-5} N^{-1}).$$

Moreover, since $|F^1_{ijk}(z)| \leq \mathcal{O}(\eta^{-1}), |\partial^{(1)}_{ijk} \operatorname{Tr}(\boldsymbol{Q}(\bar{z}))| \leq \mathcal{O}(\eta^{-2}N^{-1/2})$, then it gives that

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\left|F_{ijk}^{1}(z)\mathcal{D}\left(\partial_{ijk}^{(3)}\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c}\right)\right|\right]$$

$$\leq \eta^{-1} N^{-2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\left|a_{i}b_{j}c_{k}(Q_{ii}^{11}(\bar{z}))^{2}Q_{jj}^{22}(\bar{z})Q_{kk}^{33}(\bar{z})\right|\right] = O(\eta^{-5}N^{-1/2}), \tag{E.15}$$

and

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\left|\partial_{ijk}^{(1)} \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c} \mathscr{D}\left(\partial_{ijk}^{(2)} F_{ijk}^{1}(z)\right)\right|\right]$$

$$\leq 2\eta^{-2} N^{-2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\left|a_{i} b_{j} c_{k} Q_{ii}^{11}(z) Q_{jj}^{22}(z) Q_{kk}^{33}(z)\right|\right] = \mathcal{O}(\eta^{-5} N^{-1/2}). \tag{E.16}$$

Therefore, we only need to consider $\alpha=1$, i.e. $\partial_{ijk}^{(2)}\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))\partial_{ijk}^{(1)}F_{ijk}^{1}(z)$, by Lemma D.6, we have

$$\begin{split} N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\partial_{ijk}^{(2)} \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z})) \partial_{ijk}^{(1)} F_{ijk}^{1}(z) \right] = \\ N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\mathcal{D} \left(\partial_{ijk}^{(2)} \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z})) \right) \mathcal{D} \left(\partial_{ijk}^{(1)} F_{ijk}^{1}(z) \right) \right] + \operatorname{O}(\eta^{-5} N^{-1/2}) = \\ -2N^{-2} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{11}(z) \operatorname{diag}(\boldsymbol{Q}^{11}(\bar{z})^{2})) \left(\|\boldsymbol{c}\|_{4}^{4} \operatorname{Tr}(\operatorname{diag}(|\boldsymbol{Q}^{22}(z)|^{\circ 2})) + \|\boldsymbol{b}\|_{4}^{4} \operatorname{Tr}(\operatorname{diag}(|\boldsymbol{Q}^{33}(z)|^{\circ 2})) \right) \right] \\ -2N^{-2} \mathbb{E} \left[\|\boldsymbol{c}\|_{4}^{4} \operatorname{Tr}(\boldsymbol{Q}^{22}(z) \operatorname{diag}(\boldsymbol{Q}^{21}(\bar{z}) \boldsymbol{Q}^{12}(\bar{z}))) \operatorname{Tr}(\boldsymbol{Q}^{11}(z) \operatorname{diag}(\boldsymbol{Q}^{11}(\bar{z}))) \right] \\ -2N^{-2} \mathbb{E} \left[\|\boldsymbol{b}\|_{4}^{4} \operatorname{Tr}(\boldsymbol{Q}^{33}(z) \operatorname{diag}(\boldsymbol{Q}^{31}(\bar{z}) \boldsymbol{Q}^{13}(\bar{z}))) \operatorname{Tr}(\boldsymbol{Q}^{11}(z) \operatorname{diag}(\boldsymbol{Q}^{11}(\bar{z}))) \right] + \operatorname{O}(\eta^{-5} N^{-1/2}). \end{split}$$

Therefore, we finally obtain

$$\frac{\kappa_4}{6\sqrt{N}} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\partial_{ijk}^{(3)} \left\{ F_{ijk}^{1}(z) \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z})) \right\} \right]
= -\kappa_4 \widetilde{\mathcal{U}}_{11,N}^{(3)}(z,\bar{z}) + \mathcal{O}(\eta^{-5} N^{-1/2} + \eta^{-8} N^{-\omega} \mathcal{C}_{11,N}^{(3)}(z,z)),$$
(E.17)

where $\{i, j, k\} = \{1, 2, 3\}$ and $\boldsymbol{a}^{(l)}$ is defined in (D.2) and

$$\widetilde{\mathcal{U}}_{ij,N}^{(3)}(z_1, z_2) := N^{-2} \|\boldsymbol{a}^{(k)}\|_{4}^{4} \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{ii}(z_1) \circ \boldsymbol{Q}^{ii}(z_2)) \operatorname{Tr}(\boldsymbol{Q}^{jj}(z_1) \circ \boldsymbol{Q}^{jj}(z_2) \boldsymbol{Q}^{jj}(z_2))] \\
+ N^{-2} \|\boldsymbol{a}^{(k)}\|_{4}^{4} \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{jj}(z_1) \circ \boldsymbol{Q}^{jj}(z_2)) \operatorname{Tr}(\boldsymbol{Q}^{ii}(z_1) \circ (\boldsymbol{Q}^{ij}(z_2) \boldsymbol{Q}^{ji}(z_2)))] \\
+ N^{-2} \|\boldsymbol{a}^{(j)}\|_{4}^{4} \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{ii}(z_1) \circ \boldsymbol{Q}^{ii}(z_2)) \operatorname{Tr}(\boldsymbol{Q}^{kk}(z_1) \circ \boldsymbol{Q}^{kj}(z_2) \boldsymbol{Q}^{jk}(z_2))] \\
+ N^{-2} \|\boldsymbol{a}^{(j)}\|_{4}^{4} \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{kk}(z_1) \circ \boldsymbol{Q}^{kk}(z_2)) \operatorname{Tr}(\boldsymbol{Q}^{ii}(z_1) \circ (\boldsymbol{Q}^{ij}(z_2) \boldsymbol{Q}^{ji}(z_2)))]. \tag{E.18}$$

Readers can further refer to §E.3 for proofs of $\lim_{N\to\infty} \widetilde{\mathcal{U}}_{ij,N}^{(3)}(z_1,z_2) - \mathcal{U}_{ij,N}^{(3)}(z_1,z_2) = 0$ in (E.45).

Remainders: We claim that:

$$N^{-1/2} \left| \sum_{i,i,k=1}^{m,n,p} \mathbb{E} \left[\partial_{ijk}^{(\alpha)} F_{ijk}^{1}(z) \partial_{ijk}^{(4-\alpha)} \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^{c} \right] \right| \leq \mathcal{O}(\eta^{-6} N^{-1/2}), \ \alpha = 0, 1, \dots, 4.$$
 (E.19)

First, when $\alpha = 4$, since $|\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))| \leq O(\eta^{-1}N)$ and $\sum_{i,j,k=1}^{m,n,p} |\partial_{ijk}^{(4)} F_{ijk}^1(z)| \leq O(\eta^{-5}N^{-3/2})$ by (E.34) later, it implies that

$$N^{-1/2} \Big| \sum_{i,j,k=1}^{m,n,p} \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}))^c \partial_{ijk}^{(4)} F_{ijk}^1(z) \Big| \le O(\eta^{-6} N^{-1}).$$

Next, when $\alpha = 0$ and 3, we can repeat the same arguments as those for (E.10), (E.11), (E.12), (E.15) and (E.16) to show that

$$N^{-1/2} \left| \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\partial_{ijk}^{(3)} F_{ijk}^1(z) \partial_{ijk}^{(1)} \operatorname{Tr}(\boldsymbol{Q}(\bar{z}))^c \right] \right|, N^{-1/2} \left| \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[F_{ijk}^1(z) \partial_{ijk}^{(4)} \operatorname{Tr}(\boldsymbol{Q}(\bar{z}))^c \right] \right| \leq \mathcal{O}(\eta^{-6} N^{-1/2}).$$

Finally, when $\alpha = 1$ and 2, by Lemma D.6, it is enough to show the following terms are minor:

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\mathscr{D} \left(\partial_{ijk}^{(2)} F_{ijk}^{1}(z) \right) \mathscr{D} \left(\partial_{ijk}^{(2)} \operatorname{Tr} (\boldsymbol{Q}^{11}(\bar{z})) \right) \right], \quad N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\mathscr{D} \left(\partial_{ijk}^{(1)} F_{ijk}^{1}(z) \right) \left(\partial_{ijk}^{(3)} \operatorname{Tr} (\boldsymbol{Q}^{11}(\bar{z})) \right) \right].$$

Recall that in Lemma D.5, if $n_a, n_b, n_c > 0$, then

$$N^{-5/2} \mathbf{1}_m' \mathrm{diag}(|\boldsymbol{Q}^{11}|^{\circ n_{11}}) |\boldsymbol{a}| \mathbf{1}_n' \mathrm{diag}(|\boldsymbol{Q}^{22}|^{\circ n_{11}}) |\boldsymbol{b}| \mathbf{1}_p' \mathrm{diag}(|\boldsymbol{Q}^{33}|^{\circ n_{11}}) |\boldsymbol{c}| \leq \mathrm{O}(\eta^{-6} N^{-1}).$$

Actually, by direct calculations, $\mathscr{D}(\partial_{ijk}^{(2)}F_{ijk}^1(z)), \mathscr{D}(\partial_{ijk}^{(3)}\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z})))$ satisfy $n_a, n_b, n_c > 0$. Hence, $N^{-1/2}\sum_{i,j,k=1}^{m,n,p} |\epsilon_{ijk}^{(4)}|$ is minor.

Now, combining (E.6), (E.8), (E.14), (E.17) and (E.19), we obtain

$$(z + \mathfrak{m}_{2}(z) + \mathfrak{m}_{3}(z) + \mathcal{O}(\eta^{-8}N^{-\omega}))\mathcal{C}_{11,N}^{(3)}(z,z) = -\mathfrak{m}_{1}(z)[\mathcal{C}_{21,N}^{(3)}(z,z) + \mathcal{C}_{31,N}^{(3)}(z,z)] -2\mathcal{V}_{11,N}^{(3)}(z,\bar{z}) - \kappa_{4}\mathcal{U}_{11,N}^{(3)}(z,\bar{z}) + \mathcal{O}(\eta^{-6}N^{-1/2}).$$

Similarly, for any $s, t \in \{1, 2, 3\}$, we can obtain

$$(z + \mathfrak{m} - \mathfrak{m}_s)\mathcal{C}_{st,N}^{(3)} + \mathcal{O}(\eta^{-8}N^{-\omega})\mathcal{C}_{tt,N}^{(3)} = -\mathfrak{m}_s \sum_{l \neq s}^{3} \mathcal{C}_{lt,N}^{(3)} - (2\mathcal{V}_{st,N}^{(3)}(z,\bar{z}) + \kappa_4 \mathcal{U}_{st,N}^{(3)}(z,\bar{z})) + \mathcal{O}(\eta^{-6}N^{-1/2}),$$

where we omit the (z, z) in $\mathcal{C}_{ij,N}^{(3)}(z, z)$ and (z) in $\mathfrak{m}_i(z)$ for convenience. Next, define two matrices $\mathbf{\Theta}_N^{(3)}(z_1, z_2) = [\Theta_{ij,N}^{(3)}(z_1, z_2)]_{3\times 3} \in \mathbb{C}^{3\times 3}$ and $\mathbf{F}_N^{(3)}(z_1, z_2) = [\mathcal{F}_{ij,N}^{(3)}(z_1, z_2)]_{3\times 3} \in \mathbb{C}^{3\times 3}$ such that

$$\Theta_{ij,N}^{(3)}(z_1, z_2) = \begin{cases} z_1 + \mathfrak{m}(z_1) - \mathfrak{m}_i(z_1) & i = j \\ \mathfrak{m}_i(z_2) & i \neq j \end{cases},$$
 (E.20)

and

$$\mathcal{F}_{ii,N}^{(3)}(z_1, z_2) := 2\mathcal{V}_{ii,N}^{(3)}(z_1, z_2) + \kappa_4 \mathcal{U}_{ii,N}^{(3)}(z_1, z_2) \tag{E.21}$$

then we obtain

$$\mathbf{\Theta}_{N}^{(3)}(z,z)\mathbf{C}_{N}^{(3)}(z,z) = -\mathbf{F}_{N}^{(3)}(z,z) + \mathcal{O}(\eta^{-8}N^{-\omega})\operatorname{diag}(\mathbf{C}_{N}^{(3)}(z,z)) + \mathcal{O}(\eta_{0}^{-6}N^{-1/2})\mathbf{1}_{3\times 3}. \quad (E.22)$$

By Theorem D.2, $\|\boldsymbol{m}(z) - \boldsymbol{g}(z)\|_{\infty} = O(\eta_0^{-15} N^{-2\omega})$, it implies that

$$\|\mathbf{\Theta}_{N}^{(3)}(z,z) + \operatorname{diag}(\mathbf{c} \circ \mathbf{g}(z)^{-1})\mathbf{\Pi}^{(3)}(z,z)\|_{\infty} \le \mathrm{O}(\eta_{0}^{-15}N^{-2\omega}),$$

where $\Pi(z, z)$ is defined in (B.11). By Lemma B.1, we have

$$\|\operatorname{diag}(\mathbf{c} \circ \mathbf{g}(z)^{-1})\mathbf{\Pi}^{(3)}(z,z)\| \ge 3^{-1/2}\|\operatorname{diag}(\mathbf{c} \circ \mathbf{g}(z)^{-1})\mathbf{\Pi}^{(3)}(z,z)\|_F \ge C_{\mathbf{c}}\eta_0^3$$

then diag($\mathfrak{c} \circ g(z)^{-1}$) $\Pi^{(3)}(z,z)$ is the dominating term as $N \to \infty$. Moreover, $\Pi^{(3)}(z,z)$ is invertible by the Remark B.2, which implies that $\Theta_N^{(3)}(z,z)$ is also invertible as $N \to \infty$. Hence,

$$C_N^{(3)}(z,z) = -\mathbf{\Theta}_N^{(3)}(z,z)^{-1} F_N^{(3)}(z,z)$$

$$+ O(\eta^{-8} N^{-\omega}) \mathbf{\Theta}_N^{(3)}(z,z)^{-1} \operatorname{diag}(\mathbf{C}_N^{(3)}(z,z)) + O(\eta_0^{-6} N^{-1/2}) \mathbf{1}_{3\times 3}.$$
(E.23)

Let $\Delta^{(3)} := \mathbf{\Theta}_N^{(3)}(z,z) + \operatorname{diag}(\mathbf{c} \circ \mathbf{g}(z)^{-1})\mathbf{\Pi}^{(3)}(z,z)$, where $\|\Delta^{(3)}\|_{\infty} = \mathrm{O}(\eta_0^{-15}N^{-2\omega})$. Since

$$\begin{split} & \boldsymbol{\Theta}_{N}^{(3)}(z,z)^{-1} = -(\operatorname{diag}(\boldsymbol{\mathfrak{c}} \circ \boldsymbol{g}(z)^{-1})\boldsymbol{\Pi}^{(3)}(z,z) - \boldsymbol{\Delta}^{(3)})^{-1} \\ & = -\boldsymbol{\Pi}^{(3)}(z,z)^{-1}\operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1} \circ \boldsymbol{g}(z)) - \boldsymbol{\Pi}^{(3)}(z,z)^{-1}\operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1} \circ \boldsymbol{g}(z))\boldsymbol{\Delta}^{(3)}\boldsymbol{\Theta}_{N}^{(3)}(z,z)^{-1}, \end{split}$$

then

$$\|\boldsymbol{\Theta}_{N}^{(3)}(z,z)^{-1}\| \leq (1 - \|\boldsymbol{\Pi}^{(3)}(z,z)^{-1}\operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1} \circ \boldsymbol{g}(z))\| \cdot \|\boldsymbol{\Delta}^{(3)}\|)^{-1}\|\boldsymbol{\Pi}^{(3)}(z,z)^{-1}\operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1} \circ \boldsymbol{g}(z))\|.$$

By Proposition B.3 and Lemma B.1, it implies that $\|\mathbf{\Pi}^{(3)}(z,z)^{-1}\operatorname{diag}(\mathbf{c}^{-1}\circ\mathbf{g}(z))\| \leq C_{\mathfrak{c}}\eta_0^{-5}$. Moreover, since $\lim_{N\to\infty}\|\Delta^{(3)}\|=0$, we obtain that $\|\mathbf{\Theta}_N^{(3)}(z,z)^{-1}\|\leq C_{\mathfrak{c}}\eta_0^{-5}$. By (E.23), it further gives that

$$\|\boldsymbol{C}_{N}^{(3)}(z,z)\| \leq (1 - \mathcal{O}(\eta_{0}^{-8}N^{-\omega})\|\boldsymbol{\Theta}_{N}^{(3)}(z,z)^{-1}\|)^{-1}(\|\boldsymbol{\Theta}_{N}^{(3)}(z,z)^{-1}\boldsymbol{F}_{N}^{(3)}(z,z)\| + \mathcal{O}(\eta_{0}^{-6}N^{-1/2})),$$

then we obtain that

$$\|C_N^{(3)}(z,z)\| \le C_{\mathfrak{c}}\eta_0^{-10},$$
 (E.24)

so do its entries. Moreover, since

$$\begin{aligned} &\|\boldsymbol{\Theta}_{N}^{(3)}(z,z)^{-1} + \boldsymbol{\Pi}^{(3)}(z,z)^{-1}\operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1} \circ \boldsymbol{g}(z))\| \\ &\leq &\|\boldsymbol{\Pi}^{(3)}(z,z)^{-1}\operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1} \circ \boldsymbol{g}(z))\Delta^{(3)}\boldsymbol{\Theta}_{N}^{(3)}(z,z)^{-1}\| \leq C_{\mathfrak{c}}\eta_{0}^{-10}\|\Delta^{(3)}\|, \end{aligned}$$

then we replace all $\Theta_N^{(3)}(z,z)^{-1}$ in (E.23) by $-\Pi^{(3)}(z,z)^{-1}\operatorname{diag}(\mathfrak{c}^{-1}\circ g(z))$ and derive that

$$\lim_{N \to \infty} \|\boldsymbol{C}_N^{(3)}(z, z) - \boldsymbol{\Pi}^{(3)}(z, z)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z)) \boldsymbol{F}_N^{(3)}(z, z) \| = 0.$$
 (E.25)

Finally, for $z_1 \neq z_2 \in \mathcal{S}_{\eta_0}$, we can repeat the previous arguments to derive that

$$\begin{split} &(z_1 + \mathfrak{m}(z_1) - \mathfrak{m}_s(z_1))\mathcal{C}_{st,N}^{(3)}(z_1, z_2) \\ &= -\mathfrak{m}_s(z_1) \sum_{l \neq s}^3 \mathcal{C}_{lt,N}^{(3)}(z_1, z_2) - \mathcal{F}_{st,N}^{(3)}(z_1, \bar{z}_2) + \mathcal{O}(C_{\eta_0} N^{-\omega}) \mathcal{C}_{tt,N}^{(3)}(z_2, z_2) + \mathcal{O}(C_{\eta_0} N^{-\omega}), \end{split}$$

since we have shown that $C_{tt,N}^{(3)}(z_2,z_2)$ is bounded by $C_{\eta_0,\mathfrak{e},d}$, then we can repeat the previous arguments to derive that

$$\lim_{N\to\infty} \|\boldsymbol{C}_N^{(3)}(z_1,z_2) - \boldsymbol{\Pi}^{(3)}(z_1,z_2)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z_1)) \boldsymbol{F}_N^{(3)}(z_1,\bar{z}_2) \| = 0,$$

here we omit details to save space.

E.2 Mean function

In this section, we will derive the limiting form of $\mathbb{E}[\text{Tr}(\mathbf{Q}(z))] - Ng(z)$. For convenience, we omit (z) in $\mathbf{Q}(z)$ and its entries.

Theorem E.2. Under Assumptions A.1 and A.2, for any $\eta_0 > 0$ and $z \in \mathcal{S}_{\eta_0}$ in (C.18), let

$$\overrightarrow{M}_{N}^{(3)}(z) = (M_{1,N}^{(3)}(z), M_{2,N}^{(3)}(z), M_{3,N}^{(3)}(z))'$$

where for $1 \le i \le 3$

$$M_{i,N}^{(3)}(z) := g_i(z) \sum_{r \neq i}^{3} \sum_{w \neq i,r}^{3} W_{rw}^{(3)}(z) + \sum_{l \neq i}^{3} \left[(g(z) - g_l(z)) W_{il}^{(3)}(z) + V_{il}^{(3)}(z,z) \right]$$

$$-2\kappa_3 G_N^{(3)}(z) + \kappa_4 H_{i,N}^{(3)}(z,z),$$
(E.26)

where $W_{jk}^{(3)}(z), V_{ij}^{(3)}(z,z), G_N^{(3)}(z), H_{i,N}^{(3)}(z,z)$ are defined in (D.1), (E.40), (E.32), (E.33). Then we have

$$\lim_{N\to\infty} \|N(\boldsymbol{m}(z)-\boldsymbol{g}(z))-\boldsymbol{\Pi}^{(3)}(z,z)^{-1}\operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1}\circ\boldsymbol{g}(z))\overrightarrow{M}_N^{(3)}(z)\|=0.$$

Consequently, we obtain that

$$\lim_{N \to \infty} \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}(z))] - Ng(z) - \mu_N^{(3)}(z) = 0,$$

where

$$\mu_N^{(3)}(z) := \mathbf{1}_3' \mathbf{\Pi}^{(3)}(z, z)^{-1} \operatorname{diag}(\mathbf{c}^{-1} \circ \mathbf{g}(z)) \overrightarrow{M}_N^{(3)}(z), \tag{E.27}$$

and $\Pi^{(3)}(z,z)$ is defined in (B.11).

Before proving the above theorem, we first give the explicit forms of major terms in cumulant expansions of $\mathbb{E}[\text{Tr}(\boldsymbol{Q}]]$. It is enough to calculate $\mathbb{E}[\text{Tr}(\boldsymbol{Q}^{ii}]]$ for i=1,2,3. Without loss of generality, we only calculate $\mathbb{E}[\text{Tr}(\boldsymbol{Q}^{11})]$ in details. By notations in (D.2), the trick of $z\boldsymbol{Q} = \boldsymbol{Q}\boldsymbol{M} - \boldsymbol{I}_N$ and cumulant expansion (D.4), we have

$$z\mathbb{E}[\text{Tr}(\boldsymbol{Q}^{11}] = \frac{1}{\sqrt{N}} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}[X_{ijk}(b_j Q_{ik}^{13} + c_k Q_{ij}^{12})] - m$$

$$= \frac{1}{\sqrt{N}} \sum_{i,k=1}^{m,n,p} \left(\sum_{n=0}^{3} \frac{\kappa_{l+1}}{l!} \mathbb{E}[b_j \partial_{ijk}^{(l)} Q_{ik}^{13} + c_k \partial_{ijk}^{(l)} Q_{ij}^{12}] + \epsilon_{ijk}^{(4)} \right) - m,$$

where $|\epsilon_{ijk}^{(4)}| \leq C_{\kappa_5} \sup_{z \in \mathcal{S}_{\eta_0}} |b_j \partial_{ijk}^{(4)} Q_{ik}^{13} + c_k \partial_{ijk}^{(4)} Q_{ij}^{12}|$. By Lemma D.5, for $2 \leq l \leq 4$, we have

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \left| \mathscr{O}\left(b_j \partial_{ijk}^{(l)} Q_{ik}^{13} + c_k \partial_{ijk}^{(l)} Q_{ij}^{12}\right) \right| \le \mathcal{O}(\eta_0^{-(l+1)} N^{-(l+1)/2+1}), \tag{E.28}$$

so it is enough to focus on

$$N^{-1/2} \sum_{i,i,k=1}^{m,n,p} \mathcal{D}\left(b_j \partial_{ijk}^{(l)} Q_{ik}^{13} + c_k \partial_{ijk}^{(l)} Q_{ij}^{12}\right), \tag{E.29}$$

where the operators " \mathcal{D} , \mathcal{O} " are defined in (D.33) and (D.34).

First derivatives: When l = 1, by direct calculations, we can obtain that

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[b_{j} \partial_{ijk}^{(1)} Q_{ik}^{13} + c_{k} \partial_{ijk}^{(1)} Q_{ij}^{12}\right]$$

$$= -N^{-1} \mathbb{E}\left[\operatorname{Tr}(\boldsymbol{Q}^{11}) \operatorname{Tr}(\boldsymbol{Q}^{22}) + \operatorname{Tr}(\boldsymbol{Q}^{11}) \operatorname{Tr}(\boldsymbol{Q}^{33})\right] - \left(V_{12,N}^{(3)}(z,z) + V_{13,N}^{(3)}(z,z)\right)$$

$$-N^{-1} \mathbb{E}\left[2b'\boldsymbol{Q}^{23}\boldsymbol{c} \operatorname{Tr}(\boldsymbol{Q}^{11}) + a'\boldsymbol{Q}^{12}\boldsymbol{b} \operatorname{Tr}(\boldsymbol{Q}^{33}) + a'\boldsymbol{Q}^{13}\boldsymbol{c} \operatorname{Tr}(\boldsymbol{Q}^{22})\right] + O(\eta_{0}^{-2}N^{-1}),$$

where

$$V_{ij,N}^{(3)}(z_1, z_2) := N^{-1} \mathbb{E}[\text{tr}(\mathbf{Q}^{ij}(z_1)\mathbf{Q}^{ji}(z_2))], \ 1 \le i \le j \le 3.$$
 (E.30)

Second derivatives: When l = 2, we have

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\mathcal{D}\left(b_{j}\partial_{ijk}^{(2)}Q_{ik}^{13} + c_{k}\partial_{ijk}^{(2)}Q_{ij}^{12}\right)\right]$$

$$= 4N^{-3/2} \sum_{i,j,k=1}^{m,n,p} a_{i}b_{j}c_{k}\mathbb{E}\left[Q_{ii}^{11}Q_{jj}^{22}Q_{kk}^{33}\right] + \mathcal{O}(\eta_{0}^{-3}N^{-1/2})$$

$$= 4N^{-3/2}\mathbb{E}\left[\left(\mathbf{1}'_{m}\operatorname{diag}(\mathbf{Q}^{11})\mathbf{a}\right)\left(\mathbf{1}'_{n}\operatorname{diag}(\mathbf{Q}^{22})\mathbf{b}\right)\left(\mathbf{1}'_{p}\operatorname{diag}(\mathbf{Q}^{33})\mathbf{c}\right)\right] + \mathcal{O}(\eta_{0}^{-3}N^{-1/2}).$$
(E.31)

By Lemma D.3 and Theorem D.1, we can show that

$$\left| N^{-1/2} \mathbf{1}' \operatorname{diag}(\mathbf{Q}^{kk}(z)) \mathbf{a}^{(k)} - \mathfrak{c}_k^{-1} g_k(z) N^{-1/2} \sum_{j=1}^{n_k} a_j^{(k)} \right| \prec \operatorname{O}(C_{\eta_0} N^{-\omega}),$$

by (E.1), we define

$$G_N^{(3)}(z) := (\mathfrak{c}_1 \mathfrak{c}_2 \mathfrak{c}_3)^{-1} g_1(z) g_2(z) g_3(z) \mathfrak{b}_1^{(1)} \mathfrak{b}_2^{(1)} \mathfrak{b}_3^{(1)}, \tag{E.32}$$

and $(E.31) = 6G_N^{(3)}(z) + O(C_{\eta_0}N^{-\omega}).$

Third derivatives: When l=3, there are only two possible situations in (E.29). Without loss of generality, we use $\mathscr{D}(c_k\partial_{ijk}^{(3)}Q_{ij}^{12})$ as an example. First, if $n_{11}, n_{22}, n_{33} > 0$, then the terms $a_i^2 c_k^2 Q_{ii}^{11} (Q_{jj}^{22})^2 Q_{kk}^{33}$ and $b_j^2 c_k^2 (Q_{ii}^{11})^2 Q_{jj}^{22} Q_{kk}^{33}$ will appear in $\mathscr{D}(c_k\partial_{ijk}^{(3)}Q_{ij}^{12})$, and we can conclude that

$$N^{-2} \sum_{i,j,k=1}^{m,n,p} a_i^2 c_k^2 Q_{ii}^{11}(Q_{jj}^{22})^2 Q_{kk}^{33} \leq \boldsymbol{a}' \mathrm{diag}(\boldsymbol{Q}^{11}) \boldsymbol{a} \times \boldsymbol{c}' \mathrm{diag}(\boldsymbol{Q}^{33}) \boldsymbol{c} \times \mathrm{Tr}((\boldsymbol{Q}^{22})^{\circ 2})$$

which is bounded by $N^{-1}\|\boldsymbol{Q}\|^4$, so does $N^{-2}\sum_{i,j,k=1}^{m,n,p}a_i^2c_k^2Q_{ii}^{11}(Q_{jj}^{22})^2Q_{kk}^{33}$. And the same conclusion is also valid for $b_j\partial_{ijk}^{(3)}Q_{ik}^{13}$. On the other hand, if only two of n_{11}, n_{22}, n_{33} are nonzero, then the only possible case in $\mathscr{D}(c_k\partial_{ijk}^{(3)}Q_{ij}^{12})$ is $c_k^4(Q_{ii}^{11})^2(Q_{jj}^{22})^2$, and we finally obtain

$$N^{-2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\mathscr{D} \left(b_j \partial_{ijk}^{(3)} Q_{ik}^{13} + c_k \partial_{ijk}^{(3)} Q_{ij}^{12} \right) \right]$$

$$= -6N^{-2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[b_j^4 (Q_{ii}^{11})^2 (Q_{kk}^{33})^2 + c_k^4 (Q_{ii}^{11})^2 (Q_{jj}^{22})^2 \right] + \mathcal{O}(\eta_0^{-4} N^{-1})$$

$$= -6 \sum_{k=2}^{3} \| \boldsymbol{a}^{(5-k)} \|_4^4 N^{-2} \mathbb{E} \left[\operatorname{tr}(\boldsymbol{Q}^{11}(z) \circ \boldsymbol{Q}^{11}(z)) \operatorname{tr}(\boldsymbol{Q}^{jj}(z) \circ \boldsymbol{Q}^{jj}(z)) \right] + \mathcal{O}(\eta_0^{-4} N^{-1}).$$

By Lemma D.3 and Theorem D.1, we know that

$$Cov(N^{-1}Tr(\mathbf{Q}^{ii}(z) \circ \mathbf{Q}^{ii}(z)), N^{-1}Tr(\mathbf{Q}^{jj}(z) \circ \mathbf{Q}^{jj}(z))) = O(\eta_0^{-12}N^{-2\omega})$$

and

$$\left| N^{-1}\operatorname{Tr}(\boldsymbol{Q}^{ii}(z_1) \circ \boldsymbol{Q}^{ii}(z_2)) - \mathfrak{c}_i^{-1}g_i(z_1)g_i(z_2) \right| \prec \operatorname{O}(C_{\eta_0}N^{-\omega}).$$

By (E.2), for $1 \le i \le 3$, let

$$H_{i,N}^{(3)}(z_1, z_2) := \mathfrak{c}_i^{-1} g_i(z_1) g_k(z_2) \sum_{l \neq i}^3 \mathcal{B}_{(4)}^{(k,l)} \mathfrak{c}_l^{-1} g_l(z_1) g_l(z_2). \tag{E.33}$$

Remainders: By Lemma D.5, we rewrite (E.29) as follows:

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathscr{D} \left(b_j \partial_{ijk}^{(l)} Q_{ik}^{13} + c_k \partial_{ijk}^{(l)} Q_{ij}^{12} \right) = N^{-5/2} \sum_{i,j,k=1}^{m,n,p} (a_i)^{n_a} (b_j)^{n_b} (c_k)^{n_c} (Q_{ii}^{11})^{n_{11}} (Q_{jj}^{22})^{n_{22}} (Q_{kk}^{33})^{n_{33}},$$

where $n_a + n_b + n_c = 5$. Hence, at least one of n_a, n_b, n_c is equal or greater than 2 and above sum is bounded by $N^{-3/2} \|\boldsymbol{Q}\|^5$. Combining with (E.28), we conclude that

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} |\epsilon_{ijk}^{(4)}| \le C_{\kappa_5} N^{-1/2} \sum_{i,j,k=1}^{m,n,p} |(\mathscr{D} + \mathscr{O}) (b_j \partial_{ijk}^{(l)} Q_{ik}^{13} + c_k \partial_{ijk}^{(l)} Q_{ij}^{12})| \le O(\eta_0^{-5} N^{-3/2}).$$
(E.34)

Now, let's prove Theorem E.2.

Proof of Theorem E.2. Based on previous discussions, it gives that

$$z\mathbb{E}[\text{Tr}(\boldsymbol{Q}^{11}(z))] = -N^{-1}\mathbb{E}\left[\text{Tr}(\boldsymbol{Q}^{11})\text{Tr}(\boldsymbol{Q}^{22}) + \text{Tr}(\boldsymbol{Q}^{11})\text{Tr}(\boldsymbol{Q}^{33})\right] - \left(V_{12,N}^{(3)}(z,z) + V_{13,N}^{(3)}(z,z)\right) - N^{-1}\mathbb{E}\left[2\boldsymbol{b}'\boldsymbol{Q}^{23}\boldsymbol{c}\text{Tr}(\boldsymbol{Q}^{11}) + \boldsymbol{a}'\boldsymbol{Q}^{12}\boldsymbol{b}\text{Tr}(\boldsymbol{Q}^{33}) + \boldsymbol{a}'\boldsymbol{Q}^{13}\boldsymbol{c}\text{Tr}(\boldsymbol{Q}^{22})\right] - m + 2\kappa_3 G_N^{(3)}(z) - \kappa_4 H_{1,N}^{(3)}(z,z) + O(C_{n_0}N^{-\omega}).$$

By Lemma D.3 and Theorem E.1, for $1 \le i, j \le 3$, we have $|(\boldsymbol{a}'\boldsymbol{Q}^{12}\boldsymbol{b})^c|, |(\boldsymbol{a}'\boldsymbol{Q}^{13}\boldsymbol{c})^c|, |(\boldsymbol{b}'\boldsymbol{Q}^{23}\boldsymbol{c})^c| \prec O(\eta_0^{-5}N^{-\omega})$ and $|N^{-1}\operatorname{Tr}(\boldsymbol{Q}^{12}\boldsymbol{Q}^{21})^c|, |N^{-1}\operatorname{Tr}(\boldsymbol{Q}^{13}\boldsymbol{Q}^{31})^c| \prec O(\eta_0^{-6}N^{-\omega})$. Combining with $\operatorname{Cov}(\operatorname{Tr}(\boldsymbol{Q}^{11}, \operatorname{Tr}(\boldsymbol{Q}^{22}))) \le O(\eta_0^{-10})$ in (E.24), it implies that

$$\left|N^{-1}\mathbb{E}\left[\operatorname{Tr}(\boldsymbol{Q}^{11}(z))\operatorname{Tr}(\boldsymbol{Q}^{22}(z))\right]-\mathfrak{m}_2(z)\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{11}(z))]\right|\leq \mathrm{O}(\eta_0^{-10}N^{-1})$$

and

$$\left|\operatorname{Cov}(\rho_l(z), (\boldsymbol{a}^{(i)})' \boldsymbol{Q}^{ij} \boldsymbol{a}^{(j)})\right| \leq \operatorname{O}(\eta_0^{-10} N^{-2\omega}),$$

where $\rho_i(z) = N^{-1} \operatorname{Tr}(\mathbf{Q}^{ii}(z))$ and $\mathfrak{m}_i(z) = \mathbb{E}[\rho_i(z)]$. Hence, recall the definition of $W_{ij,N}^{(3)}(z)$ in (D.40), we can obtain

$$(z + \mathfrak{m}_{2} + \mathfrak{m}_{3})\mathbb{E}\left[\operatorname{Tr}(\boldsymbol{Q}^{11})\right] = -(m + 2\mathfrak{m}_{1}W_{23,N}^{(3)} + \mathfrak{m}_{2}W_{13,N}^{(3)} + \mathfrak{m}_{3}W_{12,N}^{(3)} + V_{12,N}^{(3)} + V_{13,N}^{(3)}) + 2\kappa_{3}G_{N}^{(3)}(z) - \kappa_{4}H_{1,N}^{(3)}(z,z) + \mathcal{O}(C_{\eta_{0}}N^{-\omega}) := -(\mathfrak{c}_{1}N + M_{1,N}^{(3)}(z)) + \mathcal{O}(C_{\eta_{0}}N^{-\omega}),$$
 (E.35)

where we omit (z,z) in $V_{ij,N}^{(3)}(z,z)$ and (z) in $W_{ij,N}^{(3)}(z)$ for convenience. Moreover, for proofs of $W_{st,N}^{(3)}(z) \to W_{st}^{(3)}(z)$ and $V_{st,N}^{(3)}(z_1,z_2) \to V_{st}^{(3)}(z_1,z_2)$, readers can find details in (E.38) and (E.40) in §E.3. Next, we can repeat previous arguments to obtain the similar results for $\mathbb{E}[\text{Tr}(\mathbf{Q}^{22})]$ and $\mathbb{E}[\text{Tr}(\mathbf{Q}^{33})]$ as follows:

$$(z + \mathfrak{m}_j(z) + \mathfrak{m}_k(z))\mathbb{E}\left[\operatorname{Tr}(\boldsymbol{Q}^{ii}(z))\right] = -(\mathfrak{c}_i N + M_{i,N}^{(3)}(z)) + \operatorname{O}(C_{\eta_0} N^{-\omega}),$$

where $\{i, j, k\} = \{1, 2, 3\}$, i.e.

$$(z + \mathfrak{m}_j(z) + \mathfrak{m}_k(z))\mathfrak{m}_i(z) = -\mathfrak{c}_i - N^{-1}M_{i,N}^{(3)}(z) + \mathcal{O}(C_{\eta_0}N^{-\omega}).$$

Next, let $\boldsymbol{h}(z) := N(\boldsymbol{m}(z) - \boldsymbol{g}(z)), h(z) := N \sum_{i=1}^{3} (\mathfrak{m}_{i}(z) - g_{i}(z)) = N(\mathfrak{m}(z) - g(z)),$ then we have

$$(z + \mathfrak{m}_{j}(z) + \mathfrak{m}_{k}(z))h_{i}(z) = -\mathfrak{c}_{i}N - M_{i,N}^{(3)}(z) - N(z + \mathfrak{m}_{j}(z) + \mathfrak{m}_{k}(z))g_{i}(z) + \mathcal{O}(C_{\eta_{0}}N^{-\omega})$$

$$= \mathfrak{c}_{i}N\left(\frac{z + \mathfrak{m}_{j}(z) + \mathfrak{m}_{k}(z)}{z + g_{j}(z) + g_{k}(z)} - 1\right) - M_{i,N}^{(3)}(z) + \mathcal{O}(C_{\eta_{0}}N^{-\omega})$$

$$= \mathfrak{c}_{i}\frac{h(z) - h_{i}(z)}{z + g_{j}(z) + g_{k}(z)} - M_{i,N}^{(3)}(z) + \mathcal{O}(C_{\eta_{0}}N^{-\omega})$$

$$= -g_{i}(z)(h(z) - h_{i}(z)) - M_{i,N}^{(3)}(z) + \mathcal{O}(C_{\eta_{0}}N^{-\omega}). \tag{E.36}$$

Let $\overrightarrow{M}_{N}^{(3)}(z) = (M_{1,N}^{(3)}(z), \cdots, M_{3,N}^{(3)}(z))'$, we have

(E.36)
$$\Rightarrow (z + \mathfrak{m}_{j}(z) + \mathfrak{m}_{i}(z))h_{i}(z) = -g_{i}(z)(S_{d}h(z))_{i} - M_{i,N}^{(3)}(z) + O(C_{\eta_{0}}N^{-\omega})$$

 $\Leftrightarrow \mathbf{\Theta}_{N}^{(3)}(z,z)\tilde{h}(z) = -\overrightarrow{M}_{N}^{(3)}(z) + O(C_{\eta_{0}}N^{-\omega}),$

where $\Theta_N^{(3)}(z,z)$ is defined in (E.20) and it is invertible such that

$$\lim_{N \to \infty} \| \boldsymbol{\Theta}_N^{(3)}(z, z)^{-1} + \boldsymbol{\Pi}^{(3)}(z, z)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z)) \| = 0,$$

where $\Pi^{(3)}(z,z)$ is defined in (B.11) and it is also invertible by Remark B.2, so we obtain

$$\lim_{N \to \infty} \|N(\boldsymbol{m}(z) - \boldsymbol{g}(z)) - \boldsymbol{\Pi}^{(3)}(z, z)^{-1} \operatorname{diag}(\boldsymbol{c}^{-1} \circ \boldsymbol{g}(z)) \overrightarrow{M}_{N}^{(3)}(z)\|_{\infty} = 0,$$
 (E.37)

and
$$\lim_{N\to\infty} \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}(z))] - Ng(z) - \mu_N^{(3)}(z) = 0.$$

E.3 System equations for (D.40), (E.30) (E.9) and (E.18)

Now, we will calculate the asymptotically explicit forms of the major terms in $\mu_N^{(3)}(z_1)$ and covariance function $\mathcal{C}_N^{(3)}(z_1, z_2)$ for $z_1, z_2 \in \mathcal{S}_{\eta_0}$. Similar as proofs of Theorems E.1 and E.2, the calculation procedures rely on the cumulant expansions (D.4). For convenience, we will omit the calculations of minor terms, e.g. the remainders $\epsilon_{ijk}^{(2)}$.

System equations for $W_{st,N}^{(3)}(z)$ in (D.40): By the cumulant expansion (D.4) and (D.39), we can obtain

$$\mathbb{E}[(\boldsymbol{a}^{(s)})'\boldsymbol{Q}^{st}(z)\boldsymbol{a}^{(t)}(z+\rho(z)-\rho_s(z))] = -\delta_{st} - \sum_{l\neq s}^{3} \mathbb{E}[(\rho(z)-\rho_s(z)-\rho_l(z))(\boldsymbol{a}^{(l)})'\boldsymbol{Q}^{lt}(z)\boldsymbol{a}^{(t)}] + \mathrm{O}(\eta_0^{-3}N^{-1/2}),$$

where $\rho_i(z)$ is defined in (A.11). By Lemma D.3, we have

$$W_{st,N}^{(3)}(z)(z+\mathfrak{m}(z)-\mathfrak{m}_s(z)) = -\delta_{st} - \sum_{l \neq s}^3 (\mathfrak{m}(z)-\mathfrak{m}_s(z)-\mathfrak{m}_l(z)) W_{lt,N}^{(3)}(z) + \mathcal{O}(\eta_0^{-6}N^{-\omega}).$$

Since all $|W_{il,N}^{(3)}(z)| \leq O(\eta_0^{-1})$ and $||g(z) - m(z)||_{\infty} = O(\eta_0^{-15}N^{-2\omega})$ by Theorem D.2, it gives that

$$W_{st,N}^{(3)}(z)(z+g(z)-g_s(z)) = -\delta_{st} - \sum_{l \neq s}^{3} (g(z)-g_s(z)-g_l(z))W_{lt,N}^{(3)}(z) + \mathcal{O}(\eta_0^{-16}N^{-\omega}),$$

Therefore, define $W_N^{(3)}(z) = [W_{st,N}^{(3)}(z)]_{3\times 3}$ and

$$\mathbf{\Gamma}^{(3)}(z) := (z + g(z))\mathbf{I}_3 - \operatorname{diag}(\mathbf{g}(z)) + g(z)\mathbf{S}_3 - \operatorname{diag}(g(z))\mathbf{S}_3 - \mathbf{S}_3\operatorname{diag}(g(z)),$$

we can obtain that

$$\Gamma^{(3)}(z)W_N^{(3)}(z) = -I_3 + O(\eta_0^{-16}N^{-\omega})\mathbf{1}_{3\times 3}.$$

For the invertibility of $\Gamma^{(3)}(z)$, readers can refer to Lemma G.5 later, so we can derive the limiting expression of $W_N^{(3)}(z)$ as follows:

$$\boldsymbol{W}^{(3)}(z) := \lim_{N \to \infty} \boldsymbol{W}_{N}^{(3)}(z) = -\boldsymbol{\Gamma}^{(3)}(z)^{-1}, \quad \|\boldsymbol{W}^{(3)}(z) - \boldsymbol{W}_{N}^{(3)}(z)\| \le O(\eta_{0}^{-17}N^{-\omega}). \tag{E.38}$$

System equations for $V_{st,N}^{(3)}(z_1,z_2)$ in (E.30): By the cumulant expansion (D.4), Lemma D.5 and Theorem D.2, we can still obtain that

$$\begin{split} z_1 V_{st,N}^{(3)}(z_1,z_2) &= \frac{1}{N^{3/2}} \sum_{l \neq s}^{3} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \big[X_{ijk} \mathcal{A}_{ijk}^{(s,l)} Q_{\bar{l}.}^{lt}(z_1) Q_{\cdot \bar{s}}^{ts}(z_2) \big] - \delta_{st} \mathfrak{m}_s(z_2) = -\frac{1}{N^2} \sum_{l \neq s}^{3} \sum_{r_1 \neq r_2}^{3} \\ & \Big(\sum_{i,j,k=1}^{m,n,p} \mathbb{E} \big[\mathcal{A}_{ijk}^{(s,l)} \mathcal{A}_{ijk}^{(r_1,r_2)} (Q_{\bar{l}\bar{r}_1}^{lr_1}(z_1) Q_{\bar{r}_2.}^{r_2t}(z_1) Q_{\cdot \bar{s}}^{ts}(z_2) + Q_{\bar{l}.}^{lt}(z_1) Q_{\cdot \bar{r}_1}^{tr_1}(z_2) Q_{\bar{r}_2\bar{s}}^{r_2s}(z_2)) \Big] + \epsilon_{ijk}^{(2)} \Big) - \delta_{st} \mathfrak{m}_s(z_2) \\ &= -\frac{1}{N^2} \sum_{l \neq s}^{3} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \big[(\mathcal{A}_{ijk}^{(s,l)})^2 (Q_{\bar{l}\bar{l}}^{ll}(z_1) Q_{\bar{s}.}^{st}(z_1) Q_{\cdot \bar{s}}^{ts}(z_2) + Q_{\bar{l}.}^{lt}(z_1) Q_{\bar{l}\bar{l}}^{tl}(z_2) Q_{\bar{s}\bar{s}}^{ss}(z_2)) \Big] - \delta_{st} \mathfrak{m}_s(z_2) + \mathcal{O}(C_{\eta_0} N^{-1/2}) \\ &= -\sum_{l \neq s}^{3} \mathfrak{m}_l(z_1) V_{st,N}^{(3)}(z_1,z_2) - \sum_{l \neq s}^{3} \mathfrak{m}_s(z_2) V_{lt,N}^{(3)}(z_1,z_2) - \delta_{st} \mathfrak{m}_s(z_2) + \mathcal{O}(C_{\eta_0} N^{-\omega}) \\ &= -V_{st,N}^{(3)}(z_1,z_2) \sum_{l \neq s}^{3} g_l(z_1) - g_s(z_2) \sum_{l \neq s}^{3} V_{lt,N}^{(3)}(z_1,z_2) - \delta_{st} g_s(z_2) + \mathcal{O}(C_{\eta_0} N^{-\omega}), \end{split}$$

i.e.

$$V_{st,N}^{(3)}(z_1,z_2) = \mathfrak{c}_s^{-1} g_s(z_1) g_s(z_2) \Big(\delta_{st} + \sum_{l \neq s}^3 V_{lt,N}^{(3)}(z_1,z_2) \Big) + \mathcal{O}(C_{\eta_0} N^{-\omega}).$$

Here, define

$$V_N^{(3)}(z_1, z_2) = [V_{st\ N}^{(3)}(z_1, z_2)]_{3\times 3},\tag{E.39}$$

and we have

$$V_N^{(3)}(z_1, z_2) = \Pi^{(3)}(z_1, z_2)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ g(z_1) \circ g(z_2)) + \operatorname{o}(\mathbf{1}_{3\times 3}),$$

where $\Pi^{(3)}(z_1, z_2)$ is defined in (B.11). Hence, we have

$$V^{(3)}(z_1, z_2) := \lim_{N \to \infty} V_N^{(3)}(z_1, z_2) = \Pi^{(3)}(z_1, z_2)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ g(z_1) \circ g(z_2)). \tag{E.40}$$

System equations for $\mathcal{V}_{ij,N}^{(3)}(z_1,z_2)$ in (E.9): First, for $i,j,k\in\{1,2,3\}$, define

$$V_{ijk,N}^{(3)}(z_1, z_2) := N^{-1} \mathbb{E}[\text{Tr}(\mathbf{Q}^{ij}(z_1) \mathbf{Q}^{jk}(z_2) \mathbf{Q}^{ki}(z_2))], \tag{E.41}$$

Since $V_{ij,N}^{(3)}(z_1,z_2) = \sum_{l\neq i}^3 V_{ijl,N}^{(3)}(z_1,z_2)$, it suffices to calculate all $V_{ijl,N}^{(3)}(z_1,z_2)$. By the cumulant expansion (D.4), we have

$$z_{1}V_{stl,N}^{(3)}(z_{1},z_{2}) = \frac{1}{N^{3/2}} \sum_{r \neq s}^{3} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}[X_{ijk}\mathcal{A}_{ijk}^{(s,r)}Q_{\tilde{r}.}^{rl}(z_{1})\boldsymbol{Q}^{lt}(z_{2})Q_{.\tilde{s}}^{ts}(z_{2})] - \delta_{sl}V_{ts,N}^{(3)}(z_{2},z_{2})$$

$$= \frac{1}{N^{3/2}} \Big(\sum_{r \neq s}^{3} \sum_{i,k=1}^{m,n,p} \mathbb{E}[\mathcal{A}_{ijk}^{(s,r)}\partial_{ijk}^{(1)}\{Q_{\tilde{r}.}^{rl}(z_{1})\boldsymbol{Q}^{lt}(z_{2})Q_{.\tilde{s}}^{ts}(z_{2})\}] + \epsilon_{ijk}^{(2)} \Big) - \delta_{sl}V_{ts,N}^{(3)}(z_{2},z_{2}),$$

where

$$\frac{1}{N^{3/2}} \sum_{r \neq s}^{3} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}[\mathcal{A}_{ijk}^{(s,r)} \partial_{ijk}^{(1)} \{Q_{\tilde{r}\cdot}^{rl}(z_1) Q^{lt}(z_2) Q_{\cdot \tilde{s}}^{ts}(z_2)\}] =$$

$$- \frac{1}{N^2} \sum_{r \neq s}^{3} \sum_{w_1 \neq w_2}^{3} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}[\mathcal{A}_{ijk}^{(s,r)} Q_{\tilde{r}\tilde{w}_1}^{rw_1}(z_1) \mathcal{A}_{ijk}^{(w_1,w_2)} Q_{\tilde{w}_2}^{w_2l}(z_1) Q^{lt}(z_2) Q_{\cdot \tilde{s}}^{ts}(z_2)]$$

$$- \frac{1}{N^2} \sum_{r \neq s}^{3} \sum_{w_1 \neq w_2}^{3} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}[\mathcal{A}_{ijk}^{(s,r)} Q_{\tilde{r}\cdot}^{rl}(z_1) Q_{\cdot \tilde{w}_1}^{lw_1}(z_2) \mathcal{A}_{ijk}^{(w_1,w_2)} Q_{\tilde{w}_2\cdot}^{w_2t}(z_2) Q_{\cdot \tilde{s}}^{ts}(z_2)]$$

$$- \frac{1}{N^2} \sum_{r \neq s}^{3} \sum_{w_1 \neq w_2}^{3} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}[\mathcal{A}_{ijk}^{(s,r)} Q_{\tilde{r}\cdot}^{rl}(z_1) Q^{lt}(z_2) Q_{\cdot \tilde{w}_1}^{tw_1}(z_2) \mathcal{A}_{ijk}^{(w_1,w_2)} Q_{\tilde{w}_2\tilde{s}}^{w_2\tilde{s}}(z_2)],$$

then by Lemmas D.5 and D.3, we have

$$\begin{split} &\frac{1}{N^2} \sum_{r \neq s}^{3} \sum_{w_1 \neq w_2}^{3} \sum_{i,j,k=1}^{m_n,p} \mathbb{E} \left[\mathcal{A}_{ijk}^{(s,r)} Q_{\tilde{r}\tilde{w}_1}^{rw_1}(z_1) \mathcal{A}_{ijk}^{(w_1,w_2)} Q_{\tilde{w}_2}^{w_2l}(z_1) \boldsymbol{Q}^{lt}(z_2) Q_{\tilde{s}}^{ts}(z_2) \right] \\ &= \frac{1}{N^2} \sum_{r \neq s}^{3} \sum_{i,j,k=1}^{m_n,p} \mathbb{E} \left[(\mathcal{A}_{ijk}^{(s,r)})^2 Q_{\tilde{r}\tilde{r}}^{rr}(z_1) Q_{\tilde{s}}^{sl}(z_1) \boldsymbol{Q}^{lt}(z_2) Q_{\tilde{s}}^{ts}(z_2) \right] + \mathcal{O}(C_{\eta_0} N^{-\omega}) \\ &= V_{stl,N}^{(3)}(z_1,z_2) \sum_{r \neq s}^{3} \mathfrak{m}_r(z_1) + \mathcal{O}(C_{\eta_0} N^{-\omega}), \end{split}$$

and

$$\frac{1}{N^{2}} \sum_{r \neq s}^{3} \sum_{w_{1} \neq w_{2}}^{3} \sum_{i,j,k=1}^{m_{n},p} \mathbb{E} \left[\mathcal{A}_{ijk}^{(s,r)} Q_{\tilde{r}.}^{rl}(z_{1}) Q_{\cdot \tilde{w}_{1}}^{lw_{1}}(z_{2}) \mathcal{A}_{ijk}^{(w_{1},w_{2})} Q_{\tilde{w}_{2}.}^{w_{2}t}(z_{2}) Q_{\cdot \tilde{s}}^{ts}(z_{2}) \right]
= \frac{1}{N^{2}} \sum_{r \neq s}^{3} \sum_{i,j,k=1}^{m_{n},p} \mathbb{E} \left[(\mathcal{A}_{ijk}^{(s,r)})^{2} Q_{\tilde{r}.}^{rl}(z_{1}) Q_{\cdot \tilde{r}}^{lr}(z_{2}) Q_{\tilde{s}.}^{st}(z_{2}) Q_{\cdot \tilde{s}}^{ts}(z_{2}) \right] + \mathcal{O}(C_{\eta_{0}} N^{-\omega})
= V_{st,N}^{(3)}(z_{1},z_{2}) \sum_{r \neq s}^{3} V_{rl,N}^{(3)}(z_{1},z_{2}) + \mathcal{O}(C_{\eta_{0}} N^{-\omega}),$$

and

$$\begin{split} &\frac{1}{N^2} \sum_{r \neq s}^{3} \sum_{m_1 \neq w_2}^{3} \sum_{i,j,k=1}^{m_n,p} \mathbb{E} \left[\mathcal{A}_{ijk}^{(s,r)} Q_{\bar{r}.}^{rl}(z_1) \boldsymbol{Q}^{lt}(z_2) Q_{.\bar{w}_1}^{tw_1}(z_2) \mathcal{A}_{ijk}^{(w_1,w_2)} Q_{\bar{w}_2\bar{s}}^{w_2\bar{s}}(z_2) \right] \\ &= \frac{1}{N^2} \sum_{r \neq s}^{3} \sum_{i,j,k=1}^{m_n,p} \mathbb{E} \left[(\mathcal{A}_{ijk}^{(s,r)})^2 Q_{\bar{r}.}^{rl}(z_1) \boldsymbol{Q}^{lt}(z_2) Q_{.\bar{r}}^{tr}(z_2) Q_{\bar{s}\bar{s}}^{ss}(z_2) \right] + \mathcal{O}(C_{\eta_0} N^{-\omega}) \\ &= \mathfrak{m}_s(z_2) \sum_{r \neq s}^{3} V_{rtl,N}^{(3)}(z_1,z_2) + \mathcal{O}(C_{\eta_0} N^{-\omega}) \end{split}$$

and $\sum_{i,j,k=1}^{m,n,p} |\epsilon_{ijk}^{(2)}| = \mathcal{O}(\eta_0^{-5} N^{-1/2})$, so it gives that

$$(z_1 + \mathfrak{m}(z_1) - \mathfrak{m}_s(z_1))V_{stl,N}^{(3)}(z_1, z_2) = -\mathfrak{m}_s(z_2) \sum_{r \neq s}^3 V_{rtl,N}^{(3)}(z_1, z_2) - \delta_{st} V_{st,N}^{(3)}(z_2, z_2) - V_{st,N}^{(3)}(z_1, z_2) \sum_{r \neq s}^3 V_{rl,N}^{(3)}(z_1, z_2) + \mathcal{O}(C_{\eta_0} N^{-\omega}),$$

combining with Theorem D.2, we have

$$V_{stl,N}^{(3)}(z_1,z_2) = \mathfrak{c}_s^{-1} g_s(z_1) \Big(\delta_{st} V_{st,N}^{(3)}(z_2,z_2) + g_s(z_2) \sum_{r \neq s}^3 V_{rtl,N}^{(3)}(z_1,z_2) + V_{st,N}^{(3)}(z_1,z_2) \sum_{r \neq s}^3 V_{rl,N}^{(3)}(z_1,z_2) \Big) + \mathcal{O}(C_{\eta_0} N^{-\omega}).$$

Now, for fixed $1 \le l \le 3$, define

$$V_{l,N}^{(3)}(z_1,z_2) := [V_{stl,N}^{(3)}(z_1,z_2)]_{3\times 3},$$

then we have

$$\lim_{N \to \infty} \boldsymbol{V}_{l,N}^{(3)}(z_1, z_2) := \boldsymbol{\Pi}^{(3)}(z_1, z_2)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z_1)) [\operatorname{diag}(\boldsymbol{V}^{(3)}(z_2, z_2))$$

$$+ \operatorname{diag}(\boldsymbol{S}_3 \boldsymbol{V}_{.l}^{(3)}(z_1, z_2)) \boldsymbol{V}^{(3)}(z_1, z_2)].$$
(E.42)

where $V_{\cdot l}^{(3)}(z_1, z_2)$ is the l-th column of $V^{(3)}(z_1, z_2)$ defined in (E.40). Hence, once we obtain the limiting value of all $V_{stl,N}^{(3)}(z_1, z_2)$, we can derive the limiting expression of $\mathcal{V}_{st,N}^{(3)}(z_1, z_2)$ as follows:

$$\mathcal{V}_{st}^{(3)}(z_1, z_2) = \sum_{l \neq s}^{3} V_{stl}^{(3)}(z_1, z_2). \tag{E.43}$$

System equations for $\widetilde{\mathcal{U}}_{st,N}^{(3)}(z_1,z_2)$ in (E.18): By Lemma D.3, we know that

$$Cov(N^{-1}Tr(\boldsymbol{Q}^{ss}(z_1) \circ \boldsymbol{Q}^{ss}(z_2)), N^{-1}Tr(\boldsymbol{Q}^{tt}(z_1) \circ (\boldsymbol{Q}^{tr}(z_2)\boldsymbol{Q}^{rt}(z_2)))) = O(C_{n_0}N^{-\omega}),$$

where $s,t,r\in\{1,2,3\}$. Hence, it is enough to compute $N^{-1}\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{tt}(z_1)\circ(\boldsymbol{Q}^{tr}(z_2)\boldsymbol{Q}^{rt}(z_2)))]$ and $N^{-1}\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{ss}(z_1)\circ\boldsymbol{Q}^{ss}(z_2))]$, respectively. By (E.33), we know that $\lim_{N\to\infty}N^{-1}\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{ss}(z_1)\circ\boldsymbol{Q}^{ss}(z_2))]$ $=\mathfrak{c}_s^{-1}g_s(z_1)g_s(z_2)$. Next, let's define

$$\mathring{V}_{st,N}^{(3)}(z_1,z_2) = N^{-1} \mathbb{E} \big[\operatorname{tr}(\boldsymbol{Q}^{ss}(z_1) \circ (\boldsymbol{Q}^{st}(z_2) \boldsymbol{Q}^{ts}(z_2))) \big].$$

Similarly, by the cumulant expansion (D.4), we have

$$\begin{split} &z_1\mathring{V}_{st,N}^{(3)}(z_1,z_2) = \frac{1}{N^{3/2}}\sum_{r\neq s}^{3}\sum_{i,j,k=1}^{m,n,p}\mathbb{E}\left[X_{ijk}\mathcal{A}_{ijk}^{(s,r)}Q_{\tilde{r}\tilde{s}}^{rs}(z_1)Q_{\tilde{s}.}^{st}(z_2)Q_{.\tilde{s}}^{ts}(z_2)\right] - V_{st,N}^{(3)}(z_1,z_2)\\ &= \frac{1}{N^{3/2}}\Big(\sum_{r\neq s}^{3}\sum_{i,j,k=1}^{m,n,p}\mathbb{E}\left[\mathcal{A}_{ijk}^{(s,r)}\partial_{ijk}^{(1)}\{Q_{\tilde{r}\tilde{s}}^{rs}(z_1)Q_{\tilde{s}.}^{st}(z_2)Q_{.\tilde{s}}^{ts}(z_2)\}\right] + \epsilon_{ijk}^{(2)}\Big) - V_{st,N}^{(3)}(z_1,z_2)\\ &= -\frac{1}{N^2}\sum_{r\neq s}^{3}\sum_{w_1\neq w_2}^{3}\sum_{i,j,k=1}^{m,n,p}\mathbb{E}\left[\mathcal{A}_{ijk}^{(s,r)}Q_{\tilde{r}\tilde{w}_1}^{rw_1}(z_1)\mathcal{A}_{ijk}^{(w_1,w_2)}Q_{\tilde{w}_2\tilde{s}}^{w_2\tilde{s}}(z_1)Q_{\tilde{s}.}^{st}(z_2)Q_{.\tilde{s}}^{ts}(z_2)\right] - V_{st,N}^{(3)}(z_1,z_2)\\ &-\frac{2}{N^2}\sum_{r\neq s}^{3}\sum_{w_1\neq w_2}^{3}\sum_{i,j,k=1}^{m,n,p}\mathbb{E}\left[\mathcal{A}_{ijk}^{(s,r)}Q_{\tilde{r}\tilde{s}}^{rs}(z_1)Q_{\tilde{s}\tilde{w}_1}^{sw_1}\mathcal{A}_{ijk}^{(w_1,w_2)}Q_{\tilde{w}_2}^{w_2t}(z_2)Q_{.\tilde{s}}^{ts}(z_2)\right], \end{split}$$

by Lemma D.5 and Theorem D.2, we have

$$\begin{split} &\frac{1}{N^2} \sum_{r \neq s}^{3} \sum_{w_1 \neq w_2}^{3} \sum_{i,j,k=1}^{m_{n,n,p}} \mathbb{E} \left[\mathcal{A}_{ijk}^{(s,r)} Q_{\tilde{r}\tilde{w}_1}^{rw_1}(z_1) \mathcal{A}_{ijk}^{(w_1,w_2)} Q_{\tilde{w}_2\tilde{s}}^{w_2s}(z_1) Q_{\tilde{s}}^{st}(z_2) Q_{\cdot \tilde{s}}^{ts}(z_2) \right] \\ &= \frac{1}{N^2} \sum_{r \neq s}^{3} \sum_{i,j,k=1}^{m_{n,p}} \mathbb{E} \left[(\mathcal{A}_{ijk}^{(s,r)})^2 Q_{\tilde{r}\tilde{r}}^{rr}(z_1) Q_{\tilde{s}\tilde{s}}^{ss}(z_1) Q_{\tilde{s}}^{st}(z_2) Q_{\cdot \tilde{s}}^{ts}(z_2) \right] + \mathcal{O}(C_{\eta_0} N^{-\omega}) \\ &= \mathring{V}_{st,N}^{(3)}(z_1,z_2) \sum_{r \neq s}^{3} \mathfrak{m}_r(z_1) + \mathcal{O}(C_{\eta_0} N^{-\omega}) = \mathring{V}_{st,N}^{(3)}(z_1,z_2) \sum_{r \neq s}^{3} g_r(z_1) + \mathcal{O}(C_{\eta_0} N^{-\omega}), \end{split}$$

and

$$\frac{1}{N^2} \sum_{r \neq s}^{3} \sum_{w_1 \neq w_2}^{3} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\mathcal{A}_{ijk}^{(s,r)} Q_{\tilde{r}\tilde{s}}^{rs}(z_1) Q_{\tilde{s}\tilde{w}_1}^{sw_1} \mathcal{A}_{ijk}^{(w_1,w_2)} Q_{\tilde{w}_2}^{w_2t}(z_2) Q_{\cdot\tilde{s}}^{ts}(z_2) \right] = \mathcal{O}(C_{\eta_0} N^{-1})$$

i.e.

$$\mathring{V}_{N}^{(3)}(z_{1}, z_{2}) = \mathfrak{c}_{s}^{-1} g_{s}(z_{1}) V_{st,N}^{(3)}(z_{1}, z_{2}) + \mathcal{O}(C_{\eta_{0}} N^{-\omega}).$$

Define $\mathring{V}_{st,N}^{(3)}(z_1,z_2) := [\mathring{V}_{st,N}^{(3)}(z_1,z_2)]_{3\times 3}$, then we can conclude that

$$\lim_{N \to \infty} \| \mathring{\boldsymbol{V}}_{N}^{(3)}(z_{1}, z_{2}) - \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z_{1})) \boldsymbol{V}^{(3)}(z_{1}, z_{2}) \| = 0, \tag{E.44}$$

where $V^{(3)}(z_1, z_2)$ is given in (E.40). Hence, by (E.18) and (E.2), $\mathcal{U}_{st,N}^{(3)}(z_1, z_2)$ is given as

$$\mathcal{U}_{st}^{(3)}(z_1, z_2) := \mathfrak{c}_s^{-1} g_s(z_1) g_s(z_2) \sum_{l \neq s}^3 \mathcal{B}_{(4)}^{(s,l)} \mathring{V}_{lt}^{(3)}(z_1, z_2) + \mathring{V}_{st}^{(3)}(z_1, z_2) \sum_{l \neq s}^3 \mathcal{B}_{(4)}^{(s,l)} \mathfrak{c}_l^{-1} g_l(z_1) g_l(z_2). \tag{E.45}$$

F CLT for the LSS when d = 3

In this section, we will establish the CLT for the linear spectral statistics (LSS) of M in (A.10) when d = 3. Precisely, let's consider the family of functions as follows:

$$\mathfrak{F}_3 := \{ f(z) : f \text{ is analytic on an open set containing the interval } [-\max\{\zeta, \mathfrak{v}_3\}, \max\{\zeta, \mathfrak{v}_3\}] \},$$
(F.1)

where ζ (C.17) is the boundary of LSD ν and \mathfrak{v}_3 is defined in Theorem C.1. For any $f \in \mathfrak{F}_3$, the LSS of M is defined as follows:

$$\mathcal{L}_{\mathbf{M}}(f) := \frac{1}{N} \sum_{l=1}^{N} f(\lambda_l) = \int_{\mathbb{R}} f(x) \nu_N(dx), \tag{F.2}$$

where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N$ are the eigenvalues of M and $\nu_N = N^{-1} \sum_{l=1}^N \delta_{\lambda_l}$ is the ESD of M. By Theorem D.2, we know that the ESD ν_N converges to the LSD ν in Theorem C.2 almost surely, so let

$$G_N(f) := N \int_{-\infty}^{\infty} f(x)(\nu_N(dx) - \nu(dx)) = N\Big(\mathcal{L}_{\mathbf{M}}(f) - \int_{-\infty}^{\infty} f(x)\nu(dx)\Big), \tag{F.3}$$

we will provide that

Theorem F.1. Under Assumptions A.1 and A.2, when d=3, let \mathfrak{C}_1 and \mathfrak{C}_2 be two disjoint rectangle contours with vertexes of $\pm E_1 \pm i\eta_1$ and $\pm E_2 \pm i\eta_2$, respectively, such that $E_1, E_2 \ge \max\{\zeta, \mathfrak{v}_3\} + t$, where t > 0 is fixed constant, and $\eta_1, \eta_2 > 0$ are sufficiently small. Then for any $f \in \mathfrak{F}_3$ in (F.1), we have

$$(G_N(f) - \xi_N^{(3)})/\sigma_N^{(d)} \stackrel{d}{\longrightarrow} \mathcal{N}(0,1),$$

where

$$\begin{split} \xi_N^{(3)} &:= -\frac{1}{2\pi \mathrm{i}} \oint_{\mathfrak{C}_1} f(z) \mu_N^{(3)}(z) dz, \\ (\sigma_N^{(3)})^2 &:= -\frac{1}{4\pi^2} \oint_{\mathfrak{C}_1} \oint_{\mathfrak{C}_2} f(z_1) f(z_2) \mathcal{C}_N^{(3)}(z_1, z_2) dz_1 dz_2, \end{split}$$

and the mean function $\mu_N^{(3)}(z)$ and covariance function $\mathcal{C}_N^{(3)}(z_1, z_2)$ are defined in (E.37) and (E.5).

By Theorem C.1, for any fixed t > 0, we have $\mathbb{P}(\|\mathbf{M}\| > \mathfrak{v}_3 + t) \leq o(N^{-l})$ for any l > 0, then $G_N(f)1_{\|\mathbf{M}\| \leq \mathfrak{v}_3 + t} \xrightarrow{\mathbb{P}} G_N(f)$. Thus, conditional on $\|\mathbf{M}\| \leq \mathfrak{v}_3$, by the Cauchy integration theorem, we have

$$G_N(f) = -\frac{1}{2\pi i} \oint_{\mathfrak{C}} f(z) \{ \operatorname{Tr}(\boldsymbol{Q}(z)) - Ng(z) \} dz,$$

where \mathfrak{C} is a rectangle contour with vertexes of $\pm E_0 \pm i\eta_0$ such that $E_0 \geq \max\{\zeta, \mathfrak{v}_3\} + t$, where t > 0 is a fixed constant and $\eta_0 > 0$ is sufficiently small, ζ is the boundary of the LSD defined in (C.17). Consequently, to establish the CLT for $G_N(f)$, it is enough to establish the CLT for $\operatorname{Tr}(\mathbf{Q}(z)) - Ng(z)$. The basic outlines are first to show the process $\operatorname{Tr}(\mathbf{Q}(z)) - \mathbb{E}[\operatorname{Tr}(\mathbf{Q}(z))]$ is tight in \mathcal{S}_{η_0} , then prove that joint characteristic function of the real part and imaginary part of $\operatorname{Tr}(\mathbf{Q}(z)) - \mathbb{E}[\operatorname{Tr}(\mathbf{Q}(z))]$ converges converges to the characteristic function of a normal vector.

F.1 Tightness

Theorem F.2. Under Assumptions A.1 and A.2, for any $\eta_0 > 0$, $\text{Tr}(\mathbf{Q}(z)) - \mathbb{E}[\text{Tr}(\mathbf{Q}(z))]$ is tight in \mathcal{S}_{η_0} , i.e.

$$\sup_{\substack{z_1, z_2 \in \mathcal{S}_{\eta_0} \\ z_1 \neq z_2}} \frac{\mathbb{E}\left[|\operatorname{Tr}(\boldsymbol{Q}(z_1) - \boldsymbol{Q}(z_2)) - \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}(z_1) - \boldsymbol{Q}(z_2))|^2\right]}{|z_1 - z_2|^2} < C_{\eta_0}.$$

Similar as the proof of Theorem E.1, there will appear several major terms like $\mathcal{V}_{st,N}^{(3)}(z_1, z_2)$ and $\widetilde{\mathcal{U}}_{st,N}^{(3)}$ in (E.9) and (E.18). For the simplicity of presentations, we first define the following terms: for any $s_1, s_2, t_1, t_2 \in \{1, 2, 3\}$ and $z_1, z_2 \in \mathcal{S}_{\eta_0}$, let

$$C_{s_1t_1,s_2t_2,N}^{(3)}(z_1,z_2) := \operatorname{Cov}\left(\operatorname{Tr}(\boldsymbol{Q}^{s_1t_1}(z_1)\boldsymbol{Q}^{t_1s_1}(z_2)),\operatorname{Tr}(\boldsymbol{Q}^{s_2t_2}(z_1)\boldsymbol{Q}^{t_2s_2}(z_2))\right),$$
(F.4)

and

$$\begin{cases}
\mathcal{C}_{s_1t_1,s_2,N}^{(3)}(z_1,z_2) := \operatorname{Cov}(\operatorname{Tr}(\boldsymbol{Q}^{s_1t_1}(z_1)\boldsymbol{Q}^{t_1s_1}(z_2)), \operatorname{Tr}(\boldsymbol{Q}^{s_2s_2}(z_1))), \\
\mathcal{C}_{s_2,s_1t_1,N}^{(3)}(z_1,z_2) := \operatorname{Cov}(\operatorname{Tr}(\boldsymbol{Q}^{s_2s_2}(z_1)), \operatorname{Tr}(\boldsymbol{Q}^{s_1t_1}(z_1)\boldsymbol{Q}^{t_1s_1}(z_2))).
\end{cases} (F.5)$$

Moreover, for $k_1, k_2, l_1, l_2 \in \{1, 2, 3\}$, we define

$$\mathcal{V}_{k_{1}l_{1},k_{2}l_{2},N}^{(3)}(z_{1},z_{2}) := \frac{1}{N} \sum_{s \neq k_{1}}^{3} \sum_{r=1}^{2} \mathbb{E} \left[\operatorname{Tr} \left(\boldsymbol{Q}^{k_{1}k_{2}}(\bar{z}_{3-r}) \boldsymbol{Q}^{k_{2}l_{2}}(\bar{z}_{r}) \boldsymbol{Q}^{l_{2}s}(\bar{z}_{3-r}) \boldsymbol{Q}^{sl_{1}}(z_{1}) \boldsymbol{Q}^{l_{1}k_{1}}(z_{2}) \right) \right],$$
(F.6)

 $\mathcal{V}_{k_1 l_1, k_2, N}^{(3)}(z_1, z_2) := N^{-1} \sum_{r \neq k_1}^{3} \mathbb{E} \left[\text{Tr}(\boldsymbol{Q}^{r l_1}(z_1) \boldsymbol{Q}^{l_1 k_1}(z_2) \boldsymbol{Q}^{k_1 k_2}(\bar{z}_1) \boldsymbol{Q}^{k_2 r}(\bar{z}_2)) \right]. \tag{F.7}$

By notations in (D.2), we further define

$$\mathcal{U}_{11,11,N}^{(3)}(z,z) \qquad (F.8)$$

$$:= \frac{1}{N^2} \sum_{r=2}^{3} \sum_{w=1}^{2} \sum_{t_1,t_2}^{(1,r)} \|\boldsymbol{a}^{(5-r)}\|_{4}^{4} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{t_2t_2}(z_2) \circ (\boldsymbol{Q}^{t_21}(\bar{z}_w) \boldsymbol{Q}^{11}(\bar{z}_{3-w}) \boldsymbol{Q}^{1t_2}(\bar{z}_w))) \cdot \operatorname{Tr}(\boldsymbol{Q}^{t_1t_1}(\bar{z}_w) \circ (\boldsymbol{Q}^{t_11}(z_1) \boldsymbol{Q}^{1t_1}(z_2))) \right] \\
+ \frac{1}{N^2} \sum_{r=2}^{3} \sum_{w=1}^{2} \sum_{t_1,t_2}^{(1,r)} \|\boldsymbol{a}^{(5-r)}\|_{4}^{4} \mathbb{E} \left[\operatorname{Tr}((\boldsymbol{Q}^{t_21}(z_1) \boldsymbol{Q}^{1t_2}(z_2)) \circ (\boldsymbol{Q}^{t_21}(\bar{z}_w) \boldsymbol{Q}^{11}(\bar{z}_{3-w}) \boldsymbol{Q}^{1t_2}(\bar{z}_w))) \cdot \operatorname{Tr}(\boldsymbol{Q}^{t_1t_1}(\bar{z}_w) \circ \boldsymbol{Q}^{t_1t_1}(z_1)) \right] \\
+ \frac{1}{N^2} \sum_{r=2}^{3} \sum_{w=1}^{2} \sum_{t_1,t_2}^{(1,r)} \|\boldsymbol{a}^{(5-r)}\|_{4}^{4} \mathbb{E} \left[\operatorname{Tr}((\boldsymbol{Q}^{11}(z_2) \circ (\boldsymbol{Q}^{11}(\bar{z}_w) \boldsymbol{Q}^{11}(\bar{z}_w))) \cdot \operatorname{Tr}((\boldsymbol{Q}^{r_1}(z_1) \boldsymbol{Q}^{1r}(z_2)) \circ (\boldsymbol{Q}^{r_1}(\bar{z}_{3-w}) \boldsymbol{Q}^{1r}(\bar{z}_{3-w}))) \right] \\
+ \frac{1}{N^2} \sum_{r=2}^{3} \sum_{w=1}^{2} \sum_{t_1,t_2}^{(1,r)} \|\boldsymbol{a}^{(5-r)}\|_{4}^{4} \mathbb{E} \left[\operatorname{Tr}((\boldsymbol{Q}^{11}(z_1) \boldsymbol{Q}^{11}(z_2)) \circ (\boldsymbol{Q}^{11}(\bar{z}_w) \boldsymbol{Q}^{11}(\bar{z}_w))) \cdot \operatorname{Tr}(\boldsymbol{Q}^{r_1}(z_1) \circ (\boldsymbol{Q}^{r_1}(\bar{z}_{3-w}) \boldsymbol{Q}^{1r}(\bar{z}_{3-w}))) \right],$$

and

$$\mathcal{U}_{11,1,N}^{(3)}(z_{1},z_{2}) \qquad (F.9)$$

$$:= \frac{1}{N^{2}} \sum_{r=2}^{3} \|\boldsymbol{a}^{(5-r)}\|_{4}^{4} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{11}(z_{1}) \circ \boldsymbol{Q}^{11}(\bar{z}_{2})) \cdot \operatorname{Tr}((\boldsymbol{Q}^{r1}(z_{1})\boldsymbol{Q}^{1r}(z_{2})) \circ (\boldsymbol{Q}^{r1}(\bar{z}_{2})\boldsymbol{Q}^{1r}(\bar{z}_{2}))) \right]$$

$$+ \frac{1}{N^{2}} \sum_{r=2}^{3} \|\boldsymbol{a}^{(5-r)}\|_{4}^{4} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{11}(z_{1}) \circ (\boldsymbol{Q}^{11}(\bar{z}_{2})\boldsymbol{Q}^{11}(\bar{z}_{2}))) \cdot \operatorname{Tr}((\boldsymbol{Q}^{r1}(z_{1})\boldsymbol{Q}^{1r}(z_{2})) \circ \boldsymbol{Q}^{rr}(\bar{z}_{2})) \right]$$

$$+ \frac{1}{N^{2}} \sum_{r=2}^{3} \|\boldsymbol{a}^{(5-r)}\|_{4}^{4} \mathbb{E} \left[\operatorname{Tr}((\boldsymbol{Q}^{11}(z_{1})\boldsymbol{Q}^{11}(z_{2})) \circ \boldsymbol{Q}^{11}(\bar{z}_{2})) \cdot \operatorname{Tr}(\boldsymbol{Q}^{rr}(z_{2}) \circ (\boldsymbol{Q}^{r1}(\bar{z}_{2})\boldsymbol{Q}^{1r}(\bar{z}_{2}))) \right]$$

$$+ \frac{1}{N^{2}} \sum_{r=2}^{3} \|\boldsymbol{a}^{(5-r)}\|_{4}^{4} \mathbb{E} \left[\operatorname{Tr}((\boldsymbol{Q}^{11}(z_{1})\boldsymbol{Q}^{11}(z_{2})) \circ (\boldsymbol{Q}^{11}(\bar{z}_{2})\boldsymbol{Q}^{11}(\bar{z}_{2}))) \cdot \operatorname{Tr}(\boldsymbol{Q}^{rr}(z_{2}) \circ \boldsymbol{Q}^{rr}(\bar{z}_{2})) \right],$$

where $t_1, t_2 \in \{1, 2, 3\}$ and the notation $\sum_{t_1, t_2}^{(1,r)}$ means that the summation of t_1 and t_2 are over $\{1, 2, 3\} \setminus \{1, r\}$.

Proof. By (II.19) in [24], we know that $Q(z_1) - Q(z_2) = (z_1 - z_2)Q(z_1)Q(z_2)$, then $(z_1 - z_2)^{-1} \operatorname{Tr} (Q(z_1) - Q(z_2)) = \operatorname{Tr} (Q(z_1)Q(z_2))$ for $z_1 \neq z_2$. Note that

$$\operatorname{Tr}\left(\boldsymbol{Q}(z_1)\boldsymbol{Q}(z_2)\right) = \sum_{i=1}^{3} \operatorname{Tr}\left(\boldsymbol{Q}^{ii}(z_1)\boldsymbol{Q}^{ii}(z_2)\right) + 2 \sum_{1 \leq i < j \leq 3} \operatorname{Tr}\left(\boldsymbol{Q}^{ij}(z_1)\boldsymbol{Q}^{ji}(z_2)\right),$$

so the tightness of $\text{Tr}(\mathbf{Q}(z)) - \mathbb{E}[\text{Tr}(\mathbf{Q}(z))]$ is indeed equivalent to

$$C_{s_1t_1, s_2t_2, N}^{(3)}(z_1, z_2) = \operatorname{Cov}\left(\operatorname{Tr}(\boldsymbol{Q}^{s_1t_1}(z_1)\boldsymbol{Q}^{t_1s_1}(z_2)), \operatorname{Tr}(\boldsymbol{Q}^{s_2t_2}(z_1)\boldsymbol{Q}^{t_2s_2}(z_2))\right) < C_{\eta_0}$$

for any $z_1, z_2 \in \mathcal{S}_{\eta_0}$ and $s_1, s_2, t_1, t_2 \in \{1, 2, 3\}$. Similar as proofs of Theorem E.1, we will derive a system equation for all $\mathcal{C}_{s_1t_1, s_2t_2, N}^{(3)}(z_1, z_2)$. For convenience, we only present the detailed calculation procedures of $\mathcal{C}_{11, 11, N}^{(3)}$ and omit the (z_1, z_2) behind it, further assume $\mathcal{C}_{11, 11, N}^{(3)} \geq 1$, otherwise it is bounded. By $\mathbf{Q}(z)\mathbf{M} - z\mathbf{Q}(z) = \mathbf{I}_N$, we obtain that

$$z_{1}C_{11,11,N}^{(3)}(z_{1},z_{2}) = \mathbb{E}\left[\operatorname{Tr}(\boldsymbol{Q}^{11}(z_{1})\boldsymbol{Q}^{11}(z_{2}))\left\{\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{1})\boldsymbol{Q}^{11}(\bar{z}_{2}))\right\}^{c}\right]$$

$$= \frac{1}{\sqrt{N}} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[X_{ijk}(c_{k}Q_{j}^{21}(z_{1})Q_{\cdot i}^{11}(z_{2}) + b_{j}Q_{k\cdot}^{31}(z_{1})Q_{\cdot i}^{11}(z_{2}))\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{1})\boldsymbol{Q}^{11}(\bar{z}_{2}))^{c}\right] - C_{1,11,N}^{(3)}(z_{1},z_{2}), \tag{F.10}$$

where $C_{1,11,N}^{(3)}(z_1,z_2) = \text{Cov}\left(\text{Tr}(\boldsymbol{Q}^{11}(z_2)), \text{Tr}(\boldsymbol{Q}^{11}(z_1)\boldsymbol{Q}^{11}(z_2))\right)$ by (F.5). Note that $C_{s_1t_1,s_2,N}^{(3)}(z_1,z_2)$ and $C_{s_2,s_1t_1,N}^{(3)}(z_1,z_2)$ are conjugate, to solve $C_{s_1t_1,s_2t_2,N}^{(3)}(z_1,z_2)$, we also need to obtain the system equation of $C_{s_1t_1,s_2,N}^{(3)}(z_1,z_2)$. Thus, we will calculate (F.10) and derive the system equations of (F.11), respectively.

(F.10): First, let

$$G^1_{ijk}(z_1,z_2) := c_k Q^{21}_{j\cdot}(z_2) Q^{11}_{\cdot i}(z_1) + b_j Q^{31}_{k\cdot}(z_2) Q^{11}_{\cdot i}(z_1).$$

By the cumulant expansion (D.4), we have

$$(\mathbf{F}.\mathbf{10}) = \frac{1}{\sqrt{N}} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[X_{ijk}G_{ijk}^{1}(z_{1},z_{2})\{\text{Tr}(\mathbf{Q}^{11}(\bar{z}_{1})\mathbf{Q}^{11}(\bar{z}_{2}))\}^{c}\right] = \frac{1}{\sqrt{N}} \sum_{i,j,k=1}^{m,n,p} \left(\sum_{\alpha=1}^{3} \frac{\kappa_{\alpha+1}}{\alpha!} \mathbb{E}\left[\partial_{ijk}^{(\alpha)}\{G_{ijk}^{1}(z_{1},z_{2})\{\text{Tr}(\mathbf{Q}^{11}(\bar{z}_{1})\mathbf{Q}^{11}(\bar{z}_{2}))\}^{c}\}\right] + \epsilon_{ijk}^{(4)}\right).$$

First derivatives: When $\alpha = 1$, similar as the proofs for l = 1 in Theorem E.1, by direct calculations, we can show the followings by Lemma D.3:

$$\begin{split} N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\partial_{ijk}^{(1)} \left\{ G_{ijk}^{1}(z_{1},z_{2}) \left\{ \text{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{1})\boldsymbol{Q}^{11}(\bar{z}_{2})) \right\}^{c} \right\} \right] = \\ - N^{-1} \mathbb{E} \left[\text{Tr}(\boldsymbol{Q}^{11}(z_{2})) \, \text{Tr}(\boldsymbol{Q}^{12}(z_{1})\boldsymbol{Q}^{21}(z_{2}) + \boldsymbol{Q}^{13}(z_{1})\boldsymbol{Q}^{31}(z_{2})) \left\{ \text{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{1})\boldsymbol{Q}^{11}(\bar{z}_{2})) \right\}^{c} \right] \\ - N^{-1} \mathbb{E} \left[\text{Tr}(\boldsymbol{Q}^{11}(z_{1})\boldsymbol{Q}^{11}(z_{2})) \, \text{Tr}(\boldsymbol{Q}^{22}(z_{1}) + \boldsymbol{Q}^{33}(z_{1})) \, \text{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{1})\boldsymbol{Q}^{11}(\bar{z}_{2}))^{c} \right] + \mathcal{O}(C_{\eta_{0}}N^{-\omega}) \\ = -(V_{12,N}^{(3)}(z_{1},z_{2}) + V_{13,N}^{(3)}(z_{1},z_{2})) \mathcal{C}_{1,11,N}^{(3)}(z_{1},z_{2}) - \mathfrak{m}_{1}(z_{2}) (\mathcal{C}_{12,11,N}^{(3)} + \mathcal{C}_{13,11,N}^{(3)}) + \mathcal{O}(C_{\eta_{0}}N^{-\omega}) \\ - V_{11,N}^{(3)}(z_{1},z_{2}) (\mathcal{C}_{2,11,N}^{(3)}(z_{1},z_{2}) + \mathcal{C}_{3,11,N}^{(3)}(z_{1},z_{2})) - (\mathfrak{m}_{2}(z_{1}) + \mathfrak{m}_{3}(z_{1}) + \mathcal{O}(C_{\eta_{0}}N^{-\omega})) \mathcal{C}_{11,11,N}^{(3)} \end{aligned}$$

where $V_{ij,N}^{(3)}(z_1,z_2)$ are defined in (E.30) and we use the same trick as (E.7). Since

$$\begin{split} &\partial_{ijk}^{(1)}\operatorname{Tr}(\boldsymbol{Q}^{11}(z_1)\boldsymbol{Q}^{11}(z_2)) = \sum_{s,t=1}^{m,m} \partial_{ijk}^{(1)} \left\{ Q_{st}^{11}(z_1) Q_{st}^{11}(z_2) \right\} = \sum_{s,t=1}^{m,m} Q_{st}^{11}(z_2) \partial_{ijk}^{(1)} Q_{st}^{11}(z_1) + Q_{st}^{11}(z_1) \partial_{ijk}^{(1)} Q_{st}^{11}(z_2) \\ &= -N^{-1/2} \sum_{r_1 \neq r_2}^{3} \mathcal{A}_{ijk}^{(r_1,r_2)} Q_{\tilde{t}_1}^{t_21}(z_1) \boldsymbol{Q}^{11}(z_2) Q_{\tilde{t}_3}^{1t_3}(z_1) - N^{-1/2} \sum_{r_1 \neq r_2}^{3} \mathcal{A}_{ijk}^{(r_1,r_2)} Q_{\tilde{s}_1}^{s_21}(z_2) \boldsymbol{Q}^{11}(z_1) Q_{\tilde{s}_3}^{1s_3}(z_2), \end{split}$$

then by Lemma D.5, we have

$$\begin{split} N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[G_{ijk}^{1}(z_{1},z_{2}) \partial_{ijk}^{(1)} \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{1}) \boldsymbol{Q}^{11}(\bar{z}_{2})) \right] &= \mathrm{O}(\eta_{0}^{-5} N^{-1/2}) \\ -2N^{-1} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{1}) \boldsymbol{Q}^{11}(\bar{z}_{2}) [\boldsymbol{Q}^{12}(\bar{z}_{1}) \boldsymbol{Q}^{21}(z_{1}) \boldsymbol{Q}^{11}(z_{2}) + \boldsymbol{Q}^{13}(\bar{z}_{1}) \boldsymbol{Q}^{31}(z_{1}) \boldsymbol{Q}^{11}(z_{2})] \right) \right] \\ -2N^{-1} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{2}) \boldsymbol{Q}^{11}(\bar{z}_{1}) [\boldsymbol{Q}^{12}(\bar{z}_{2}) \boldsymbol{Q}^{21}(z_{1}) \boldsymbol{Q}^{11}(z_{2}) + \boldsymbol{Q}^{13}(\bar{z}_{2}) \boldsymbol{Q}^{31}(z_{1}) \boldsymbol{Q}^{11}(z_{2})] \right) \right]. \end{split}$$

For simplicity, we define

$$\mathcal{V}_{k_1 l_1, k_2 l_2, N}^{(3)}(z_1, z_2) := \frac{1}{N} \sum_{s \neq k_1}^{3} \sum_{r=1}^{2} \mathbb{E} \left[\operatorname{Tr} \left(\boldsymbol{Q}^{k_1 k_2}(\bar{z}_{3-r}) \boldsymbol{Q}^{k_2 l_2}(\bar{z}_r) \boldsymbol{Q}^{l_2 s}(\bar{z}_{3-r}) \boldsymbol{Q}^{s l_1}(z_1) \boldsymbol{Q}^{l_1 k_1}(z_2) \right) \right],$$

then we have

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\partial_{ijk}^{(1)} \left\{ G_{ijk}^{1}(z_{1},z_{2}) \left\{ \text{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{1})\boldsymbol{Q}^{11}(\bar{z}_{2})) \right\}^{c} \right\} \right] =$$

$$-2\mathcal{V}_{11,11,N}^{(3)}(z_{1},z_{2}) - (1 + V_{12,N}^{(3)}(z_{1},z_{2}) + V_{13,N}^{(3)}(z_{1},z_{2}))\mathcal{C}_{1,11,N}^{(3)} - \mathfrak{m}_{1}(z_{2})(\mathcal{C}_{12,11,N}^{(3)} + \mathcal{C}_{13,11,N}^{(3)})$$

$$-V_{11,N}^{(3)}(z_{1},z_{2})(\mathcal{C}_{2,11,N}^{(3)} + \mathcal{C}_{3,11,N}^{(3)}) - (\mathfrak{m}_{2}(z_{1}) + \mathfrak{m}_{3}(z_{1}) + \mathcal{O}(\mathcal{C}_{\eta_{0}}N^{-\omega}))\mathcal{C}_{11,11,N}^{(3)} + \mathcal{O}(\mathcal{C}_{\eta_{0}}N^{-\omega}),$$
(F.12)

where we omit (z_1, z_2) behind $C_{st,11,N}^{(3)}(z_1, z_2)$ and $C_{s,11,N}^{(3)}(z_1, z_2)$ to save space.

Second derivatives: When $\alpha=2$, similar as the proofs for l=2 in Theorem E.1, we claim that there is no major terms. Since $|G_{ijk}^1(z_1,z_2)| \leq \mathrm{O}(\eta_0^{-2})$ and $|\partial_{ijk}^{(1)}\mathrm{Tr}(\boldsymbol{Q}^{11}(\bar{z}_1)\boldsymbol{Q}^{11}(\bar{z}_2))| \leq \mathrm{O}(\eta_0^{-3}N^{-1/2})$, we can show the sum over all i,j,k of following terms are minor by Lemma D.5:

$$G_{ijk}^{1}(z_{1},z_{2})\mathscr{O}\left\{\partial_{ijk}^{(2)}\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{1})\boldsymbol{Q}^{11}(\bar{z}_{2}))\right\} \quad \text{and} \quad \partial_{ijk}^{(1)}\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{1})\boldsymbol{Q}^{11}(\bar{z}_{2}))\mathscr{O}\left\{\partial_{ijk}^{(1)}G_{ijk}^{1}(z_{1},z_{2})\right\},$$

where \mathcal{O} is defined in (D.34). Otherwise, let's consider

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} G^1_{ijk}(z_1,z_2) \mathcal{D} \{ \partial^{(2)}_{ijk} \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_1) \boldsymbol{Q}^{11}(\bar{z}_2)) \},$$

since

$$\begin{split} &\partial_{ijk}^{(2)} \{ \text{Tr}(\boldsymbol{Q}^{11}(z_1) \boldsymbol{Q}^{11}(z_2)) \} \\ &= \frac{2}{N} \sum_{\substack{t_1 \neq t_2 \\ t_3 \neq t_4}}^{3} \sum_{r=1}^{2} \mathcal{A}_{ijk}^{(t_1,t_2)} Q_{\tilde{t}_2\tilde{t}_3}^{t_2t_3}(z_r) \mathcal{A}_{ijk}^{(t_3,t_4)} Q_{\tilde{t}_4}^{t_41}(z_r) \boldsymbol{Q}^{11}(z_{3-r}) Q_{.\tilde{t}_1}^{1t_1}(z_r) \\ &+ \frac{2}{N} \sum_{\substack{t_1 \neq t_2 \\ t_3 \neq t_4}}^{d} \mathcal{A}_{ijk}^{(t_1,t_2)} Q_{\tilde{t}_2}^{t_21}(z_1) Q_{.\tilde{t}_3}^{1t_3}(z_1) \mathcal{A}_{ijk}^{(t_3,t_4)} Q_{\tilde{t}_4}^{t_41}(z_2) Q_{.\tilde{t}_1}^{1t_1}(z_2), \end{split}$$

then $\mathscr{D}\left\{\partial_{ijk}^{(2)}\operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_1)\boldsymbol{Q}^{11}(\bar{z}_2))\right\}$ contains (e.g.) $N^{-1}c_k^2Q_{ii}^{11}(\bar{z}_1)Q_{j\cdot}^{21}(\bar{z}_1)\boldsymbol{Q}^{11}(\bar{z}_2)Q_{\cdot j}^{12}(\bar{z}_1)$ and

$$N^{-3/2} \sum_{i,j,k=1}^{m,n,p} c_k^3 Q_{i\cdot}^{11}(z_2) Q_{\cdot j}^{12}(z_1) Q_{ii}^{11}(\bar{z}_1) Q_{j\cdot}^{21}(\bar{z}_1) \boldsymbol{Q}^{11}(\bar{z}_2) Q_{\cdot j}^{12}(\bar{z}_1)$$

$$= N^{-3/2} \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_1) \circ (\boldsymbol{Q}^{11}(z_2) \boldsymbol{Q}^{12}(z_1) \boldsymbol{Q}^{21}(\bar{z}_1) \boldsymbol{Q}^{11}(\bar{z}_2) \boldsymbol{Q}^{11}(\bar{z}_1))) = O(\eta_0^{-6} N^{-1/2}),$$

and we can also show other situations are also minor. Finally, since $N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \partial_{ijk}^{(2)} G_{ijk}^1(z_1,z_2)$ contains the following major term:

$$N^{-3/2} \sum_{i,j,k=1}^{m,n,p} a_i b_j c_k Q_{i\cdot}^{11}(z_2) Q_{\cdot i}^{11}(z_1) Q_{kk}^{33}(z_1) Q_{jj}^{22}(z_1) = N^{-3/2} \mathbf{1}_m' \boldsymbol{Q}^{11}(z_1) \boldsymbol{Q}^{11}(z_2) \boldsymbol{a} \cdot \mathbf{1}_n' \boldsymbol{Q}^{22}(z_1) \boldsymbol{b} \cdot \mathbf{1}_p' \boldsymbol{Q}^{22}(z_1) \boldsymbol{c},$$

so by Lemma D.3, it yields that

$$\left| \mathbb{E} \left[\text{Tr}(\boldsymbol{Q}^{11}(\bar{z}_1) \boldsymbol{Q}^{11}(\bar{z}_2))^c \left\{ N^{-3/2} \mathbf{1}_m' \boldsymbol{Q}^{11}(z_1) \boldsymbol{Q}^{11}(z_2) \boldsymbol{a} \cdot \mathbf{1}_n' \boldsymbol{Q}^{22}(z_1) \boldsymbol{b} \cdot \mathbf{1}_p' \boldsymbol{Q}^{22}(z_1) \right\}^c \right] \right| \leq \mathcal{O}(C_{\eta_0} N^{-\omega}) \mathcal{C}_{11,11,N}^{(3)},$$

where we apply the same trick as the part l=2 of Theorem E.1. For other terms, the results are same, so we obtain

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\text{Tr}(\boldsymbol{Q}^{11}(\bar{z}_1)\boldsymbol{Q}^{11}(\bar{z}_2))^c \partial_{ijk}^{(2)} G_{ijk}^1(z_1,z_2) \right] \leq \mathcal{O}(C_{\eta_0} N^{-\omega}) \mathcal{C}_{11,11,N}^{(3)}.$$

Therefore, combining with previous results, we have

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[\partial_{ijk}^{(2)} \left\{ G_{ijk}^{1}(z_{1},z_{2}) \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{1})\boldsymbol{Q}^{11}(\bar{z}_{2})) \right\} \right] \leq \mathcal{O}(C_{\eta_{0}} N^{-\omega}) \mathcal{C}_{11,11,N}^{(3)}. \tag{F.13}$$

Third derivatives: When $\alpha = 3$, by the same proofs as those for l = 3 in Theorem E.1, we can conclude that for $\alpha = 0, 1, 3$

$$N^{-1/2} \left| \sum_{i,j,k=1}^{m,n,p} \partial_{ijk}^{(\alpha)} \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_1) \boldsymbol{Q}^{11}(\bar{z}_2)) \partial_{ijk}^{(3-\alpha)} G_{ijk}^1(z_1,z_2) \right| \leq \mathcal{O}(C_{\eta_0} N^{-\omega}) \mathcal{C}_{11,11,N}^{(3)},$$

here we omit the details to save space. Now, we only focus on the case of $\alpha = 2$. Since

$$\begin{split} &\partial_{ijk}^{(2)} \{ \mathrm{Tr}(\boldsymbol{Q}^{11}(z_1) \boldsymbol{Q}^{11}(z_2)) \} \\ &= \frac{2}{N} \sum_{\substack{t_1 \neq t_2 \\ t_3 \neq t_4}}^{3} \sum_{r=1}^{2} \mathcal{A}_{ijk}^{(t_1,t_2)} Q_{\tilde{t}_2\tilde{t}_3}^{t_2t_3}(z_r) \mathcal{A}_{ijk}^{(t_3,t_4)} Q_{\tilde{t}_4}^{t_41}(z_r) \boldsymbol{Q}^{11}(z_{3-r}) Q_{.\tilde{t}_1}^{1t_1}(z_r) \\ &+ \frac{2}{N} \sum_{\substack{t_1 \neq t_2 \\ t_3 \neq t_4}}^{d} \mathcal{A}_{ijk}^{(t_1,t_2)} Q_{\tilde{t}_2}^{t_21}(z_1) Q_{.\tilde{t}_3}^{1t_3}(z_1) \mathcal{A}_{ijk}^{(t_3,t_4)} Q_{\tilde{t}_4}^{t_41}(z_2) Q_{.\tilde{t}_1}^{1t_1}(z_2), \end{split}$$

and

$$\partial_{ijk}^{(1)}\{G_{ijk}^{1}(z_{1},z_{2})\} = -\frac{1}{\sqrt{N}}\sum_{r\neq 1}^{3}\mathcal{A}_{ijk}^{(1,r)}\mathcal{A}_{ijk}^{(t_{1},t_{2})}\left(Q_{i\tilde{t}_{1}}^{1t_{1}}(z_{2})Q_{i\tilde{t}_{2}}^{t_{2}1}(z_{2})Q_{\cdot\tilde{r}}^{1r}(z_{1}) + Q_{i\cdot}^{11}(z_{2})Q_{\cdot\tilde{t}_{1}}^{1t_{1}}(z_{1})Q_{i\tilde{t}_{2}\tilde{r}}^{t_{2}r}(z_{1})\right),$$

then by Lemmas D.6 and D.5, we have

$$\begin{split} &\frac{1}{\sqrt{N}} \sum_{i,j,k=1}^{m,n,p} \sum_{t_3 \neq t_4}^{3} \mathbb{E} \left[\partial_{ijk}^{(1)} \{G_{ijk}^1(z_1,z_2)\} \partial_{ijk}^{(2)} \{ \text{Tr}(\boldsymbol{Q}^{11}(z_1) \boldsymbol{Q}^{11}(z_2)) \} \right] = \mathcal{O}(C_{\eta_0} N^{-1/2}) \\ &- \frac{2}{N^2} \sum_{i,j,k=1}^{m,n,p} \sum_{r \neq 1}^{3} \sum_{t_1,t_2}^{(1,r)} \sum_{w=1}^{2} \mathbb{E} \left[(\mathcal{A}_{ijk}^{(1,r)})^4 Q_{ii}^{11}(z_2) Q_{r.}^{r.l}(z_1) Q_{r.}^{1r}(z_2) Q_{t_1t_1}^{t_1t_1}(\bar{z}_w) Q_{t_2}^{t_21}(\bar{z}_w) \boldsymbol{Q}^{11}(\bar{z}_{3-w}) Q_{.t_2}^{1t_2}(\bar{z}_w) \right] \\ &- \frac{2}{N^2} \sum_{i,j,k=1}^{m,n,p} \sum_{r \neq 1}^{3} \sum_{t_1,t_2}^{2} \mathbb{E} \left[(\mathcal{A}_{ijk}^{(1,r)})^4 Q_{i}^{11}(z_2) Q_{.i}^{r.l}(z_1) Q_{rr}^{r.r}(z_1) Q_{t_1t_1}^{r.r}(\bar{z}_w) Q_{t_2}^{t_21}(\bar{z}_w) \boldsymbol{Q}^{11}(\bar{z}_{3-w}) Q_{.t_2}^{1t_2}(\bar{z}_w) \right] \\ &- \frac{2}{N^2} \sum_{i,j,k=1}^{m,n,p} \sum_{r \neq 1}^{3} \sum_{t_1,t_2}^{2} \mathbb{E} \left[(\mathcal{A}_{ijk}^{(1,r)})^4 Q_{i}^{11}(z_2) Q_{r.}^{r.l}(z_1) Q_{rr}^{r.r}(z_2) Q_{t_1}^{t_1}(\bar{z}_1) Q_{t_2}^{t_21}(\bar{z}_2) Q_{.t_2}^{1t_2}(\bar{z}_2) Q_{.t_2}^{1t_2}(\bar{z}_2) \right] \\ &- \frac{2}{N^2} \sum_{i,j,k=1}^{m,n,p} \sum_{r \neq 1}^{3} \sum_{t_1,t_2}^{1,r.r} \mathbb{E} \left[(\mathcal{A}_{ijk}^{(1,r)})^4 Q_{i}^{11}(z_2) Q_{r.}^{r.l}(z_1) Q_{rr}^{r.r}(z_2) Q_{t_1}^{t_1}(\bar{z}_1) Q_{t_2}^{1t_1}(\bar{z}_1) Q_{t_2}^{t_2}(\bar{z}_2) Q_{.t_2}^{1t_2}(\bar{z}_2) \right] \\ &- \frac{2}{N^2} \sum_{r=2}^{3} \sum_{w=1}^{3} \sum_{t_1,t_2}^{1,r.r} \mathbb{E} \left[(\mathcal{A}_{ijk}^{(1,r)})^4 Q_{i}^{11}(z_2) Q_{r.}^{11}(z_1) Q_{rr}^{r.r}(z_1) Q_{t_1}^{t_1}(\bar{z}_1) Q_{t_2}^{t_2}(\bar{z}_2) Q_{.t_2}^{1t_2}(\bar{z}_2) Q_{.t_2}^{1t_2}(\bar{z}_2) \right] \\ &- \frac{2}{N^2} \sum_{r=2}^{3} \sum_{w=1}^{3} \sum_{t_1,t_2}^{1,r.r} \| \boldsymbol{a}^{(5-r)} \|_4^4 \mathbb{E} \left[\text{Tr}(\boldsymbol{Q}^{t_2t_2}(z_2) \circ (\boldsymbol{Q}^{t_2t_1}(\bar{z}_w) \boldsymbol{Q}^{11}(\bar{z}_w) \boldsymbol{Q}^{11}(\bar{z}_3-w) \boldsymbol{Q}^{1t_2}(\bar{z}_w))) \cdot \text{Tr}(\boldsymbol{Q}^{r.t}(z_1) Q_{1}^{r.t}(z_1)) \right] \\ &- \frac{2}{N^2} \sum_{r=2}^{3} \sum_{w=1}^{3} \sum_{t_1,t_2}^{1,r.} \| \boldsymbol{a}^{(5-r)} \|_4^4 \mathbb{E} \left[\text{Tr}(\boldsymbol{Q}^{11}(z_2) \circ (\boldsymbol{Q}^{11}(\bar{z}_w) \boldsymbol{Q}^{11}(\bar{z}_w))) \cdot \text{Tr}(\boldsymbol{Q}^{r.t}(z_1) Q_{1}^{r.t}(z_2)) \circ (\boldsymbol{Q}^{r.t}(\bar{z}_3-w) \boldsymbol{Q}^{1r}(\bar{z}_3-w)) \right) \right] \\ &- \frac{2}{N^2} \sum_{r=2}^{3} \sum_{t_1,t_2}^{1,r.} \| \boldsymbol{a}^{(5-r)} \|_4^4 \mathbb{E} \left[\text{Tr}(\boldsymbol{Q}^{11}(z_2) \circ (\boldsymbol{Q}^{11}(\bar{z}_w) \boldsymbol{Q}^{11}(\bar{z}_w) \boldsymbol{Q}^{11}(\bar$$

where the notation $\sum_{t_1,t_2}^{(1,r)}$ means the summation of t_1 and t_2 are over $\{1,2,3\}\setminus\{1,r\}$, $\mathcal{U}_{11,11,N}^{(3)}(z,z)$ is defined in (F.8).

Remainders: When $\alpha = 4$, we can repeat the same proof argument as those for the part l = 4 of Theorem E.1 to show that the sum over all i, j, k of $\epsilon_{ijk}^{(4)}$ is minor, here we omit details to save space.

Now, combining (F.12), (F.13) and (F.8), we obtain

$$\begin{split} &(z_1+\mathfrak{m}(z_1)-\mathfrak{m}_1(z_1)+\mathcal{O}(C_{\eta_0}N^{-\omega}))\mathcal{C}_{11,11,N}^{(3)}=-2\mathcal{V}_{11,11,N}^{(3)}(z_1,z_2)-\kappa_4\mathcal{G}_{11,11,N}^{(3)}(z_1,z_2)-\mathfrak{m}_1(z_2)(\mathcal{C}_{12,11,N}^{(3)}+\mathcal{C}_{13,11,N}^{(3)})\\ &-(1+V_{12,N}^{(3)}(z_1,z_2)+V_{13,N}^{(3)}(z_1,z_2))\mathcal{C}_{1,11,N}^{(3)}-V_{11,N}^{(3)}(z_1,z_2)(\mathcal{C}_{2,11,N}^{(3)}+\mathcal{C}_{3,11,N}^{(3)})+\mathcal{O}(C_{\eta_0}N^{-\omega}). \end{split}$$

Similarly, for any $s,t \in \{1,2,3\}$ and $\mathcal{C}^{(3)}_{st,11,N}(z,z)$, we have

$$(z_1 + \mathfrak{m}(z_1) - \mathfrak{m}_s(z_1))\mathcal{C}_{st,11,N}^{(3)} = -2\mathcal{V}_{st,11,N}^{(3)}(z_1, z_2) - \kappa_4 \mathcal{U}_{st,11,N}^{(3)}(z_1, z_2) - \mathfrak{m}_s(z_2) \sum_{l \neq s}^{3} \mathcal{C}_{lt,11,N}^{(3)}$$
(F.14)

$$-\left(\delta_{st} + \sum_{l \neq s}^{3} V_{lt,N}^{(3)}(z_1, z_2)\right) \mathcal{C}_{s,11,N}^{(3)} - V_{st,N}^{(3)}(z_1, z_2) \sum_{l \neq s}^{3} \mathcal{C}_{l,11,N}^{(3)} + \mathcal{O}(C_{\eta_0} N^{-\omega}) \mathcal{C}_{11,11,N}^{(3)} + \mathcal{O}(C_{\eta_0} N^{-\omega}).$$

(F.11): Next, we will derive the system equations for all $C_{l,11,N}^{(3)}$. Here, we only present the detailed calculation procedure for $C_{11,1}^{(3)}(z_1, z_2)$, since others are the same. By the cumulant expansion (D.4),

we can obtain

$$z_1 \mathcal{C}_{11,1,N}^{(3)}(z_1, z_2) = \frac{1}{\sqrt{N}} \sum_{i,j,k=1}^{m,n,p} \left(\sum_{\alpha=1}^{3} \frac{\kappa_{\alpha+1}}{\alpha!} \mathbb{E}\left[\partial_{ijk}^{(\alpha)} \left\{ G_{ijk}^1(z_1, z_2) \operatorname{Tr}(\boldsymbol{Q}(\bar{z}_2))^c \right\} \right] + \epsilon_{ijk}^{(4)} \right) - \mathcal{C}_{1,1,N}^{(3)}(z_1, z_2),$$

where $C_{1,1,N}^{(3)}(z_1, z_2)$ is defined in (E.3) and it is already bounded by C_{η_0} . Actually, we can repeat the proofs in Theorem E.1, and major terms only appear in cases of $\alpha = 1$ and 3, so we omit other cases to save space.

First derivatives: When $\alpha = 1$, by Lemma D.5 and Theorem D.3, we can show that

$$\begin{split} N^{-1/2} \sum_{l=1}^{m} \mathbb{E} \left[\partial_{ijk}^{(1)} \{ G_{ijk}^{1}(z_{1}, z_{2}) \} \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{2}))^{c} \right] = \\ - N^{-1} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{11}(z_{2})) \operatorname{Tr}(\boldsymbol{Q}^{12}(z_{2}) \boldsymbol{Q}^{21}(z_{1}) + \boldsymbol{Q}^{13}(z_{2}) \boldsymbol{Q}^{31}(z_{1})) \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{2}))^{c} \right] \\ - N^{-1} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{11}(z_{1}) \boldsymbol{Q}^{11}(z_{2})) \operatorname{Tr}(\boldsymbol{Q}^{22}(z_{1}) + \boldsymbol{Q}^{33}(z_{1})) \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{2}))^{c} \right] + \operatorname{O}(C_{\eta_{0}} N^{-1/2}) \\ = -(V_{12,N}^{(3)}(z_{1}, z_{2}) + V_{13,N}^{(3)}(z_{1}, z_{2})) \mathcal{C}_{1,1,N}^{(3)}(z_{2}, z_{2}) - V_{11}(z_{1}, z_{2}) (\mathcal{C}_{2,1,N}^{(3)}(z_{1}, z_{2}) + \mathcal{C}_{3,1,N}^{(3)}(z_{1}, z_{2})) \\ - \mathfrak{m}_{1}(z_{2}) (\mathcal{C}_{12,1,N}^{(3)}(z_{1}, z_{2}) + \mathcal{C}_{13,1}^{(3)}(z_{1}, z_{2})) - (\mathfrak{m}_{2}(z_{1}) + \mathfrak{m}_{3}(z_{1})) \mathcal{C}_{11,1,N}^{(3)}(z_{1}, z_{2}) + \operatorname{O}(C_{\eta_{0}} N^{-\omega}) \end{split}$$

and

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[G_{ijk}^{1}(z_{1},z_{2})\partial_{ijk}^{(1)}\{\text{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{2}))^{c}\}\right] = \\ -2N^{-1}\mathbb{E}\left[\text{Tr}(\boldsymbol{Q}^{11}(z_{2})\boldsymbol{Q}^{12}(z_{1})\boldsymbol{Q}^{21}(\bar{z}_{2})\boldsymbol{Q}^{11}(\bar{z}_{2}) + \boldsymbol{Q}^{11}(z_{2})\boldsymbol{Q}^{13}(z_{1})\boldsymbol{Q}^{31}(\bar{z}_{2})\boldsymbol{Q}^{11}(\bar{z}_{2}))\right] + C_{n_{0}}N^{-1/2}$$

For simplicity, we denote

$$\mathcal{V}_{k_1 l_1, k_2, N}^{(3)}(z_1, z_2) := N^{-1} \sum_{r \neq k_1}^{3} \mathbb{E} \left[\text{Tr}(\boldsymbol{Q}^{r l_1}(z_1) \boldsymbol{Q}^{l_1 k_1}(z_2) \boldsymbol{Q}^{k_1 k_2}(\bar{z}_1) \boldsymbol{Q}^{k_2 r}(\bar{z}_2)) \right],$$

where $k_1, l_1, k_2 \in \{1, 2, 3\}$, then we have

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[G_{ijk}^{1}(z_{1},z_{2}) \partial_{ijk}^{(1)} \{ \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{2}))^{c} \} \right] = -2 \mathcal{V}_{11,1,N}^{(3)}(z_{1},z_{2})$$

$$- (V_{12,N}^{(3)}(z_{1},z_{2}) + V_{13,N}^{(3)}(z_{1},z_{2})) \mathcal{C}_{1,1,N}^{(3)}(z_{2},z_{2}) - V_{11}(z_{1},z_{2}) (\mathcal{C}_{2,1,N}^{(3)}(z_{1},z_{2}) + \mathcal{C}_{3,1,N}^{(3)}(z_{1},z_{2}))$$

$$- \mathfrak{m}_{1}(z_{2}) (\mathcal{C}_{12,1,N}^{(3)}(z_{1},z_{2}) + \mathcal{C}_{13,1}^{(3)}(z_{1},z_{2})) - (\mathfrak{m}_{2}(z_{1}) + \mathfrak{m}_{3}(z_{1})) \mathcal{C}_{11,1,N}^{(3)}(z_{1},z_{2}) + \mathcal{O}(C_{n0}N^{-\omega}).$$
(F.15)

Second derivatives: The calculations of second derivatives are similar as those in proofs of Theorem E.1, we can also show that

$$N^{-1/2} \left| \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\partial_{ijk}^{(2)} \{ G_{ijk}^1(z_1, z_2) \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_2))^c \} \right] \right| \le \mathcal{O}(C_{\eta_0} N^{-\omega}),$$

we omit details here to save space.

Third derivatives: When $\alpha = 3$, similar as previous arguments for $C_{11,11,N}^{(3)}$, the major terms will only appear in

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\partial_{ijk}^{(1)} G_{ijk}^1(z_1,z_2) \partial_{ijk}^{(2)} \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_2))^c \right],$$

where

$$\partial_{ijk}^{(2)}\operatorname{Tr}(\boldsymbol{Q}^{11}(z)) = 2N^{-1} \sum_{t_1 \neq t_2}^{3} \sum_{t_3 \neq t_4}^{3} \mathcal{A}_{ijk}^{(t_1, t_2)} Q_{\tilde{t}_2 \tilde{t}_3}^{t_2 t_3}(z) \mathcal{A}_{ijk}^{(t_3, t_4)} Q_{\tilde{t}_4}^{t_4 1}(z) Q_{.\tilde{t}_1}^{1t_1}(z),$$

and

$$\partial_{ijk}^{(1)}\{G_{ijk}^{1}(z_{1},z_{2})\} = -\frac{1}{\sqrt{N}}\sum_{r\neq 1}^{3}\mathcal{A}_{ijk}^{(1,r)}\mathcal{A}_{ijk}^{(t_{1},t_{2})}\big(Q_{i\tilde{t}_{1}}^{1t_{1}}(z_{1})Q_{i\tilde{t}_{2}}^{t_{2}1}(z_{1})Q_{\cdot\tilde{r}}^{1r}(z_{2}) + Q_{i\cdot}^{11}(z_{1})Q_{\cdot\tilde{t}_{1}}^{1t_{1}}(z_{2})Q_{i\tilde{t}_{2}\tilde{r}}^{t_{2}r}(z_{2})\big),$$

then we have

$$\begin{split} N^{-1/2} & \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\partial_{ijk}^{(1)} G_{ijk}^{1}(z_{1},z_{2}) \partial_{ijk}^{(2)} \operatorname{Tr}(\boldsymbol{Q}^{11}(\bar{z}_{2}))^{c} \right] = \mathcal{O}(C_{\eta_{0}} N^{-\omega}) \\ & - \frac{2}{N^{2}} \sum_{i,j,k=1}^{m,n,p} \sum_{r\neq 1}^{3} \mathbb{E} \left[(\mathcal{A}_{ijk}^{(1,r)})^{4} Q_{ii}^{11}(z_{1}) Q_{r}^{r1}(z_{1}) Q_{r}^{1r}(z_{2}) Q_{ii}^{11}(\bar{z}_{2}) Q_{r}^{r1}(\bar{z}_{2}) Q_{r}^{1r}(\bar{z}_{2}) \right] \\ & - \frac{2}{N^{2}} \sum_{i,j,k=1}^{m,n,p} \sum_{r\neq 1}^{3} \mathbb{E} \left[(\mathcal{A}_{ijk}^{(1,r)})^{4} Q_{ii}^{11}(z_{1}) Q_{r}^{r1}(z_{1}) Q_{r}^{1r}(z_{2}) Q_{rr}^{rp}(z_{2}) Q_{ii}^{11}(\bar{z}_{2}) Q_{ii}^{11}(\bar{z}_{2}) Q_{ii}^{11}(\bar{z}_{2}) \right] \\ & - \frac{2}{N^{2}} \sum_{i,j,k=1}^{m,n,p} \sum_{r\neq 1}^{3} \mathbb{E} \left[(\mathcal{A}_{ijk}^{(1,r)})^{4} Q_{i}^{11}(z_{1}) Q_{i}^{11}(z_{2}) Q_{rr}^{rr}(z_{2}) Q_{ii}^{11}(\bar{z}_{2}) Q_{r}^{rr}(\bar{z}_{2}) Q_{i}^{1r}(\bar{z}_{2}) \right] \\ & - \frac{2}{N^{2}} \sum_{i,j,k=1}^{m,n,p} \sum_{r\neq 1}^{3} \mathbb{E} \left[(\mathcal{A}_{ijk}^{(1,r)})^{4} Q_{i}^{11}(z_{1}) Q_{i}^{11}(z_{2}) Q_{rr}^{rr}(z_{2}) Q_{rr}^{rr}(\bar{z}_{2}) Q_{i}^{11}(\bar{z}_{2}) Q_{i}^{1r}(\bar{z}_{2}) \right] \\ & - \frac{2}{N^{2}} \sum_{r=2}^{3} \|\boldsymbol{a}^{(5-r)}\|_{4}^{4} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{11}(z_{1}) \circ \boldsymbol{Q}^{11}(\bar{z}_{2})) \cdot \operatorname{Tr}((\boldsymbol{Q}^{r1}(z_{1}) \boldsymbol{Q}^{1r}(z_{2})) \circ (\boldsymbol{Q}^{rr}(\bar{z}_{2}) Q_{i}^{1r}(\bar{z}_{2})) \right] \\ & - \frac{2}{N^{2}} \sum_{r=2}^{3} \|\boldsymbol{a}^{(5-r)}\|_{4}^{4} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{11}(z_{1}) \circ (\boldsymbol{Q}^{11}(\bar{z}_{2}) \boldsymbol{Q}^{11}(\bar{z}_{2})) \cdot \operatorname{Tr}(\boldsymbol{Q}^{rr}(z_{2}) \circ (\boldsymbol{Q}^{rr}(\bar{z}_{2}) Q_{i}^{1r}(\bar{z}_{2})) \right] \\ & - \frac{2}{N^{2}} \sum_{r=2}^{3} \|\boldsymbol{a}^{(5-r)}\|_{4}^{4} \mathbb{E} \left[\operatorname{Tr}((\boldsymbol{Q}^{11}(z_{1}) \boldsymbol{Q}^{11}(z_{2})) \circ \boldsymbol{Q}^{11}(\bar{z}_{2})) \cdot \operatorname{Tr}(\boldsymbol{Q}^{rr}(z_{2}) \circ (\boldsymbol{Q}^{rr}(\bar{z}_{2}) \boldsymbol{Q}^{1r}(\bar{z}_{2})) \right] \\ & - \frac{2}{N^{2}} \sum_{r=2}^{3} \|\boldsymbol{a}^{(5-r)}\|_{4}^{4} \mathbb{E} \left[\operatorname{Tr}((\boldsymbol{Q}^{11}(z_{1}) \boldsymbol{Q}^{11}(z_{2})) \circ (\boldsymbol{Q}^{11}(\bar{z}_{2})) \cdot \operatorname{Tr}(\boldsymbol{Q}^{rr}(z_{2}) \circ (\boldsymbol{Q}^{rr}(\bar{z}_{2}) \boldsymbol{Q}^{1r}(\bar{z}_{2})) \right] \\ & - \frac{2}{N^{2}} \sum_{r=2}^{3} \|\boldsymbol{a}^{(5-r)}\|_{4}^{4} \mathbb{E} \left[\operatorname{Tr}((\boldsymbol{Q}^{11}(z_{1}) \boldsymbol{Q}^{11}(z_{2})) \circ (\boldsymbol{Q}^{11}(\bar{z}_{2})) \cdot \operatorname{Tr}(\boldsymbol{Q}^{rr}(z_{2}) \circ \boldsymbol{Q}^{rr}(\bar{z}_{2})) \right] \\ & - \frac{2}{N^{2}} \sum_{r=2}^{3} \|\boldsymbol{a}^{(5-r)}\|_{4}^{4} \mathbb{E} \left[\operatorname{Tr}((\boldsymbol{Q$$

where $\mathcal{U}_{11,1,N}^{(3)}(z_1,z_2)$ is defined in (F.9).

Remainders: We can repeat the same proof argument as those for the part l=4 of Theorem E.1 to show that the sum over all i, j, k of $\epsilon_{ijk}^{(4)}$ is minor, here we omit details to save space.

Now, combining (F.15) and (F.9), we obtain that

$$\begin{split} &(z_1+\mathfrak{m}_2(z_1)+\mathfrak{m}_3(z_1))\mathcal{C}_{11,1,N}^{(3)}(z_1,z_2) = -2\mathcal{V}_{11,1,N}^{(3)}(z_1,z_2) - \kappa_4\mathcal{U}_{11,1,N}^{(3)}(z_1,z_2) \\ &- (V_{12,N}^{(3)}(z_1,z_2) + V_{13,N}^{(3)}(z_1,z_2))\mathcal{C}_{1,1,N}^{(3)}(z_2,z_2) - V_{11,N}^{(3)}(z_1,z_2)(\mathcal{C}_{2,1,N}^{(3)}(z_1,z_2) + \mathcal{C}_{3,1,N}^{(3)}(z_1,z_2)) \\ &- \mathfrak{m}_1(z_2)(\mathcal{C}_{12,1,N}^{(3)}(z_1,z_2) + \mathcal{C}_{13,1,N}^{(3)}(z_1,z_2)) + \mathcal{O}(C_{\eta_0}N^{-\omega}) \\ &:= -\mathfrak{m}_1(z_2)(\mathcal{C}_{12,1,N}^{(3)}(z_1,z_2) + \mathcal{C}_{13,1,N}^{(3)}(z_1,z_2)) - \mathcal{F}_{11,1,N}^{(3)}(z_1,z_2) + \mathcal{O}(C_{\eta_0}N^{-\omega}) \end{split}$$

Define

$$C_{1,N}^{(3)}(z_1,z_2) := [\mathcal{C}_{st,1,N}^{(3)}(z_1,z_2)]_{3\times 3}$$
 and $F_{1,N}^{(3)}(z_1,z_2) := [\mathcal{F}_{st,1,N}^{(3)}(z_1,z_2)]_{3\times 3}$.

By system equations in §E.3 and Theorem E.1, $\mathcal{V}_{st,1,N}^{(3)}(z_1,z_2), \mathcal{U}_{st,1,N}^{(3)}(z_1,z_2), V_{st,N}^{(3)}(z_1,z_2)$ and $\mathcal{C}_{s,t,N}^{(3)}(z_1,z_2)$ are all bounded by C_{η_0} , so $\|\boldsymbol{F}_{1,N}^{(3)}(z_1,z_2)\| < C_{\eta_0}$. Moreover, since

$$\boldsymbol{\Theta}_{N}^{(3)}(z_{1},z_{2})\boldsymbol{C}_{1,N}^{(3)}(z_{1},z_{2}) = -\boldsymbol{F}_{1,N}^{(3)}(z_{1},z_{2}) + \mathrm{o}(\boldsymbol{1}_{3\times3})$$

where $\boldsymbol{\Theta}_{N}^{(3)}(z_{1}, z_{2})$ is defined in (E.20). By Theorem E.1, we have $\lim_{N\to\infty} \|\boldsymbol{\Theta}_{N}^{(3)}(z_{1}, z_{2})^{-1} + \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1} \circ \boldsymbol{g}(z))\boldsymbol{\Pi}^{(3)}(z_{1}, z_{2})^{-1}\| = 0$, so $\|\boldsymbol{\Theta}_{N}^{(3)}(z_{1}, z_{2})^{-1}\| \leq C_{\mathfrak{c}}\eta_{0}^{-5}$, which implies that

$$\lim_{N\to\infty} \|\boldsymbol{C}_{1,N}^{(3)}(z_1,z_2)\| \le \lim_{N\to\infty} \|\boldsymbol{\Theta}_N^{(3)}(z_1,z_2)^{-1}\| \cdot \|\boldsymbol{F}_{1,N}^{(3)}(z_1,z_2)\| \le C_{\eta_0},$$

i.e. all $|\mathcal{C}_{st,1,N}^{(3)}(z_1,z_2)| \leq C_{\eta_0}$ for $1 \leq s,t \leq 3$. Similarly, we can repeat the previous procedures to show that $|\mathcal{C}_{st,l,N}^{(3)}(z_1,z_2)| \leq C_{\eta_0}$ for $1 \leq s,t,l \leq 3$. Finally, let's back to (F.14), define

$$\begin{split} \mathcal{F}_{st,11,N}^{(3)}(z_1,z_2) &:= 2\mathcal{V}_{st,11,N}^{(3)}(z_1,z_2) + \kappa_4 \mathcal{U}_{st,11,N}^{(3)}(z_1,z_2) \\ &+ \Big(\delta_{st} + \sum_{l \neq c}^3 V_{lt,N}^{(3)}(z_1,z_2) \Big) \mathcal{C}_{s,11,N}^{(3)}(z_1,z_2) + V_{st,N}^{(3)}(z_1,z_2) \sum_{l \neq c}^3 \mathcal{C}_{l,11,N}^{(3)}(z_1,z_2), \end{split}$$

and

$$C_{11\ N}^{(3)}(z_1,z_2) := [\mathcal{C}_{st\ 11\ N}^{(3)}(z_1,z_2)]_{3\times 3}$$
 and $F_{11\ N}^{(3)}(z_1,z_2) := [\mathcal{F}_{st\ 11\ N}^{(3)}(z_1,z_2)]_{3\times 3}$,

then write (F.14) into matrix notations, i.e.

$$\boldsymbol{\Theta}_{N}^{(3)}(z_{1},z_{2})\boldsymbol{C}_{11,N}^{(3)}(z_{1},z_{2}) = -\boldsymbol{F}_{11,N}^{(3)}(z_{1},z_{2}) + \mathrm{o}(\boldsymbol{1}_{3\times3}) + \mathrm{O}(C_{\eta_{0}}N^{-\omega})\mathcal{C}_{11,11,N}^{(3)}(z_{1},z_{2})\boldsymbol{1}_{3\times3}.$$

Since we have shown $|\mathcal{C}_{l,11,N}^{(3)}(z_1,z_2)| < C_{\eta_0}$, and $|\mathcal{V}_{st,11,N}^{(3)}(z_1,z_2)|, |\mathcal{U}_{st,11,N}^{(3)}(z_1,z_2)| \leq C_{\eta_0}$ by definitions in (F.6) and (F.8), so $|\mathcal{F}_{st,11,N}^{(3)}(z_1,z_2)| \leq C_{\eta_0}$ and $||\mathbf{F}_{11,N}^{(3)}(z_1,z_2)|| \leq C_{\eta_0}$. Thus,

$$\lim_{N\to\infty} \|\boldsymbol{C}_{11,N}^{(3)}(z_1,z_2)\| \le \lim_{N\to\infty} \|\boldsymbol{\Theta}_N^{(3)}(z_1,z_2)^{-1}\| \cdot \|\boldsymbol{F}_{11,N}^{(3)}(z_1,z_2)\| \le C_{\eta_0}.$$

For other $C_{s_1t_1,s_2t_2,N}^{(3)}(z_1,z_2)$, we can repeat the previous procedures to derive the system equations of $C_{s_2t_2,N}^{(3)}(z_1,z_2) := [\mathcal{C}_{s_1t_1,s_2t_2,N}^{(3)}(z_1,z_2)]_{3\times 3}$ for each fixed $1 \leq s_2, t_2 \leq 3$, since the arguments are totally the same, we omit details here.

F.2 Characteristic function

Theorem F.3. Under Assumptions A.1 and A.2, when d = 3, $\text{Tr}(\mathbf{Q}(z)) - \mathbb{E}[\text{Tr}(\mathbf{Q}(z))]$ weakly converges to a Gaussian random process in \mathcal{S}_{η_0} (C.18).

Proof. First, we define

$$\gamma_l(z) := \operatorname{Tr}(\boldsymbol{Q}^{ll}(z)) - \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{ll}(z))], \quad (\mathfrak{a}(\tau), \mathfrak{b}(\tau)) := \begin{cases} (1/2, 1/2) & \tau = 1\\ (1/2\mathrm{i}, -1/2\mathrm{i}) & \tau = \mathrm{i} \end{cases}$$

where l=1,2,3 and $\gamma(z):=\sum_{l=1}^3 \gamma_l(z).$ Besides, let

$$e_q := e_q(\boldsymbol{t}_q, \boldsymbol{\tau}_q, \boldsymbol{z}_q) := \exp\left(\mathrm{i} \sum_{s=1}^q t_s \left(\mathfrak{a}(\tau_s) \gamma(z_s) + \mathfrak{b}(\tau_s) \gamma(\bar{z}_s)\right)\right) \quad \text{for } q \in \mathbb{N}^+, \tag{F.16}$$

where $\boldsymbol{t}_q := (t_1, \dots, t_q)', \boldsymbol{\tau}_q := (\tau_1, \dots, \tau_q), \boldsymbol{z}_q = (z_1, \dots, z_q)$ and $\tau_s \in \{1, i\}, z_s \in \mathcal{S}_{\eta_0}$. Notice that

$$\frac{\partial}{\partial t_s} \mathbb{E}[e_q] = i \mathbb{E}\left[e_q\left(\mathfrak{a}(\tau_s)\gamma(z_s) + \mathfrak{b}(\tau_s)\gamma(\bar{z}_s)\right)\right],$$

and we will show that there exists a set of covariance coefficients $A_{st}, s, t = 1, \dots, q$ such that for each fixed T_q

$$\lim_{N \to \infty} \left| \mathbb{E} \left[e_q \left(\mathfrak{a}(\tau_s) \gamma(z_s) + \mathfrak{b}(\tau_s) \gamma(\bar{z}_s) \right) \right] + \mathbb{E} [e_q] \sum_{w=1}^q t_w A_{sw} \right| = 0.$$
 (F.17)

Since

$$\mathbb{E}[e_q \gamma_l(z)] = \frac{z^{-1}}{\sqrt{N}} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}[X_{ijk} e_q^c F_{ijk}^l(z)], \text{ where } F_{ijk}^l(z) := \begin{cases} c_k Q_{ij}^{12}(z) + b_j Q_{ik}^{13}(z) & l = 1\\ c_k Q_{ij}^{12}(z) + a_i Q_{jk}^{23}(z) & l = 2\\ a_i Q_{jk}^{23}(z) + b_j Q_{ik}^{13}(z) & l = 3 \end{cases}$$

for $z, z_1, \dots, z_q \in \mathcal{S}_{\eta_0}$. Next, we only compute $\mathbb{E}[e_q \gamma_1(z)]$ since the proof argument is the same for $\mathbb{E}[e_q \gamma_2(z)], \mathbb{E}[e_q \gamma_3(z)]$. For convenience, we define

$$C_{l,e,N}^{(3)}(z; \boldsymbol{t}_q, \boldsymbol{\tau}_q, \boldsymbol{z}_q) := C_{l,e,N}^{(3)} := \text{Cov}(\text{Tr}(\boldsymbol{Q}^{ll}(z)), e_q) \quad \text{for } l = 1, 2, 3.$$
 (F.18)

By the cumulant expansion (D.4), it gives that

$$z\mathbb{E}[e_q \gamma_l(z)] = z \operatorname{Cov}(\gamma_1(z), e_q) = \mathcal{C}_{1,e,N}^{(3)}(z; \boldsymbol{t}_q, \boldsymbol{\tau}_q, \boldsymbol{z}_q)$$
$$= \frac{1}{\sqrt{N}} \sum_{i,j,k=1}^{m,n,p} \left(\sum_{l=0}^{3} \frac{\kappa_{l+1}}{l!} \mathbb{E}\left[\partial_{ijk}^{(l)} \left\{ F_{ijk}^{1}(z) e_q^c \right\} \right] + \epsilon_{ijk}^{(4)} \right).$$

Similar as proofs of Theorem E.1, we can show that only $\partial_{ijk}^{(1)} \{F_{ijk}^1(z)e_q^c\}$ and $\partial_{ijk}^{(3)} \{F_{ijk}^1(z)e_q^c\}$ contain major terms, we omit the details here and only present the final results:

First derivatives: When l=1, by Lemma D.3 and the fact that $|e_q| \leq 1$, we can obtain

$$\mathbb{E}[\partial_{ijk}^{(1)}\{F_{ijk}^{1}(z)\}e_{q}^{c}] = -N^{-1}\mathbb{E}[\mathrm{Tr}(\boldsymbol{Q}^{11}(z))\,\mathrm{Tr}(\boldsymbol{Q}^{22}(z) + \boldsymbol{Q}^{33}(z))e_{q}^{c}] + \mathrm{O}(C_{\eta_{0}}N^{-\omega}).$$

By the same trick as (E.7), we have

$$\begin{aligned} &\operatorname{Cov}(N^{-1}\operatorname{Tr}(\boldsymbol{Q}^{11}(z))\operatorname{Tr}(\boldsymbol{Q}^{22}(z)), e_q) = \mathbb{E}\Big[\big(N^{-1}\operatorname{Tr}(\boldsymbol{Q}^{11}(z))\operatorname{Tr}(\boldsymbol{Q}^{22}(z)) - N^{-1}\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{11}(z))]\operatorname{Tr}(\boldsymbol{Q}^{22}(z)) \\ &+ N^{-1}\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{11}(z))]\operatorname{Tr}(\boldsymbol{Q}^{22}(z)) - N^{-1}\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{11}(z))]\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{22}(z))] + N^{-1}\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{11}(z))]\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{22}(z))] \\ &- N^{-1}\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{11}(z))\operatorname{Tr}(\boldsymbol{Q}^{22}(z))]\big)e_q^c\Big] = \mathfrak{m}_1(z)\mathcal{C}_{2,e,N}^{(3)} + \mathbb{E}\left[N^{-1}\operatorname{Tr}(\boldsymbol{Q}^{22}(z))\operatorname{Tr}(\boldsymbol{Q}^{11}(z))^ce_q^c\right]. \end{aligned}$$

where $\mathfrak{m}_l(z) = N^{-1}\mathbb{E}[\text{Tr}(\boldsymbol{Q}^{ll}(z))]$. According to Lemma D.3, it gives that

$$\begin{split} & \left| \mathbb{E} \left[N^{-1} \operatorname{Tr}(\boldsymbol{Q}^{22}(z)) \operatorname{Tr}(\boldsymbol{Q}^{11}(z))^{c} \overline{e_{q}^{c}} \right] - m_{2}(z) \operatorname{Cov}(\operatorname{Tr}(\boldsymbol{Q}^{11}(z)), e_{q}) \right| \\ & \leq \operatorname{O}(\eta_{0}^{-5} N^{-\omega}) \mathbb{E} \left[|\operatorname{Tr}(\boldsymbol{Q}^{11}(z))^{c} \overline{e_{q}^{c}}| \right] + \mathbb{E} \left[|N^{-1} \operatorname{Tr}(\boldsymbol{Q}^{22}(z)) \operatorname{Tr}(\boldsymbol{Q}^{11}(z))^{c} \overline{e_{q}^{c}}| 1_{|\operatorname{Tr}(\boldsymbol{Q}^{22}(z))^{c}| > \eta_{0}^{-5} N^{1-\omega}} \right] \\ & \leq \operatorname{O}(\eta_{0}^{-5} N^{-\omega}) \sqrt{\operatorname{Var}(\operatorname{Tr}(\boldsymbol{Q}^{11}(z))) \operatorname{Var}(e_{q})} + N^{2} \exp(-CN^{1-2\omega}) = \operatorname{O}(C_{\eta_{0}} N^{-\omega}), \end{split}$$

where we use the fact that $Var(e_q) \leq \mathbb{E}[|e_q|^2] \leq 1$. As a result, we conclude that

$$Cov(N^{-1}\operatorname{Tr}(\boldsymbol{Q}^{11}(z))\operatorname{Tr}(\boldsymbol{Q}^{22}(z)), e_q) = \mathfrak{m}_1(z)\mathcal{C}_{2,e,N}^{(3)} + \mathfrak{m}_2(z)\mathcal{C}_{1,e,N}^{(3)} + \mathcal{O}(C_{\eta_0}N^{-\omega})$$

Similarly, the following equation is also valid:

$$\mathrm{Cov}(N^{-1}\operatorname{Tr}(\boldsymbol{Q}^{11}(z))\operatorname{Tr}(\boldsymbol{Q}^{33}(z)),e_q)=\mathfrak{m}_1(z)\mathcal{C}_{3,e,N}^{(3)}+\mathfrak{m}_3(z)\mathcal{C}_{1,e,N}^{(3)}+\mathrm{O}(C_{\eta_0}N^{-\omega})$$

Moreover, since

$$\partial_{ijk}^{(1)}\{e_q\} = -\frac{\mathrm{i} e_q}{\sqrt{N}} \sum_{q=1}^s \sum_{w=1}^3 \sum_{s_1 \neq s_2}^3 t_s \mathcal{A}_{ijk}^{(s_1,s_2)} \big[\mathfrak{a}(\tau_s) Q_{\tilde{s}_1\cdot}^{s_1w}(z_s) Q_{\cdot \tilde{s}_2}^{ws_2}(z_s) + \mathfrak{b}(\tau_s) Q_{\tilde{s}_1\cdot}^{s_1w}(\bar{z}_s) Q_{\cdot \tilde{s}_2}^{ws_2}(\bar{z}_s) \big],$$

by Lemmas D.5 and D.6, we have

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}[\partial_{ijk}^{(1)} \{e_q\} F_{ijk}^1(z)] = \mathcal{O}(C_{\eta_0} N^{-1/2})$$

$$- \frac{2i}{N} \sum_{s=1}^{q} \sum_{l\neq 1}^{3} \sum_{w=1}^{3} t_s \mathbb{E}[\text{Tr}(\mathbf{Q}^{1l}(z)(\mathfrak{a}(\tau_s) \mathbf{Q}^{lw}(z_s) \mathbf{Q}^{w1}(z_s) + \mathfrak{b}(\tau_s) \mathbf{Q}^{lw}(\bar{z}_s) \mathbf{Q}^{w1}(\bar{z}_s))) \cdot e_q].$$

By Lemma D.3 and the fact of $|e_q| \leq 1$, it gives that

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}[\partial_{ijk}^{(1)} \{e_q\} F_{ijk}^1(z)] = \mathcal{O}(C_{\eta_0} N^{-\omega})$$

$$-\frac{2i}{N} \sum_{s=1}^q \sum_{l\neq 1}^3 \sum_{w=1}^3 t_s \mathbb{E}[\text{Tr}(\mathbf{Q}^{1l}(z)(\mathfrak{a}(\tau_s) \mathbf{Q}^{lw}(z_s) \mathbf{Q}^{w1}(z_s) + \mathfrak{b}(\tau_s) \mathbf{Q}^{lw}(\bar{z}_s) \mathbf{Q}^{w1}(\bar{z}_s)))] \cdot \mathbb{E}[e_q].$$

Hence, for $i \in \{1, 2, 3\}$, we define

$$\mathcal{V}_{i,e,N}^{(3)}(z,z_s) := rac{1}{N} \sum_{l
eq i}^3 \sum_{w=1}^3 \mathbb{E}[\boldsymbol{Q}^{il}(z) \boldsymbol{Q}^{lw}(z_s) \boldsymbol{Q}^{wi}(z_s)],$$

we can obtain that

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}[\partial_{ijk}^{(1)} \{ F_{ijk}^{1}(z) e_{q}^{c} \}] = -\mathfrak{m}_{1}(z) \left(\mathcal{C}_{2,e,N}^{(3)} + \mathcal{C}_{3,e,N}^{(3)} \right) - \mathcal{C}_{1,e,N}^{(3)}(\mathfrak{m}_{2}(z) + \mathfrak{m}_{3}(z))$$

$$-2i\mathbb{E}[e_{q}] \sum_{s=1}^{q} t_{s} \left(\mathfrak{a}(\tau_{s}) \mathcal{V}_{1,e,N}^{(3)}(z,z_{s}) + \mathfrak{b}(\tau_{s}) \mathcal{V}_{1,e,N}^{(3)}(z,\bar{z}_{s}) \right) + \mathcal{O}(C_{\eta_{0}} N^{-\omega}).$$
(F.19)

Second derivatives: The calculations for the second derivatives are the same as those in Theorem E.1, we can show that

$$N^{-1/2} \left| \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[\partial_{ijk}^{(2)} \{ F_{ijk}^1(z) e_q^c \} \right] \right| \le \mathcal{O}(C_{\eta_0} N^{-\omega}),$$

here we omit details to save space.

Third derivatives: When l=3, only the following one contains the major terms:

$$N^{-1/2} \sum_{\substack{i,j,k-1}}^{m,n,p} \mathbb{E} \left[\partial_{ijk}^{(2)} \{ e_q^c \} \partial_{ijk}^{(1)} \{ F_{ijk}^1(z) \} \right],$$

where

$$\partial_{ijk}^{(2)} \{e_q^c\} = -e_q A_1 - 2ie_q A_2$$

and

$$\begin{split} A_1 := \frac{1}{N} \Big(\sum_{q=1}^s \sum_{w=1}^3 \sum_{s_1 \neq s_2}^3 t_s \mathcal{A}_{ijk}^{(s_1,s_2)} \big[\mathfrak{a}(\tau_s) Q_{\tilde{s}_1\cdot}^{s_1w}(z_s) Q_{\cdot \tilde{s}_2}^{ws_2}(z_s) + \mathfrak{b}(\tau_s) Q_{\tilde{s}_1\cdot}^{s_1w}(\bar{z}_s) Q_{\cdot \tilde{s}_2}^{ws_2}(\bar{z}_s) \big] \Big)^2, \\ A_2 := \frac{1}{N} \sum_{q=1}^s \sum_{w=1}^3 \sum_{s_1 \neq s_2}^3 t_s \mathcal{A}_{ijk}^{(s_1,s_2)} \mathcal{A}_{ijk}^{(s_3,s_4)} \big[\mathfrak{a}(\tau_s) Q_{\tilde{s}_1\tilde{s}_3}^{s_1s_3}(z_s) Q_{\tilde{s}_4\cdot}^{s_4w}(z_s) Q_{\cdot \tilde{s}_2}^{ws_2}(z_s) + \mathfrak{b}(\tau_s) Q_{\tilde{s}_1\tilde{s}_3}^{s_1s_3}(\bar{z}_s) Q_{\tilde{s}_4\cdot}^{s_4w}(\bar{z}_s) Q_{\cdot \tilde{s}_2}^{ws_2}(\bar{z}_s) \big]. \end{split}$$

and

$$\partial_{ijk}^{(1)}\{F_{ijk}^{1}(z)\} = -\frac{1}{\sqrt{N}}\sum_{s_1 \neq s_2}^3 \sum_{l \neq 1}^3 \mathcal{A}_{ijk}^{(1,l)} \mathcal{A}_{ijk}^{(s_1,s_2)} Q_{i\tilde{s}_1}^{1s_1}(z) Q_{\tilde{s}_2\tilde{l}}^{s_2l}(z).$$

For the A_1 in $\partial_{ijk}^{(2)}\{e_q^c\}$, it is easy to see it only contains the off-diagonal terms since $s_1 \neq s_2$, so by Lemma D.6, if it associates with $\partial_{ijk}^{(1)}\{F_{ijk}^1(z)\}$, the summation over all i, j, k will be minor with order of $C_{\eta_0}N^{-1/2}$. In fact, although A_1 is a square of the summation of off-diagonal terms, we can use the Cauchy's inequality to transform it as the summation of square of off-diagonal terms, then we can claim it is minor by Lemma D.6. Next, by Lemma D.5, we have

$$\begin{split} N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E} \left[A_2 e_q \partial_{ijk}^{(1)} \{ F_{ijk}^1(z) \} \right] \\ &= -\frac{1}{N^2} \sum_{i,j,k=1}^{m,n,p} \sum_{q=1}^{s} \sum_{w=1}^{3} \sum_{l \neq 1}^{3} \sum_{s_1,s_2}^{(1,l)} t_s (\mathcal{A}_{ijk}^{(1,l)})^4 \mathbb{E} \left[(Q_{ii}^{11}(z) Q_{l\bar{l}}^{ll}(z)) \cdot \left(\mathfrak{a}(\tau_s) Q_{\tilde{s}_1 \tilde{s}_1}^{s_1 s_1}(z_s) Q_{\tilde{s}_2}^{s_2 w}(z_s) Q_{.\tilde{s}_2}^{ws_2}(z_s) \right. \\ &+ \mathfrak{b}(\tau_s) Q_{\tilde{s}_1 \tilde{s}_1}^{s_1 s_1}(\bar{z}_s) Q_{\tilde{s}_2}^{s_2 w}(\bar{z}_s) Q_{.\tilde{s}_2}^{ws_2}(\bar{z}_s) \right) \cdot e_q \right] + \mathcal{O}(C_{\eta_0} N^{-1/2}) \\ &= -\frac{1}{N^2} \sum_{q=1}^{s} \sum_{w=1}^{3} \sum_{l \neq 1}^{3} \sum_{s_1,s_2}^{1} t_s \| \boldsymbol{a}^{(5-l)} \|_4^4 \mathbb{E} \left[\left(\mathfrak{a}(\tau_s) \operatorname{Tr}(\boldsymbol{Q}^{s_1 s_1}(z) \circ \boldsymbol{Q}^{s_1 s_1}(z_s)) \operatorname{Tr}(\boldsymbol{Q}^{s_2 s_2}(z) \circ (\boldsymbol{Q}^{s_2 w}(z_s) \boldsymbol{Q}^{ws_2}(z_s))) \right. \\ &+ \mathfrak{b}(\tau_s) \operatorname{Tr}(\boldsymbol{Q}^{s_1 s_1}(z) \circ \boldsymbol{Q}^{s_1 s_1}(\bar{z}_s)) \operatorname{Tr}(\boldsymbol{Q}^{s_2 s_2}(z) \circ (\boldsymbol{Q}^{s_2 w}(\bar{z}_s) \boldsymbol{Q}^{ws_2}(\bar{z}_s))) \right) \cdot e_q \right] + \mathcal{O}(C_{\eta_0} N^{-1/2}). \end{split}$$

For simplicity, for $i \in \{1, 2, 3\}$, we define

$$\mathcal{U}_{i,e,N}^{(3)}(z,z_s) := \frac{1}{N^2} \sum_{w=1}^{3} \sum_{l \neq i}^{3} \sum_{s_1,s_2}^{(1,i)} \|\boldsymbol{a}^{(5-l)}\|_4^4 \mathbb{E}[\text{Tr}(\boldsymbol{Q}^{s_1s_1}(z) \circ \boldsymbol{Q}^{s_1s_1}(z_s)) \, \text{Tr}(\boldsymbol{Q}^{s_2s_2}(z) \circ (\boldsymbol{Q}^{s_2w}(z_s)\boldsymbol{Q}^{ws_2}(z_s))]).$$

where the notation $\sum_{s_1,s_2}^{(i,l)}$ means that the summation of s_1 and s_2 are over $\{1,2,3\}\setminus\{i,r\}$. Then by Lemma D.3, we can further obtain

$$N^{-1/2} \sum_{i,j,k=1}^{m,n,p} \mathbb{E}\left[A_2 e_q \partial_{ijk}^{(1)} \{F_{ijk}^1(z)\}\right]$$

$$= \mathbb{E}[e_q] \sum_{q=1}^{s} t_s \left(\mathfrak{a}(\tau_s) \mathcal{U}_{1,e,N}^{(3)}(z,z_s) + \mathfrak{b}(\tau_s) \mathcal{U}_{1,e,N}^{(3)}(z,\bar{z}_s)\right) + \mathcal{O}(C_{\eta_0} N^{-1/2}). \tag{F.20}$$

Now, let

$$\mathcal{F}_{l,e,N}^{(3)}(z,z_s) := \mathcal{V}_{l,e,N}^{(3)}(z,z_s) + \kappa_4 \mathcal{U}_{l,e,N}^{(3)}(z,z_s),$$

then combining (F.19) and (F.20), we have

$$\begin{split} &(z+\mathfrak{m}(z)-\mathfrak{m}_{1}(z))\mathcal{C}_{1,e,N}^{(3)} \\ &=-\mathfrak{m}_{1}(z)\big(\mathcal{C}_{2,e,N}^{(3)}+\mathcal{C}_{3,e,N}^{(3)}\big)-\mathrm{i}\mathbb{E}[e_{q}]\sum_{s=1}^{q}t_{s}\big[\mathfrak{a}(\tau_{s})\mathcal{F}_{1,e,N}^{(3)}(z,z_{s})+\mathfrak{b}(\tau_{s})\mathcal{F}_{1,e,N}^{(3)}(z,\bar{z}_{s})\big]+\mathrm{O}(C_{\eta_{0}}N^{-\omega}). \end{split}$$

Similarly, for other $r \in \{1, 2, 3\}$, we have

$$(z + \mathfrak{m}(z) - \mathfrak{m}_{r}(z))C_{r,e,N}^{(3)} = -\mathfrak{m}_{r}(z)\sum_{l \neq r}^{3} C_{l,e,N}^{(3)} + \mathcal{O}(C_{\eta_{0}}N^{-\omega})$$
$$-i\mathbb{E}[e_{q}]\sum_{r=1}^{q} t_{s} \left[\mathfrak{a}(\tau_{s})\mathcal{F}_{r,e,N}^{(3)}(z,z_{s}) + \mathfrak{b}(\tau_{s})\mathcal{F}_{r,e,N}^{(3)}(z,\bar{z}_{s})\right].$$

Next, define

$$\boldsymbol{C}_{e,N}^{(3)}(z) := [\mathcal{C}_{r,e,N}^{(3)}(z;\boldsymbol{t}_q,\boldsymbol{\tau}_q,\boldsymbol{z}_q)]_{3\times 1} \quad \text{and} \quad \boldsymbol{F}_{e,N}^{(3)}(z,z_s) := [\mathcal{F}_{r,e,N}^{(3)}(z;z_s)]_{3\times 1},$$

so

$$\boldsymbol{\Theta}_{N}^{(3)}(z,z)\boldsymbol{C}_{e,N}^{(3)}(z) = -\mathrm{i}\mathbb{E}[e_{q}]\sum_{s=1}^{q}t_{s}\left[\mathfrak{a}(\tau_{s})\boldsymbol{F}_{e,N}^{(3)}(z,z_{s}) + \mathfrak{b}(\tau_{s})\boldsymbol{F}_{e,N}^{(3)}(z,\bar{z}_{s})\right] + \mathrm{o}(\boldsymbol{1}_{3\times3}),$$

where $\mathbf{\Theta}_N^{(3)}(z,z)$ defined in (E.20) is invertible, and we have shown that $\lim_{N\to\infty} \|\mathbf{\Theta}_N^{(3)}(z,z)^{-1} + \mathbf{\Pi}^{(3)}(z,z)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z))\| = 0$. Thus, we obtain that

$$\lim_{N \to \infty} \left\| \boldsymbol{C}_{e,N}^{(3)}(z) - \mathrm{i} \mathbb{E}[e_q] \sum_{s=1}^q t_s \boldsymbol{\Pi}^{(3)}(z,z)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z)) \left[\mathfrak{a}(\tau_s) \boldsymbol{F}_{e,N}^{(3)}(z,z_s) + \mathfrak{b}(\tau_s) \boldsymbol{F}_{e,N}^{(3)}(z,\bar{z}_s) \right] \right\| = 0.$$

As a result,

$$\begin{split} &\frac{\partial}{\partial t_s} \mathbb{E}[e_q] = \mathrm{i} \mathbb{E}\left[e_q\left(\mathfrak{a}(\tau_s)\gamma(z_s) + \mathfrak{b}(\tau_s)\gamma(\bar{z}_s)\right)\right] = \mathrm{i} \sum_{r=1}^3 \left(\mathfrak{a}(\tau_s)\mathcal{C}_{r,e,N}^{(3)}(z_s) + \mathfrak{a}(\tau_s)\mathcal{C}_{r,e,N}^{(3)}(\bar{z}_s)\right) \\ &= -\mathbb{E}[e_q] \sum_{w=1}^q t_w \left(\mathfrak{a}(\tau_s)\mathbf{1}_3'\mathbf{\Pi}^{(3)}(z_s,z_s)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z_s)) \left[\mathfrak{a}(\tau_w)\boldsymbol{F}_{e,N}^{(3)}(z_s,z_w) + \mathfrak{b}(\tau_w)\boldsymbol{F}_{e,N}^{(3)}(z_s,\bar{z}_w)\right] \\ &+ \mathfrak{b}(\tau_s)\mathbf{1}_3'\mathbf{\Pi}^{(3)}(\bar{z}_s,\bar{z}_s)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(\bar{z}_s)) \left[\mathfrak{a}(\tau_w)\boldsymbol{F}_{e,N}^{(3)}(\bar{z}_s,z_w) + \mathfrak{b}(\tau_w)\boldsymbol{F}_{e,N}^{(3)}(\bar{z}_s,\bar{z}_w)\right] \right) + \mathrm{o}(1), \end{split}$$

which concludes (F.17). Hence, combining with Theorem F.2, we can conclude that $\text{Tr}(\boldsymbol{Q}(z)) - \mathbb{E}[\text{Tr}(\boldsymbol{Q}(z))]$ weakly converges to a Gaussian process in \mathcal{S}_{η_0} .

F.3 Proof of Theorem F.1

Proof of Theorem F.1. First, since

$$G_N(f) \xrightarrow{\mathbb{P}} -\frac{1}{2\pi i} \oint_{\mathfrak{C}} f(z) \{ \operatorname{Tr}(\boldsymbol{Q}(z)) - Ng(z) \} dz$$

$$= -\frac{1}{2\pi i} \oint_{\mathfrak{C}} f(z) \{ \operatorname{Tr}(\boldsymbol{Q}(z)) - \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}(z))] \} dz - \frac{1}{2\pi i} \oint_{\mathfrak{C}} f(z) \{ \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}(z))] - Ng(z) \} dz.$$

Here, let's split \mathfrak{C} by $\mathfrak{C}^v \cup \mathfrak{C}^h$, where

$$\mathfrak{C}^v := \{ z = \pm E_0 + i\eta \in \mathbb{C} : |\eta| \in [0, \eta_0] \} \text{ and } \mathfrak{C}^h := \{ z = E \pm i\eta_0 \in \mathbb{C} : |E| \in [0, E_0] \}.$$

First, by Theorems F.3, E.1 and E.2, we know that $\text{Tr}(\boldsymbol{Q}(z)) - Ng(z)$ weakly converges to a Gaussian process in \mathcal{S}_{η_0} (C.18) with mean $\mu_N^{(3)}(z)$ (E.27) and variance $\mathcal{C}_N^{(3)}(z,z)$ (E.5). Hence, since $\mathfrak{C}^v \subset \mathcal{S}_{\eta_0}$, we can conclude that

$$(\sigma_N^{(3)})^{-1}\left(\frac{1}{2\pi \mathrm{i}}\oint_{\sigma^h}f(z)\{\mathrm{Tr}(\boldsymbol{Q}(z))-Ng(z)\}dz-\xi_N^{(3)}\right)\stackrel{d}{\longrightarrow}\mathcal{N}(0,1),$$

where

$$\xi_N^{(3)} := \frac{1}{2\pi i} \oint_{\sigma} f(z) \mu_N^{(3)}(z) dz, \tag{F.21}$$

$$(\sigma_N^{(3)})^2 := -\frac{1}{4\pi^2} \oint_{\mathfrak{C}_1} \oint_{\mathfrak{C}_2} f(z_1) f(z_2) \mathcal{C}_N^{(3)}(z_1, z_2) dz_1 dz_2, \tag{F.22}$$

where $\mathfrak{C}_{1,2}$ are two disjoint rectangle contours with vertexes of $\pm E_{1,2} \pm i\eta_{1,2}$ such that $E_{1,2} \ge \max\{\zeta, \mathfrak{v}_3\} + t$ and $\eta_{1,2} > 0$ are sufficiently small. Next, we will show that

$$\lim_{\eta_0\downarrow 0} \limsup_{N\to\infty} \frac{1}{2\pi \mathrm{i}} \oint_{\mathfrak{C}^v} f(z) \{ \mathrm{Tr}(\boldsymbol{Q}(z)) - Ng(z) \} dz \stackrel{\mathbb{P}}{\longrightarrow} 0,$$

it is enough to prove

$$\lim_{\eta_0\downarrow 0} \limsup_{N\to\infty} \mathbb{E} \Big| \int_{\mathfrak{C}^v} 1_{\mathcal{E}_M} f(z) \{ \operatorname{Tr}(\boldsymbol{Q}(z)) - \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}(z))] \} dz \Big|^2 = 0, \tag{F.23}$$

$$\lim_{\eta_0\downarrow 0} \limsup_{N\to\infty} \Big| \int_{\mathfrak{C}^v} 1_{\mathcal{E}_M} f(z) \{ \mathbb{E}[\text{Tr}(\boldsymbol{Q}(z))] - Ng(z) \} dz \Big|^2 = 0, \tag{F.24}$$

where the event $\mathcal{E}_{M} := \{ \|M\| \leq \max\{\mathfrak{v}_{3},\zeta\} + t \}$, \mathfrak{v}_{3},ζ are defined in Theorem C.1 and (C.17), respectively, and t > 0 is a fixed constant. By Theorem C.1, we know that $\mathbb{P}(\mathcal{E}_{M}) \geq 1 - \mathrm{o}(N^{-l})$ for any l > 0. Now, let's first prove (F.24). By the definition of \mathfrak{C}^{v} , we know that $\mathrm{dist}(z, [-\mathfrak{v}_{3}, \mathfrak{v}_{3}]) > t$ conditional on \mathcal{E}_{M} , so $\|Q(z)\| \leq t^{-1}$ for any $z \in \mathfrak{C}^{v}$. Hence, we can use the same proofs of Theorem E.2 to conculde that

$$\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}(z))] - Ng(z) = \mu_N^{(3)}(z) + \mathcal{O}(C_t N^{-\omega}),$$

where the error term $O(C_t N^{-\omega})$ is independent with η_0 . Moreover, by Lemma F.1 later, we know that $\mu_N^{(3)}(z)$ is analytic on \mathfrak{C}^v . And f(z) is also analytic on \mathfrak{C}^v due to $f \in \mathfrak{F}_3$ in (F.1). Therefore, conditional on \mathcal{E}_M , we have

$$\begin{split} &(\mathbf{F}.\mathbf{24}) \leq \lim_{\eta_0\downarrow 0^+} \limsup_{N\to\infty} \Big(\oint_{\mathfrak{C}^v} \big| f(z) (\mathbb{E}[\mathrm{Tr}(\boldsymbol{Q}(z))] - Ng(z)) \big| dz \Big)^2 \\ &\leq \lim_{\eta_0\downarrow 0^+} \limsup_{N\to\infty} \Big(\oint_{\mathfrak{C}^v} \big| f(z) \mu_N^{(3)}(z) \big| dz \Big)^2 + 2 \lim_{\eta_0\downarrow 0^+} \limsup_{N\to\infty} \eta_0 C_t N^{-\omega} \sup_{z\in\mathfrak{C}^v} |f(z)| = 0, \end{split}$$

where we use the fact that $\lim_{\eta_0\downarrow 0^+} \oint_{\mathfrak{C}^v} |f(z)\mu_N^{(3)}(z)| dz = 0$ due to $f(z)\mu_N^{(3)}(z)$ is analytic on \mathfrak{C}^v and the length of \mathfrak{C}^v tends to 0. Next, for (F.23), conditional on \mathcal{E}_M , we have

$$\begin{split} & (\mathbf{F}.\mathbf{23}) \leq \lim_{\eta_0\downarrow 0^+} \limsup_{N\to\infty} \oint_{\mathfrak{C}^v} \mathbb{E}\big[\big|f(z)(\mathrm{Tr}(\boldsymbol{Q}(z)) - \mathbb{E}[\mathrm{Tr}(\boldsymbol{Q}(z))])\big|^2\big] dz \\ & = \lim_{\eta_0\downarrow 0^+} \limsup_{N\to\infty} \oint_{\mathfrak{C}^v} |f(z)|^2 \, \mathrm{Var}(\mathrm{Tr}(\boldsymbol{Q}(z))) dz. \end{split}$$

By the same proofs of Theorem E.1, we know that

$$Var(Tr(\mathbf{Q}(z))) = \mathcal{C}_N^{(3)}(z, z) + O(C_t N^{-\omega}).$$

Similarly, since $C_N^{(3)}(z,z)$ is analytic by Lemma F.1, so it gives that

$$(F.23) \le \lim_{\eta_0\downarrow 0^+} \limsup_{N\to\infty} \oint_{\mathfrak{C}^v} |f(z)|^2 \operatorname{Var}(\operatorname{Tr}(\boldsymbol{Q}(z))) dz = 0.$$

Hence, we conclude (F.23) and (F.24), which completes our proof.

Lemma F.1. The mean function $\mu_N(z)$ in (E.27) and covariance function $\mathcal{C}_N^{(3)}(z_1, z_2)$ in (E.5) are analytical for $z, z_1, z_2 \in \mathfrak{C}^v$.

Proof. We first need to ensure that $\Pi^{(3)}(z_1, z_2)$ is still invertible when $z \in \mathfrak{C}^v$. Based on the definition of $\Pi^{(3)}(z_1, z_2)$ in (B.11) the proof of Proposition B.2, it is enough to show that $\operatorname{diag}(e^{-2iq}) - \mathbf{F}^{(3)}(z)$ is invertible, where $\mathbf{q}, \mathbf{F}^{(3)}(z)$ are defined in (B.8) and (B.5). For convenience, we simplify $\mathbf{F}^{(3)}(z)$ by \mathbf{F} . Let's first show that $||\mathbf{F}(z)|| < 1$ for all $z \in \mathfrak{C}^v$. Since

$$\|\mathbf{F}\| = 1 - \frac{\Im(z)\langle \mathbf{f}, \mathbf{c}^{-1} \circ |\mathbf{g}|\rangle}{\langle \mathbf{f}, \sin \mathbf{g}\rangle},$$

where $\sin q = \frac{\Im(g)}{|g|}$ and f is the unit eigenvector of F with eigenvalue of ||F||. Denote ν_i be the measure deduced by $g_i(z)$ for $i = 1, \dots, d$, whose support is bounded by ζ defined in (C.17), then

$$\Im(g_i(z)) = \int_{-\xi}^{\xi} \frac{\eta}{(E_0 - x)^2 + \eta^2} \nu_i(dx),$$

where $z = E_0 + i\eta \in \mathfrak{C}^v$ and $|E_0| - \xi = t > 0, \eta \in [0, \eta_0]$. Hence,

$$\sup_{\eta \in [0,\eta_0]} \eta^{-1} \Im(g_i(z)) \le \int_{-\xi}^{\xi} \frac{1}{(E_0 - x)^2} \nu_i(dx) < t^{-2} \mathfrak{c}_i.$$

On the other hand, we have

$$\inf_{\eta \in [0,\eta_0]} |g_i(E_0 + i\eta)| \ge \inf_{\eta \in [0,\eta_0]} |\Re(g_i(E_0 + i\eta))| \ge \int_{-\xi}^{\xi} \frac{|E_0 - x|}{|E_0 - x|^2 + \eta_0^2} \nu_i(dx)
> \frac{t\mathfrak{c}_i}{t^2 + \eta_0^2} > \mathfrak{c}_i/(2t),$$

so it gives that $\sup_{z \in \mathfrak{C}^v} \frac{\Im(z)^{-1}\Im(g_i(z))}{|g_i(z)|} \leq 2t^{-1}$ and $\Im(z)^{-1}\langle \boldsymbol{f}, \sin \boldsymbol{q} \rangle < 2t^{-1}\langle \boldsymbol{f}, 1 \rangle$. In addition, since

$$\inf_{\eta \in [0,\eta_0]} \mathfrak{c}_i^{-1} |g_i(E_0 + \mathrm{i} \eta)| = \mathfrak{c}_i^{-1} \inf_{\eta \in [0,\eta_0]} |\Re(g_i(E_0 + \mathrm{i} \eta))| > \frac{t}{t^2 + \eta_0^2},$$

then

$$\langle oldsymbol{f}, oldsymbol{\mathfrak{c}}^{-1} \circ |oldsymbol{g}|
angle > rac{t}{t^2 + \eta_0^2} \langle oldsymbol{f}, oldsymbol{1}
angle.$$

Therefore, we conclude that

$$\sup_{\eta \in [0,\eta_0]} \| \boldsymbol{F}(E + \mathrm{i} \eta) \| \le 1 - \frac{t^2}{2(t^2 + \eta_0^2)} < 1,$$

combining with Lemma B.2, we can further conclude that that $\operatorname{diag}(e^{-2\mathrm{i}q}) - F(z)$ is invertible for $z \in \mathfrak{C}^v$, so does $\Pi^{(3)}(z,z)$. Moreover, by the same proofs of Proposition B.2, we can show that $\Pi^{(3)}(z_1,z_2)$ for $z_1,z_2 \in \mathfrak{C}^v$. Since $g_i(z)$ are analytical on \mathfrak{C}^v , then the entries of $\Pi^{-1}(z,z)$ are also analytical; further based on the system equations in §E.3, $W_{ij}^{(3)}(z)$ (E.38) and $V_{ij}^{(3)}(z,z)$ (E.39) are all analytical, so the mean function $\mu_N(z)$ in (E.27) is also analytical. Similarly, by Theorem E.1 and system equations in §E.3, $\mathcal{C}_N^{(3)}(z_1,z_2)$ is analytic on \mathfrak{C}^v due to the system equations of $\mathcal{V}_{ij}^{(3)}(z_1,z_2)$ (E.43) and $\mathcal{U}_{ij,N}^{(3)}(z_1,z_2)$ (E.45) only depend on $g(z),\Pi^{(3)}(z_1,z_2)$, so the covariance function $\mathcal{C}_N^{(3)}(z_1,z_2)$ in (E.5) is also analytical, which completes our proof.

G General cases

Now, we will extend all results in §D, §E and §F for general $d \geq 3$. Since the proofs procedures for $d \geq 3$ are the same as those for d = 3, we will not introduce them in details for convenience. Moreover, in proofs of these generalized results, we only present the key calculations to highlight the differences. Before presenting the details, let's make some notations. Recall the blockwise tensor contraction mapping Φ_d defined in (A.8), denote

$$oldsymbol{M} = rac{1}{\sqrt{N}} oldsymbol{\Phi}_d(oldsymbol{X}, oldsymbol{a}^{(1)}, \cdots oldsymbol{a}^{(d)}) \quad ext{and} \quad oldsymbol{Q}(z) = (oldsymbol{M} - z oldsymbol{I}_N)^{-1},$$

where $\boldsymbol{a}^{(i)} \in \mathbb{S}^{(n_i-1)}, i=1\cdots,d$ are d fixed unit deterministic vectors with bounded L^2 norms and $N=\sum_{i=1}^d n_i$, the dimension n_1,\cdots,n_d satisfy Assumption A.2, $\boldsymbol{X}=[X_{i_1\cdots i_d}]_{n_1\times\cdots\times n_d}\in\mathbb{R}^{n_1\times\cdots\times n_d}$ is the random tensor such that $X_{i_1\cdots i_d}$ are i.i.d. satisfying Assumption A.1. Similar as (C.18), for any sufficiently small $\eta_0>0$, we define

$$S_{\eta_0} := \{ z \in \mathbb{C}^+ : \text{dist}(z, [-\max\{\mathfrak{v}_d, \zeta\}, \max\{\mathfrak{v}_d, \zeta\}]) \ge \eta_0, |\Re(z)|, |\Im(z)| \le \eta_0^{-1} \}.$$
 (G.1)

Without special mention, the constant $\omega \in (1/2 - \delta, 1/2)$, where $\delta > 0$ is a sufficient small constant. For any matrix A, A_i and $A_{\cdot j}$ means the i-th row and j-th column of A, respectively.

G.1 Preliminary Lemmas

First, we will extend Lemmas D.3, D.5 and D.6 for general $d \ge 3$. Similar as (D.12), we have

$$\partial_{i_{1}\cdots i_{d}}^{(1)} \boldsymbol{M} = \frac{1}{\sqrt{N}} \left(\begin{array}{cccc} \mathbf{0}_{n_{1}\times n_{1}} & \mathcal{A}_{i_{1}\cdots i_{d}}^{(1,2)} \boldsymbol{e}_{i_{1}}^{n_{1}}(\boldsymbol{e}_{i_{2}}^{n_{2}})' & \cdots & \mathcal{A}_{i_{1}\cdots i_{d}}^{(1,d)} \boldsymbol{e}_{i_{1}}^{n_{1}}(\boldsymbol{e}_{i_{d}}^{n_{d}})' \\ \mathcal{A}_{i_{1}\cdots i_{d}}^{(2,1)} \boldsymbol{e}_{i_{2}}^{n_{2}}(\boldsymbol{e}_{i_{1}}^{n_{1}})' & \mathbf{0}_{n_{2}\times n_{2}} & \cdots & \mathcal{A}_{i_{1}\cdots i_{d}}^{(2,d)} \boldsymbol{e}_{i_{2}}^{n_{2}}(\boldsymbol{e}_{i_{d}}^{n_{d}})' \\ \vdots & \ddots & \ddots & \vdots \\ \mathcal{A}_{i_{1}\cdots i_{d}}^{(d,1)} \boldsymbol{e}_{i_{d}}^{n_{d}}(\boldsymbol{e}_{i_{1}}^{n_{1}})' & \cdots & \mathcal{A}_{i_{1}\cdots i_{d}}^{(d,d-1)} \boldsymbol{e}_{i_{d-1}}^{n_{d-1}}(\boldsymbol{e}_{i_{d}}^{n_{d}})' & \mathbf{0}_{n_{d}\times n_{d}} \end{array} \right),$$

where $e_{i_k}^{n_k} \in \mathbb{R}^{n_k}$ such that its i_k -th entry is 1 while others are 0, and $\partial_{i_1\cdots i_d}^{(l)} := \frac{\partial^l}{\partial X_{i_1\cdots i_d}^l}$ is the generalization of (D.5). Since we also split $Q(z) = [Q^{st}(z)]_{d\times d}$ into $d\times d$ blocks such that $Q^{st}(z) \in \mathbb{C}^{n_s\times n_t}$ for $s,t\in\{1,\cdots,d\}$, we say $Q^{st}(z)$ comes from the off-diagonal block if $s\neq t$, otherwise it belongs to the diagonal block. Before proving Lemma D.3 for general $d\geq 3$, we need extend Lemma D.4 first:

Lemma G.1. For any $K \in \mathbb{N}^+$ and $z \in \mathbb{C}^+$, let $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{C}^N$ be two deterministic vectors with bounded L^2 norms, then for l = 1, 2, 3, we have

$$\sum_{i_1\cdots i_d}^{n_1\cdots n_d} \left| \boldsymbol{x}' \partial_{i_1\cdots i_d}^{(l)} \left(\prod_{k=1}^K \boldsymbol{Q}(z) \right) \boldsymbol{y} \right|^2 < \begin{cases} C_l \|\boldsymbol{Q}(z)\|^{2(l+K)} N^{-1} & l = 1, 2, \\ C_l \|\boldsymbol{Q}(z)\|^{2(l+K)} N^{-2} & l = 3. \end{cases}$$

 $\textit{Proof.} \ \ \text{Note that} \ \ \partial^{(l)}_{i_1\cdots i_d} \boldsymbol{Q} = (-1)^l l! (\boldsymbol{Q} \partial^{(1)}_{i_1\cdots i_d} \boldsymbol{M})^l \boldsymbol{Q} \ \ \text{for} \ \ l \in \mathbb{N}^+, \ \text{then let's consider:}$

First derivatives: When l = 1, we have

$$\begin{split} &\sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}}|(\boldsymbol{x}^{(l_{0})})'\partial_{i_{1}\cdots i_{d}}^{(1)}\boldsymbol{Q}^{s_{l_{0}}s_{l_{0}+1}}\boldsymbol{y}^{(l_{0})}|^{2} \leq N^{-1}C_{d}\sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}}\sum_{t_{1}\neq t_{2}}^{d}|(\boldsymbol{x}^{(l_{0})})'Q_{\cdot i_{t_{1}}}^{s_{l_{0}}t_{1}}\mathcal{A}_{i_{1}\cdots i_{d}}^{(t_{1},t_{2})}Q_{i_{t_{2}}}^{t_{2}s_{l_{0}+1}}\boldsymbol{y}^{(l_{0})}|^{2} \\ &\leq C_{d}N^{-1}\sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}}\sum_{t_{1}\neq t_{2}}^{d}\prod_{l\neq t_{1},t_{2}}^{d}|(\boldsymbol{x}^{(l_{0})})'Q_{\cdot i_{t_{1}}}^{s_{l_{0}}t_{1}}a_{i_{l}}^{(l)}Q_{i_{t_{2}}}^{t_{2}s_{l_{0}+1}}\boldsymbol{y}^{(l_{0})}|^{2} \\ &\leq C_{d}N^{-1}\sum_{t_{1}\neq t_{2}}^{d}\|\boldsymbol{Q}^{t_{1}s_{l_{0}}}\boldsymbol{x}^{(l_{0})}\|_{2}^{2}\cdot\|\boldsymbol{Q}^{t_{2}s_{l_{0}+1}}\boldsymbol{y}^{(l_{0})}\|_{2}^{2}\leq C_{d}N^{-1}\|\boldsymbol{Q}\|^{2(K+1)}. \end{split}$$

Second derivatives: When l = 2, we have

$$\begin{split} &\sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}}|(\boldsymbol{x}^{j_{1}})'\partial_{i_{1}\cdots i_{d}}^{(2)}\boldsymbol{Q}^{j_{1}j_{2}}\boldsymbol{y}^{j_{2}}|^{2} \leq C_{d}\sum_{s_{1}\neq s_{2}}^{d}\sum_{s_{3}\neq s_{4}}^{d}N^{-2}\sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}}|(\boldsymbol{x}^{j_{1}})'Q_{\cdot i_{s_{1}}}^{j_{1}s_{1}}\mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{1},s_{2})}Q_{i_{s_{2}}i_{s_{3}}}^{s_{2}s_{3}}\mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{3},s_{4})}Q_{i_{s_{4}}}^{s_{4}j_{2}}\boldsymbol{y}^{j_{2}}|^{2}\\ &:=C_{d}\sum_{s_{1}\neq s_{2}}^{d}\sum_{s_{3}\neq s_{4}}^{d}\mathcal{P}_{s_{1}\cdots s_{4}}(j_{1},j_{2}) \end{split}$$

By the proof of Lemma D.4, $\mathcal{P}_{s_1 \dots s_4}(j_1, j_2)$ will have the maximal order of N when $s_2 = s_3$ and $s_1 = s_4$

$$\begin{split} N^{-2} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} |(\boldsymbol{x}^{j_{1}})' Q_{\cdot i_{s_{1}}}^{j_{1} s_{1}} \mathcal{A}_{i_{1} \cdots i_{d}}^{(s_{1}, s_{2})} Q_{i_{s_{2}} i_{s_{3}}}^{s_{2} s_{3}} \mathcal{A}_{i_{1} \cdots i_{d}}^{(s_{3}, s_{4})} Q_{i_{s_{4}}}^{s_{4} j_{2}} \boldsymbol{y}^{j_{2}}|^{2} \\ & \leq N^{-2} \operatorname{Tr}(|\boldsymbol{Q}^{s_{2} s_{2}}|^{\circ 2}) \cdot (|\boldsymbol{x}^{j_{1}}|^{\circ 2})' |\boldsymbol{Q}^{j_{1} s_{1}}|^{\circ 2} |\boldsymbol{Q}^{s_{1} j_{2}}|^{\circ 2} (|\boldsymbol{y}^{j_{2}}|^{\circ 2}) \leq N^{-1} \|\boldsymbol{Q}\|^{2(K+2)}, \end{split}$$

and $s_2 \neq s_3$ and $s_1 = s_4$

$$N^{-2} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} |(\boldsymbol{x}^{j_{1}})' Q_{\cdot i_{s_{1}}}^{j_{1} s_{1}} \mathcal{A}_{i_{1} \cdots i_{d}}^{(s_{1}, s_{2})} Q_{i_{s_{2}} i_{s_{3}}}^{s_{2} s_{3}} \mathcal{A}_{i_{1} \cdots i_{d}}^{(s_{3}, s_{4})} Q_{i_{s_{4}}}^{s_{4} j_{2}} \boldsymbol{y}^{j_{2}}|^{2}$$

$$\leq N^{-2} \operatorname{Tr}(|\boldsymbol{Q}^{s_{2} s_{2}}|^{\circ 2}) \cdot (|\boldsymbol{x}^{j_{1}}|^{\circ 2})' |\boldsymbol{Q}^{j_{1} s_{1}}|^{\circ 2} |\boldsymbol{a}^{(s_{1})}|^{\circ 2} \cdot (|\boldsymbol{y}^{j_{2}}|^{\circ 2})' |\boldsymbol{Q}^{j_{2} s_{3}}|^{\circ 2} |\boldsymbol{a}^{(s_{3})}|^{\circ 2} \leq N^{-1} \|\boldsymbol{Q}\|^{2(K+2)}$$

for other situations, $\mathcal{P}_{s_1 \cdots s_4}(j_1, j_2) \leq N^{-2} ||Q||^{2(k+2)}$.

Third derivatives: l=3: similarly, it is enough to bound

$$\mathcal{P}_{s_1\cdots s_6}(j_1,j_2) := N^{-3} \sum_{i_1\cdots i_d}^{n_1\cdots n_d} |(\boldsymbol{x}^{j_1})'Q_{\cdot i_{s_1}}^{j_1s_1} \mathcal{A}_{i_1\cdots i_d}^{(s_1,s_2)} Q_{i_{s_2}i_{s_3}}^{s_2s_3} \mathcal{A}_{i_1\cdots i_d}^{(s_3,s_4)} Q_{i_{s_4}i_{s_5}}^{s_4s_5} \mathcal{A}_{i_1\cdots i_d}^{(s_5,s_6)} Q_{i_{s_6}}^{s_6j_2} \boldsymbol{y}^{j_2}|^2,$$

and $\mathcal{P}_{s_1\cdots s_6}(j_1,j_2)$ will have the maximal order of N when $s_2=s_3=s_6,s_1=s_4=s_5$

$$\begin{split} N^{-3} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} |(\boldsymbol{x}^{j_{1}})' Q_{\cdot i_{s_{1}}}^{j_{1} s_{1}} \mathcal{A}_{i_{1} \cdots i_{d}}^{(s_{1}, s_{2})} Q_{i_{s_{2}} i_{s_{2}}}^{s_{2} s_{2}} \mathcal{A}_{i_{1} \cdots i_{d}}^{(s_{2}, s_{1})} Q_{i_{s_{1}} i_{s_{1}}}^{s_{1} s_{1}} \mathcal{A}_{i_{1} \cdots i_{d}}^{(s_{1}, s_{2})} Q_{i_{s_{2}}}^{s_{2} j_{2}} \boldsymbol{y}^{j_{2}}|^{2} \\ \leq N^{-3} (|\boldsymbol{x}^{j_{1}}|^{\circ 2})' |\boldsymbol{Q}^{j_{1} s_{1}}|^{\circ 2} |\boldsymbol{Q}^{s_{1} s_{1}}|^{\circ 2} \mathbf{1}_{n_{s_{1}}} \cdot (|\boldsymbol{y}^{j_{2}}|^{\circ 2})' |\boldsymbol{Q}^{j_{2} s_{2}}|^{\circ 2} |\boldsymbol{Q}^{s_{2} s_{2}}|^{\circ 2} \mathbf{1}_{n_{s_{2}}} \leq N^{-2} \|\boldsymbol{Q}\|^{2(K+3)}, \end{split}$$

which completes the proof of Lemma G.1.

Now, based on the above lemma, we can further prove that

Lemma G.2. Under Assumptions A.1 and A.2, for any $K \in \mathbb{N}^+$ and $z_1, \dots, z_K \in \mathcal{S}_{\eta_0}$ in (G.1), let $s_i \in \{1, \dots, d\}$ for $1 \leq i \leq K$ such that $s_{2j} \neq s_{2j+1}$ and $\boldsymbol{x} \in \mathbb{C}^{n_{s_1}}, \boldsymbol{y} \in \mathbb{C}^{n_{s_{K+1}}}$ be two deterministic vectors with bounded L^2 norms, then for any $\omega \in (1/2 - \delta, 1/2)$, where $\delta > 0$ is a sufficiently small number, we have

$$\left| x' \prod_{i=1}^{K} Q^{s_i s_{i+1}}(z_i) y - \mathbb{E} \left[x' \prod_{i=1}^{K} Q^{s_i s_{i+1}}(z_i) y \right] \right| \prec C_K \eta_0^{-(K+4)} N^{-\omega}.$$

In particular, if $s_1 = s_K$, we further have

$$\left| \boldsymbol{x}' \operatorname{diag} \left(\prod_{i=1}^K \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \right) \boldsymbol{y} - \mathbb{E} \left[\boldsymbol{x}' \operatorname{diag} \left(\prod_{i=1}^K \boldsymbol{Q}^{s_i s_{i+1}}(z_i) \right) \boldsymbol{y} \right] \right| \prec C_K \eta_0^{-(K+4)} N^{-\omega}.$$

By the proofs of Lemma D.3, it is easy to see the condition d = 3 is not essential, so we omit the detailed proofs of Lemma G.2. Next, let's give the extension of Lemma D.5:

Lemma G.3. For any $z \in \mathbb{C}^+$ and $l \in \mathbb{N}^+, 1 \leq l \leq 4$, let $t_1, \dots, t_{2(l+1)} \in \{1, \dots, d\}$ such that $t_{2\alpha} \neq t_{2\alpha+1}$ and $t_1 \neq t_{2(l+1)}$ for $1 \leq \alpha \leq l$, let

$$\sum_{i_1\cdots i_d}^{n_1\cdots n_d} \mathcal{A}_{i_1\cdots i_d}^{(t_1,t_{2l+2})} Q_{i_{t_1}i_{t_2}}^{t_1t_2} \Big(\prod_{\alpha=1}^l \mathcal{A}_{i_1\cdots i_d}^{(t_{2\alpha},t_{2\alpha+1})} Q_{i_{t_{2\alpha+1}}i_{t_{2\alpha+2}}}^{t_{2\alpha+1}t_{2\alpha+2}} \Big), \tag{G.2}$$

where $Q_{i\cdot}, Q_{\cdot i}$ means the i-th row and column of \mathbf{Q} , $\mathcal{A}_{i_1\cdots i_d}^{(t_{2l},t_{2l+1})}$ is defined in (D.6). If there is at least one terms in

$$\left\{Q_{i_{t_{2\alpha-1}}i_{t_{2\alpha}}}^{t_{2\alpha-1}t_{2\alpha}}:\alpha=1,\cdots,l+1\right\},$$

coming from the off-diagonal blocks, then the norms of (G.2) are bounded by $O(\|Q\|^{l+1}N)$.

Proof. Without loss of generality, we only give the detail proofs for l=4, i.e.

$$\sum_{i_1\cdots i_d}^{n_1\cdots n_d} \mathcal{A}_{i_1\cdots i_d}^{(t_1,t_{2l+2})} Q_{i_{t_1}i_{t_2}}^{t_1t_2} \Big(\prod_{\alpha=1}^4 \mathcal{A}_{i_1\cdots i_d}^{(t_{2\alpha},t_{2\alpha+1})} Q_{i_{t_2\alpha+1}i_{t_2\alpha+2}}^{t_{2\alpha+1}t_{2\alpha+2}} \Big), \tag{G.3}$$

Denote

 $n_{\mathbf{a}}^{(r)}$ and n_{r_1,r_2} to be the number of $a_{i_r}^{(r)}$ and $Q_{i_r,i_{r_2}}^{r_1r_2}$ in (G.3) respectively.

By the definition of $\mathcal{A}_{i_1\cdots i_d}^{(t_{2\alpha-1},t_{2\alpha})}$, there are at most two $r_1 \neq r_2$ such that $n_{\boldsymbol{a}}^{(r_1)} = n_{\boldsymbol{a}}^{(r_2)} = 0$. Let's consider the following three cases:

Case 1: If there exists $r_1, r_2 \in \{1, \dots, d\}$ such that $r_1 < r_2$ and $n_{\boldsymbol{a}}^{(r_1)} = n_{\boldsymbol{a}}^{(r_2)} = 0$, then all $\mathcal{A}_{i_1 \dots i_d}^{(t_{2\alpha-1}, t_{2\alpha})}$ should be equal, i.e. $t_{2\alpha-1} = r_1, t_{2\alpha} = r_2$ or $t_{2\alpha-1} = r_2, t_{2\alpha} = r_1$. Hence, for all $Q_{i_{1\alpha}i_{2\alpha+1}}^{t_{2\alpha}t_{2\alpha+1}}$, it must equal to $Q_{i_{r_1}i_{r_1}}^{r_1r_1}, Q_{i_{r_2}i_{r_2}}^{r_2r_2}$ or $Q_{\tilde{r}_1\tilde{r}_2}^{r_1r_2}$. Since we have at least one off-diagonal term, then we have at least one $Q_{i_{r_1}i_{r_2}}^{r_1r_2}$, i.e. $n_{r_1,r_2} \geq 1$. Hence if $n_{r_1,r_1}, n_{r_2,r_2} \geq 1$,

$$\begin{aligned} &|(G.3)| \leq \sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}} |\mathcal{A}_{i_{1}\cdots i_{d}}^{(r_{1},r_{2})}|^{l} |Q_{i_{r_{1}}i_{r_{1}}}^{r_{1}r_{1}}|^{n_{r_{1},r_{1}}} |Q_{i_{r_{2}}i_{r_{2}}}^{r_{2}r_{2}}|^{n_{r_{2},r_{2}}} |Q_{i_{r_{1}}i_{r_{2}}}^{r_{1}r_{2}}|^{n_{r_{1},r_{2}}} \\ &\leq \mathbf{1}' \operatorname{diag}(|\mathbf{Q}^{r_{1}r_{1}}|^{\circ n_{r_{1},r_{1}}}) |\mathbf{Q}^{r_{1}r_{2}}|^{\circ n_{r_{1},r_{2}}} \operatorname{diag}(|\mathbf{Q}^{r_{2}r_{2}}|^{\circ n_{r_{2},r_{2}}}) \mathbf{1} \leq N ||\mathbf{Q}||^{l+1} \end{aligned}$$

Otherwise, if at most one of n_{r_1,r_1}, n_{r_2,r_2} is nonzero, then we have $n_{r_1,r_2} \geq 2$

$$|(G.3)| \le \operatorname{Tr}\left(|Q^{r_2r_1}|\operatorname{diag}(|Q^{r_1r_1}|^{\circ n_{r_1,r_1}})|Q^{r_1r_2}|^{\circ(n_{r_1,r_2}-1)}\right) \le N||Q||^{l+1}$$

Case 2: If there is an $r_1 \in \{1, \dots, d\}$ such that $n_{\boldsymbol{a}}^{(r_1)} = 0$, then for any $\mathcal{A}_{i_1 \dots i_d}^{(t_{2\alpha}, t_{2\alpha+1})}$, we have $t_{2\alpha} = r_1$ or $t_{2\alpha+1} = r_1$. Without loss of generality, let $r_1 = 1$. If there is no diagonal terms, then we have all $n_{\boldsymbol{a}}^{(r)} \geq 1$ for r > 1 and

$$|(G.3)| \le \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \prod_{j=1}^{l+1} |\mathcal{A}^{(1,s_j)} Q_{i_1 \tilde{s}_j}^{1s_j}| \le \sum_{i_1}^{n_1} \prod_{j=1}^{l+1} |Q_{i_1}^{1s_j}| |\boldsymbol{a}^{(s_j)}| \le N \|\boldsymbol{Q}\|^{l+1}, \tag{G.4}$$

where $s_j \neq 1$ and $s_j \in \{1, \dots, d\}$. Hence, it is enough to consider there exists diagonal terms, and we claim that (G.3) must contain $Q_{i_1i_1}^{11}$. Otherwise, suppose (G.3) contains a diagonal term $Q_{i_1i_1i_1}^{t_1}$ such that $t_1 = t_2 \neq 1$, then $t_3, t_{10} = 1$ and $t_4 \neq 1$, since $A_{i_1 \cdots i_d}^{(4,5)}$ does not contain $a_{i_1}^{(1)}$, then $t_5 = 1, t_6 \neq 1$, otherwise $Q_{i_{t_5}i_{t_6}}^{t_5t_6} = Q_{i_1i_1}^{11}$. Similarly, since $A_{i_1 \cdots i_d}^{(6,7)}$ does not contain $a_{i_1}^{(1)}$, then $t_7 = 1, t_8 \neq 1$ and $t_9 = 1, t_{10} \neq 1$, which is a contradiction. Moreover, since we have at least one off-diagonal term, there are at most three types of diagonal terms. First, if there exists three different kinds of diagonal terms, without loss of generality, let them be $Q_{i_1i_1}^{11}, Q_{i_2i_2}^{22}$ and $Q_{i_3i_3}^{33}$ the only possible case is as follows:

$$(G.3) = \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \mathcal{A}_{i_1 \cdots i_d}^{(1,s_1)} Q_{i_1 i_1}^{11} \mathcal{A}_{i_1 \cdots i_d}^{(1,2)} Q_{i_2 i_2}^{22} \mathcal{A}_{i_1 \cdots i_d}^{(2,1)} Q_{i_1 i_1}^{11} \mathcal{A}_{i_1 \cdots i_d}^{(1,3)} Q_{i_3 i_3}^{33} \mathcal{A}_{i_1 \cdots i_d}^{(3,1)} Q_{i_1 i_{s_1}}^{1s_1} \mathcal{A}_{i_1 \cdots i_d}^{(1,2)} Q_{i_1 i_{s_1}}^{1s_1} \mathcal{A}_{i_1 \cdots i_d}^{(1,2)} Q_{i_1 i_1}^{1s_1} \mathcal{A}_{i_1 \cdots i_d}^{(1,2)} Q_{i_1 i_1 i_1 \cdots i_d}^{1s_1} \mathcal{A}_{i_1 \cdots i_d}^{1s_1}$$

where $s_1 \neq 1$. Since both $n_{\boldsymbol{a}}^{(2)}, n_{\boldsymbol{a}}^{(3)} \geq 2$. If $s_1 \neq 2$ or $s_1 \neq 3$, it gives that

$$|(G.3)| \le \mathbf{1}' \operatorname{diag}(|Q^{11}|^{\circ 2})|Q^{1s_1}||a^{(s_1)}| \cdot |a^{(2)}|' \operatorname{diag}(|Q^{22}|)|a^{(2)}|$$

 $\cdot |a^{(3)}|' \operatorname{diag}(|Q^{33}|)|a^{(3)}| \le N||Q||^{l+1}.$

Otherwise, suppose $s_1 = 2$, it gives that

$$|(\boldsymbol{G}.3)| \leq \mathbf{1}' \operatorname{diag}(|\boldsymbol{Q}^{11}|^{\circ 2})|Q^{12}| \operatorname{diag}(|\boldsymbol{Q}^{22}|)|\boldsymbol{a}^{(2)}| \cdot |\boldsymbol{a}^{(3)}|' \operatorname{diag}(|\boldsymbol{Q}^{33}|)|\boldsymbol{a}^{(3)}| \leq N \|\boldsymbol{Q}\|^{l+1}.$$

Next, suppose there are only two kinds of diagonal terms, then

$$\begin{aligned} |(G.3)| &= \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} |\mathcal{A}_{i_1 \cdots i_d}^{(1,s_3)} Q_{i_1 i_1}^{11} \mathcal{A}_{i_1 \cdots i_d}^{(1,s_1)} Q_{i_{s_1} i_{s_1}}^{s_1 s_1} \mathcal{A}_{i_1 \cdots i_d}^{(s_1,1)} Q_{i_1 i_1}^{11} \mathcal{A}_{i_1 \cdots i_d}^{(1,s_1)} Q_{i_{s_1} i_{s_1}}^{s_1 s_1} \mathcal{A}_{i_1 \cdots i_d}^{(s_1,1)} Q_{i_1 i_{s_3}}^{1s_3}| \\ &\leq \mathbf{1}' \operatorname{diag}(|\mathbf{Q}^{11}|^{\circ 2}) |Q^{1s_3}| |\mathbf{a}^{(s_3)}| \cdot \mathbf{1}' \operatorname{diag}(|\mathbf{Q}^{s_1 s_1}|^{\circ 2}) ||\mathbf{a}^{(s_1)}| \leq N \|\mathbf{Q}\|^{l+1}. \end{aligned}$$

Finally, if there is only one type of diagonal term which is $Q^{11}_{i_1i_1}$, then

$$\begin{split} &|(G.3)| \leq \sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}} |\mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{5},1)}Q_{i_{1}i_{1}}^{11}\mathcal{A}_{i_{1}\cdots i_{d}}^{(1,s_{1})}Q_{i_{s_{1}}i_{s_{2}}}^{s_{1}s_{2}}\mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{2},1)}Q_{i_{1}i_{1}}^{11}\mathcal{A}_{i_{1}\cdots i_{d}}^{(1,s_{3})}Q_{i_{s_{3}}i_{s_{3}}}^{s_{3}s_{4}}\mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{4},1)}Q_{i_{1}i_{s_{3}}}^{1s_{5}}|\\ &\leq \mathbf{1}'\operatorname{diag}(|\mathbf{Q}|^{11})|\mathbf{Q}^{1s_{5}}||\mathbf{a}^{(s_{5})}|\cdot|\mathbf{a}^{(s_{1})}|'|\mathbf{Q}^{s_{1}s_{2}}||\mathbf{a}^{(s_{2})}|\cdot|\mathbf{a}^{(s_{3})}|'|\mathbf{Q}^{s_{3}s_{4}}||\mathbf{a}^{(s_{4})}|\leq N\|\mathbf{Q}\|^{l+1} \end{split}$$

where $s_1 \neq s_2, s_3 \neq s_4$ and $s_1, \dots, s_5 \neq 1$.

Case 3: Suppose all $n_{(r)} \geq 1$. In this case, for any off-diagonal terms, notice that all $\mathcal{A}_{i_1\cdots i_d}^{(t_{2\alpha},t_{2\alpha+1})}$ and $\mathcal{A}_{i_1\cdots i_d}^{(t_1,t_{2l+2})}$ can not be equal, otherwise it is the first situation. Hence, there exists at most two $r_1 < r_2$ such that $n_{\boldsymbol{a}}^{(r_1)} = n_{\boldsymbol{a}}^{(r_2)} = 1$. Without loss of generality, let $r_1 = 1$ and $r_2 = 2$, then there are two situations. First, we have four $\mathcal{A}_{i_1\cdots i_d}^{(1,2)}$ and an $\mathcal{A}_{i_1\cdots i_d}^{(s_1,s_2)}$, where $s_1,s_2\neq 1,2$. Then we will have two off-diagonal terms $Q_{s_1i_1}^{s_1i_1},Q_{s_2i_2}^{s_2i_2}$ and

$$\begin{aligned} |(G.3)| &\leq \sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}} |(\mathcal{A}_{i_{1}\cdots i_{d}}^{(1,2)})^{4} (Q_{i_{1}i_{1}}^{11})^{n_{1,1}} (Q_{i_{2}i_{2}}^{22})^{n_{2,2}} (Q_{i_{1}i_{2}}^{12})^{n_{1,2}} \mathcal{A}_{i_{1}\cdots i_{d}}^{(1,2)} Q_{i_{s_{1}}i_{1}}^{s_{1}1} Q_{i_{s_{2}}i_{2}}^{s_{2}2} | \\ &\leq |\boldsymbol{a}^{(s_{1})}|' |\boldsymbol{Q}^{s_{1}1}| \operatorname{diag}(|\boldsymbol{Q}^{11}|^{\circ n_{1,1}}) |\boldsymbol{Q}^{12}|^{\circ n_{1,2}} \operatorname{diag}(|\boldsymbol{Q}^{22}|^{\circ n_{2,2}}) |\boldsymbol{Q}^{2s_{2}}| |\boldsymbol{a}^{(s_{2})}| \leq |\boldsymbol{Q}|^{l+1}. \end{aligned}$$

$$(G.5)$$

Otherwise, we have three $\mathcal{A}^{(1,2)}_{i_1\cdots i_d}$, one $\mathcal{A}^{1,s_1}_{i_1\cdots i_d}$ and $\mathcal{A}^{2,s_2}_{i_1\cdots i_d}$, so we will have one $Q^{s_1s_2}_{i_{s_1}i_{s_2}}$ or two off-diagonal terms like $Q^{s_11}_{i_{s_1}i_1}, Q^{s_22}_{i_{s_2}i_2}$ or $Q^{s_11}_{i_{s_1}i_1}, Q^{s_21}_{i_{s_2}i_1}$ or $Q^{s_12}_{i_{s_1}i_2}, Q^{s_22}_{i_{s_2}i_2}$. For the case of one $Q^{s_1s_2}_{i_{s_1}i_{s_2}}$, since it will associate with $\mathbf{a}^{(s_1)}, \mathbf{a}^{(s_2)}$ as $|\mathbf{a}^{(s_1)}|'|Q^{s_1s_2}||\mathbf{a}^{(s_2)}| \leq ||\mathbf{Q}||$, then we can use the same trick in (G.4) to conclude our claim. For the case of two $Q^{s_11}_{i_{s_1}i_1}, Q^{s_22}_{i_{s_2}i_2}$, it is the same as (G.5). So we only give the case of $Q^{s_11}_{i_{s_1}i_1}, Q^{s_21}_{i_{s_2}i_1}$ as follows (the other one is totally the same):

$$|(G.3)| \leq \sum_{i_1}^{n_1} |a_{i_1}^{(1)}| |Q_{i_1i_1}^{11}|^{n_{1,1}} |Q_{i_1\cdot}^{12}|^{\circ n_{1,2}} \operatorname{diag}(|\boldsymbol{Q}^{22}|^{n_{2,2}}) |\boldsymbol{a}^{(2)}| \cdot |Q_{i_1\cdot}^{1s_1}| |\boldsymbol{a}^{(s_1)}| \cdot |Q_{i_1\cdot}^{1s_2}| |\boldsymbol{a}^{(s_2)}| \leq N \|\boldsymbol{Q}\|^{l+1}.$$

Next, assume $n_{\bm{a}}^{(1)}=1$ and $n_{\bm{a}}^{(r)}\geq 2$ for all $r\neq 1$. In this case, we have at most three $Q_{i_{s_1}i_{s_2}}^{s_1s_2},Q_{i_{s_3}i_{s_4}}^{s_3s_4},Q_{i_{s_5}i_{s_6}}^{s_5s_6}$ such that $s_1,\cdots,s_6\neq 1$, i.e.

$$\mathcal{A}_{i_{1}\cdots i_{d}}^{(1,s_{1})}Q_{i_{s_{1}}i_{s_{2}}}^{s_{1}s_{2}}\mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{2},s_{3})}Q_{i_{s_{3}}i_{s_{4}}}^{s_{3}s_{4}}\mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{4},1)}Q_{i_{1}i_{1}}^{11}\mathcal{A}_{i_{1}\cdots i_{d}}^{(1,s_{5})}Q_{i_{s_{5}}i_{s_{6}}}^{s_{5}s_{6}}\mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{6},1)}Q_{i_{1}i_{1}}^{11}.$$

Since $Q_{i_1i_1}^{11}$ will associate with $\boldsymbol{a}^{(1)}$ as $\mathbf{1}$ diag($|\boldsymbol{Q}^{11}|^{\circ 2}$) $|\boldsymbol{a}^{(1)}| \leq N^{1/2} \|\boldsymbol{Q}\|^2$, and $Q_{i_{s_1}i_{s_2}}^{s_1s_2}$ will associate with $\boldsymbol{a}^{(s_1)}$ or other terms like $Q_{i_{s_3}i_{s_4}}^{s_3s_4}$ as (for example) $|\boldsymbol{a}^{(s_1)}|'|\boldsymbol{Q}^{(s_1,s_2)}||\boldsymbol{a}^{(s_2)}|$ or $|\boldsymbol{a}^{(s_1)}|'|\boldsymbol{Q}^{(s_1,s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||\boldsymbol{a}^{(s_2)}||$

$$\mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{6},1)}Q_{i_{1}i_{s_{5}}}^{1s_{5}}\mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{5},s_{1})}Q_{i_{s_{1}}i_{s_{2}}}^{s_{1}s_{2}}\mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{4},1)}Q_{i_{1}i_{1}}^{11}\mathcal{A}_{i_{1}\cdots i_{d}}^{(1,s_{3})}Q_{i_{s_{3}}i_{s_{4}}}^{s_{3}s_{4}}\mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{4},1)}Q_{i_{1}i_{s_{6}}}^{1s_{6}}$$

Therefore, for $Q_{i_{s_1}i_{s_2}}^{s_1s_2}$, it will associate with $\boldsymbol{a}^{(s_1)}, \boldsymbol{a}^{(s_2)}$ as $|\boldsymbol{a}^{(s_1)}|'|\boldsymbol{Q}^{s_1s_2}||\boldsymbol{a}^{(s_2)}| \leq \|\boldsymbol{Q}\|$ if $s_1, s_2 \neq s_5, s_6$ or one $Q_{i_1i_{s_5}}^{1s_5}$ as $Q_{i_1}^{1s_1}\boldsymbol{Q}^{s_1s_2}\boldsymbol{a}^{(s_2)}$. Whatever which situations, it must have (e.g. $s_1, \dots, s_4 \neq s_5, s_6$)

$$|(G.3)| \leq |\boldsymbol{a}^{(s_5)}|'|\boldsymbol{Q}^{s_51}|\operatorname{diag}(|\boldsymbol{Q}|^{11})|\boldsymbol{Q}^{1s_6}||\boldsymbol{a}^{(s_6)}| \cdot |\boldsymbol{a}^{(s_1)}|'|\boldsymbol{Q}^{s_1s_2}||\boldsymbol{a}^{(s_2)}| \cdot |\boldsymbol{a}^{(s_3)}|'|\boldsymbol{Q}^{s_3s_4}||\boldsymbol{a}^{(s_4)}| \leq \|\boldsymbol{Q}\|^{l+1}.$$

Now, if we have one $Q_{i_{s_1}i_{s_2}}^{s_1s_2}$. Similar as the above result, $Q_{i_{s_1}i_{s_2}}^{s_1s_2}$ can associate with $Q_{i_1s_1}^{1s_1}$ as $Q_{i_1}^{1s_1} Q^{s_1s_2} a^{(s_2)}$, or associate with $a^{(s_1)}, a^{(s_2)}$ as $|a^{(s_1)}|' |Q^{s_1s_2}| |a^{(s_2)}| \le ||Q||$. So, it gives that

$$|(\boldsymbol{G}.3)| \leq |\boldsymbol{a}^{(s_1)}|'|\boldsymbol{Q}^{s_1s_2}||\boldsymbol{a}^{(s_2)}| \sum_{i_1}^{n_1} |a_{i_1}^{(1)}||Q_{i_1i_1}^{11}|^{n_{1,1}} \cdot \prod_{j=1}^{l_0} |Q_{i_1}^{1s_j}||\boldsymbol{a}^{(j)}| \leq N \|\boldsymbol{Q}\|^{l+1},$$

where we use the fact that all $|Q_{i_1}^{1s_j}||a^{(j)}| \leq ||Q||$ and $\mathbf{1}' \operatorname{diag}(|Q^{11}|^{\circ n_{1,1}})|a^{(1)}| \leq N||Q||^{n_{1,1}}$. Finally, suppose all $n_{\boldsymbol{a}}^{(r)} \geq 2$. Since l=4, given an $r \in \{1, \cdots, d\}$, there will be at most three $\mathcal{A}_{i_1 \cdots i_d}^{(t_{2\alpha-1}, t_{2\alpha})}$ contain r. As a result, for any diagonal terms $Q_{i_r i_r}^{rr}$ in (G.3), we have two situations. First, all $(t_{2\alpha}, t_{2\alpha+1})$ from $Q_{i_{2\alpha}i_{2\alpha+1}}^{t_{2\alpha+1}}$ does not contain r, then there is only one $Q_{i_r i_r}^{rr}$ in (G.3), which will associate with $\boldsymbol{a}^{(r)}$ as follows:

$$|a^{(r)}|' \operatorname{diag}(|Q^{rr}|)|a^{(r)}|^{\circ (n_a^{(r)}-1)} \le ||Q||^{n_{r,r}}.$$

Otherwise, there exists only one $Q_{i_r i_{s_1}}^{rs_1}$ such that $s_1 \neq r$, then $Q_{i_r i_r}^{rr}$ will associate with $\boldsymbol{a}^{(r)}$ and $Q_{i_r i_{s_1}}^{rs_1}$ as follows (e.g.):

$$(|\boldsymbol{a}^{(r)}|^{\circ n_{(r)}})' \operatorname{diag}(|\boldsymbol{Q}^{rr}|)|\boldsymbol{Q}^{rs_1}||\boldsymbol{a}^{(s_1)}| \leq ||\boldsymbol{Q}||^2.$$

Lastly, for the off-diagonal terms, since l=4, there are at most three $Q_{i_ri_{s_1}}^{rs_1}, Q_{i_ri_{s_2}}^{rs_2}, Q_{i_ri_{s_3}}^{rs_3}$ such that $s_1, s_2, s_3 \neq r$. For each of them, it will associate with $\boldsymbol{a}^{(s_1)}$ as $|Q_{i_r}^{rs_1}||\boldsymbol{a}^{(s_1)}|$ or other $Q_{i_{s_1}i_{s_4}}^{s_1s_4}$ as $|Q_{i_r}^{rs_1}||\boldsymbol{Q}^{s_1s_4}||\boldsymbol{a}^{(s_4)}|$. No matter which cases, we have (e.g.)

$$|(\boldsymbol{G}.3)| \leq \sum_{i_{r}}^{n_{r}} |a_{i_{r}}^{(r)}|^{2} |Q_{i_{r}}^{rs_{1}}||\boldsymbol{Q}^{s_{1}s_{4}}||\boldsymbol{a}^{(s_{4})}| \cdot |Q_{i_{r}}^{rs_{2}}||\boldsymbol{Q}^{s_{2}s_{5}}||\boldsymbol{a}^{(s_{5})}| \cdot |Q_{i_{r}}^{rs_{3}}||\boldsymbol{a}^{(s_{3})}| \leq \|\boldsymbol{Q}\|^{l+1}.$$

Now, we complete our proof.

Finally, we present the extension of Lemma D.6 as follows:

Lemma G.4. For any $z \in \mathbb{C}_{\eta}^+$ and $1 \le l_1, l_2 \le 4$, let $t_i, s_j \in \{1, \dots, d\}$ for $1 \le i \le 2l_1 + 1, 1 \le j \le 2l_2 + 1$ such that $t_{2\alpha} \ne t_{2\alpha+1}$ and $s_{2\gamma} \ne s_{2\gamma+1}$ for $1 \le \alpha \le l_1, 1 \le \gamma \le l_2$ and $t_1 \ne t_{2l_1+2}, s_1 \ne s_{2l_2+2}$ the define

$$\begin{cases} P_1(z) := \mathcal{A}_{ijk}^{(t_1,t_{2l_1+2})} Q_{i_1i_2}^{t_1t_2}(z) \left(\prod_{\alpha=1}^{l_1} \mathcal{A}_{i_1\cdots i_d}^{(t_{2\alpha},t_{2\alpha+1})} Q_{i_{2\alpha+1}i_{2\alpha+2}}^{t_{2\alpha+1}t_{2\alpha+2}}(z) \right), \\ P_2(z) := \mathcal{A}_{ijk}^{(s_1,s_{2l_2+2})} Q_{i_{s_1}i_{s_2}}^{s_1s_2}(z) \left(\prod_{\gamma=1}^{l_2} \mathcal{A}_{i_1\cdots i_d}^{(s_{2\gamma},s_{2\gamma+1})} Q_{i_{s_{2\gamma+1}i_{s_{2\gamma+2}}}^{s_{2\gamma+1}s_{2\gamma+2}}(z) \right). \end{cases}$$

If there are at least one term in

$$\left\{Q_{i_{t_{2\alpha+1}}i_{t_{2\alpha+2}}}^{t_{2\alpha+1}t_{2\alpha+2}}(z):\alpha=1,\cdots,l_1+1\right\}\quad\text{or}\quad \left\{Q_{i_{s_{2\gamma+1}}i_{s_{2\gamma+2}}}^{s_{2\gamma+1}s_{2\gamma+2}}(z):\gamma=1,\cdots,l_2+1\right\},$$

coming from the off-diagonal blocks, then the norm of $\sum_{i,j,k=1}^{m,n,p} P_1(z)P_2(z)$ is bounded by $O(\|\boldsymbol{Q}\|^{l_1+l_2+2}N)$.

Proof. Denote

$$n_{r_1,r_2}^{(i)}$$
 to be the number of $Q_{i_{r_1}i_{r_3}}^{r_1r_2}$ in $P_i(z)$ for $i=1,2$.

Since we can apply the Cauchy's inequality to show $\sum_{i_1\cdots i_d}^{n_1\cdots i_d} P_1(z)P_2(z)$ is bounded by $C\|\mathbf{Q}\|^{l_1+l_2+2}N$, without loss of generality, assume only $P_2(z)$ contains off-diagonal blocks. Therefore, for each $Q_{it_{\alpha}it_{\alpha}}^{t_{\alpha}}(z)$ in $P_1(z)$, denoting $n_{t_{\alpha},t_{\alpha}}^{(1)}$ and $n_{t_{\alpha},t_{\alpha}}^{(2)}$ to be the number of $Q_{it_{\alpha}it_{\alpha}}^{t_{\alpha}}(z)$ in $P_1(z)$ and $P_2(z)$, respectively, then consider the following two cases:

Case 1: If there exists $Q_{i_{s_2\gamma+1}i_{s_2\gamma+2}}^{s_2\gamma+1}(z)$ in $P_2(z)$ equal to $Q_{i_{t_{\alpha}}i_{t_{\alpha}}}^{t_{\alpha}t_{\alpha}}(z)$, then all arguments in Remark G.3 will be almost unchanged, just replacing the original power $n_{t_{\alpha},t_{\alpha}}^{(2)}$ by $n_{t_{\alpha},t_{\alpha}}^{(1)}+n_{t_{\alpha},t_{\alpha}}^{(2)}$.

Case 2: Otherwise, if $Q_{i_{t_{\alpha}}i_{t_{\alpha}}}^{t_{\alpha}t_{\alpha}}(z)$ does not exist in $P_{2}(z)$, then all $\mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{2\gamma},s_{2\gamma+1})}$ must contain $a_{i_{t_{\alpha}}}^{(t_{\alpha})}$. Therefore, when $l_{2} \geq 2$, the number of $a_{i_{t_{\alpha}}}^{(t_{\alpha})}$ in $P_{2}(z)$ must be no smaller than 2, then all $Q_{i_{t_{\alpha}}i_{t_{\alpha}}}^{t_{\alpha}t_{\alpha}}(z)$ will associate with $a_{i_{t_{\alpha}}}^{(t_{\alpha})}$ by $|\boldsymbol{a}^{(t_{\alpha})}|'$ diag $(|\boldsymbol{Q}^{t_{\alpha}t_{\alpha}}|^{\circ n_{t_{\alpha},t_{\alpha}}^{(1)}})|\boldsymbol{a}^{(t_{\alpha})}| \leq \|\boldsymbol{Q}\|^{n_{t_{\alpha},t_{\alpha}}^{(1)}}$. Finally, when $l_{2}=1$, i.e. $P_{2}(z) = \mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{1},s_{2})}Q_{i_{s_{1}}i_{s_{2}}}^{s_{1}s_{2}}(z)$ and $s_{1} \neq s_{2}$, since $P_{1}(z)$ only contains diagonal terms, then $l_{1} \geq 2$ and we have at least two kinds of diagonal terms, let's consider the following two possible cases:

• $P_1(z)$ only contains $Q_{i_{t_1}i_{t_1}}^{t_1t_1}(z)$ and $Q_{i_{t_2}i_{t_2}}^{t_2t_2}(z)$, i.e.

$$P_1(z) = \mathcal{A}_{i_1 \cdots i_d}^{(t_2, t_1)} Q_{i_t, i_t}^{t_1 t_1}(z) \mathcal{A}_{i_1 \cdots i_d}^{(t_1, t_2)} Q_{i_t, i_t}^{t_2 t_2}(z) \mathcal{A}_{i_1 \cdots i_d}^{(t_2, t_1)} \cdots$$

Since $s_1, s_2 \neq t_1$ and $s_1, s_2 \neq t_2$, then there exists $a_{i_{t_1}}^{(t_1)}, a_{i_{t_2}}^{(t_2)}$ and $a_{i_{s_1}}^{(s_1)}, a_{i_{s_2}}^{(s_2)}$, we can conclude that

$$\sum_{i_1\cdots i_d}^{n_1\cdots n_d} |P_1(z)P_2(z)| \le |\boldsymbol{a}^{(s_1)}|'|\boldsymbol{Q}^{s_1s_2}||\boldsymbol{a}^{(s_2)}| \cdot \mathbf{1}'\operatorname{diag}(|\boldsymbol{Q}^{t_1t_1}|^{\circ n_{t_1,t_1}^{(1)}})|\boldsymbol{a}^{(t_1)}| \cdot \mathbf{1}'\operatorname{diag}(|\boldsymbol{Q}^{t_2t_2}|^{\circ n_{t_2,t_2}^{(1)}})|\boldsymbol{a}^{(t_2)}| < \|\boldsymbol{Q}\|^{l_1+l_2+2}N.$$

• $P_1(z)$ contains at least three different $Q_{i_1i_1}^{t_1t_1}(z), Q_{i_2i_2}^{t_2t_2}(z), Q_{i_3i_3}^{t_3t_3}(z), \cdots$ coming from diagonal blocks, where $t_1 \neq t_2 \neq t_3 \cdots$ and all $t_j \neq s_1, t_j \neq s_2$, then for each t_j , there will be at most one $a_{it_j}^{(t_j)}$ not existing in $P_1(z)$, otherwise we back to the previous situation. Without loss generality, assume $P_1(z)$ does not contain $a_{it_1}^{(t_1)}$, then for each $a_{it_j}^{(t_j)}$ where $j \geq 2$, it will appear in $\mathcal{A}_{i_1\cdots i_d}^{(s_1,s_2)}$ and $P_1(z)$ at least once, so $Q_{it_ji_j}^{t_jt_j}(z)$ will associate with at least two $a_{it_j}^{(t_j)}$ by $|\boldsymbol{a}^{(t_j)}|' \operatorname{diag}(|\boldsymbol{Q}^{t_jt_j}|^{\circ n_{i_j,t_j}^{(1)}})|\boldsymbol{a}^{(t_j)}| \leq \|\boldsymbol{Q}\|^{n_{i_j,t_j}^{(1)}}$. For $Q_{it_1i_1}^{t_1t_1}(z)$, it will associate with one $a_{it_1}^{(t_1)}$ by $\mathbf{1}' \operatorname{diag}(|\boldsymbol{Q}^{t_1t_1}|^{\circ n_{i_1,t_1}^{(1)}})|\boldsymbol{a}^{(t_1)}| \leq N^{1/2}\|\boldsymbol{Q}\|^{n_{i_1,t_1}^{(1)}}$, which can conclude our claim. Finally, if $P_1(z)$ contains $a_{it_1}^{(t_1)}$, then all $Q_{it_ji_j}^{t_jt_j}(z)$ will associate with at least two $a_{it_j}^{(t_j)}$ by $|\boldsymbol{a}^{(t_j)}|' \operatorname{diag}(|\boldsymbol{Q}^{t_jt_j}|^{\circ n_{i_j,t_j}^{(1)}})|\boldsymbol{a}^{(t_j)}| \leq \|\boldsymbol{Q}\|^{n_{i_j,t_j}^{(1)}}$.

Now, we complete the extension of Lemma D.6 for general $d \geq 3$.

G.2 Entrywise law

Theorem G.1. Under Assumptions A.1 and A.2, for any $\eta_0 > 0$, $z \in \mathcal{S}_{\eta_0}$ in (G.1) and $\omega \in (1/2 - \delta, 1/2)$, where $\delta > 0$ is a sufficiently small number, let

$$\boldsymbol{W}^{(d)}(z) = -((z+g(z))\boldsymbol{I}_d - \operatorname{diag}(\boldsymbol{g}(z)) + g(z)\boldsymbol{S}_d - \operatorname{diag}(\boldsymbol{g}(z))\boldsymbol{S}_d - \boldsymbol{S}_d\operatorname{diag}(\boldsymbol{g}(z)))^{-1}.$$
 (G.6)

For $s, t \in \{1, \dots, d\}$, we have

$$\left| Q_{i_s i_t}^{st}(z) - \mathfrak{c}_s^{-1} g_s(z) \left[\delta_{st} \delta_{i_s i_t} + (a_{i_s}^{(s)})^2 \sum_{k \neq s}^d (g(z) - g_s(z) - g_k(z)) W_{sk}^{(d)}(z) \right] \right| \prec \mathcal{O}(\eta_0^{-21} N^{-\omega}),$$

where $Q_{i_si_t}^{st}(z)$ is the (i_s, i_t) -th entry of \mathbf{Q}^{st} and $a_{i_s}^{(s)}$ is the i-th entry of $\mathbf{a}^{(s)}$, so does $W_{sk}^{(d)}(z)$, and $\mathbf{g}(z) = (g_1(z), \dots, g_d(z))'$ is the solution of (B.1).

Proof. The existence of $W^{(d)}(z)$ on S_{η_0} is proven in Lemma G.5 later. Similar as (D.40), we define

$$W_{st,N}^{(d)}(z) = \mathbb{E}[(\boldsymbol{a}^{(s)})'\boldsymbol{Q}^{st}(z)\boldsymbol{a}^{(t)}], \text{ for } 1 \leq s, t \leq d.$$

Recall that $\|Q(z)\| \le \eta_0^{-1}$ for any $z \in \mathcal{S}_{\eta_0}$ in (G.1) Here, we will omit (z) in the following contents for convenience. Similar as what we have done in §D.2, we first prove that for any $\omega \in (1/2 - \delta, 1/2)$

$$\sup_{z \in \mathcal{S}_{\eta_0}} \| g(z) - m(z) \|_{\infty} = O(\eta_0^{-15} N^{-2\omega}).$$
 (G.7)

By $MQ - zQ = I_N$ and cumulant expansion (D.4), we have

$$\begin{split} z\mathbb{E}[Q_{i_{s}i_{t}}^{st}] &= \frac{1}{\sqrt{N}} \sum_{l \neq s}^{d} \sum_{i_{1} \cdots i_{d}}^{(s,t)} \mathbb{E}[X_{i_{1} \cdots i_{d}} \mathcal{A}_{i_{1} \cdots i_{d}}^{(s,l)} Q_{i_{l}i_{t}}^{lt}] - \delta_{st} \delta_{i_{s}i_{t}} \\ &= \frac{1}{\sqrt{N}} \sum_{i_{1} \cdots i_{d}}^{(s,t)} \left(\sum_{l \neq s}^{d} \mathbb{E}[\partial_{i_{1} \cdots i_{d}}^{(1)} \{\mathcal{A}_{i_{1} \cdots i_{d}}^{(s,l)} Q_{i_{l}i_{t}}^{lt}\}] + \epsilon_{i_{1} \cdots i_{d}}^{(2)} \right) - \delta_{st} \delta_{i_{s}i_{t}}, \end{split}$$

where the notation $\sum_{i_1\cdots i_d}^{(s,t)}$ means the summation is over all $i_r=1,\cdots,n_r$ except $i_s=1,\cdots,n_s$ and $i_t=1,\cdots,n_t$. Similar as proofs of (D.37) in Theorem D.1, we can show that $N^{-1/2}|\sum_{i_1\cdots i_d}^{(s,t)}\epsilon_{i_1\cdots i_d}^{(2)}|$ = $O(a_{i_s}^{(s)}\eta_0^{-3}N^{-1/2}+\eta_0^{-3}N^{-1})$. Here we omit details for convenience, and readers can refer to (G.11) in Theorem G.2 for an example of calculating remainders. Next, by direct calculation, it gives that

$$\frac{1}{\sqrt{N}} \sum_{l \neq s}^{d} \sum_{i_{1} \cdots i_{d}}^{(s,t)} \mathbb{E} \left[\partial_{i_{1} \cdots i_{d}}^{(1)} \left\{ \mathcal{A}_{i_{1} \cdots i_{d}}^{(s,l)} Q_{i_{l}i_{t}}^{lt} \right\} \right] = -\frac{1}{N} \sum_{l \neq s}^{d} \sum_{i_{1} \cdots i_{d}}^{(s,t)} \left[\mathcal{A}_{i_{1} \cdots i_{d}}^{(s,l)} Q_{i_{l}i_{r_{1}}}^{lr_{1}} \mathcal{A}_{i_{1} \cdots i_{d}}^{(r_{1},r_{2})} Q_{i_{r_{2}}i_{t}}^{r_{2}t} \right]$$

$$= -\sum_{l \neq s}^{d} \mathbb{E} \left[Q_{i_{s}i_{t}}^{st} \rho_{l}(z) \right] - \sum_{l \neq s}^{d} \sum_{r \neq s}^{d} a_{i_{s}}^{(s)} \mathbb{E} \left[Q_{i_{t}}^{tr} \boldsymbol{a}^{(r)} \rho_{l}(z) \right] + \mathcal{O}(\eta_{0}^{-2} N^{-1}),$$

where $\rho_l(z) = N^{-1} \operatorname{Tr}(\boldsymbol{Q}^{ll}(z))$ and $Q_{i_t}^{tr}(z)$ is the i_t -th row of \boldsymbol{Q}^{tr} . By Lemma G.2, we can derive

$$(z + \mathfrak{m}(z) - \mathfrak{m}_s(z))\mathbb{E}[Q_{i_s i_t}^{st}] = -\delta_{st}\delta_{i_s i_t} - \sum_{l \neq s}^{d} \mathfrak{m}_l(z) \sum_{r \neq s, l}^{d} a_{i_s}^{(s)} \mathbb{E}[Q_{i_t}^{tr} \boldsymbol{a}^{(r)}] + \mathcal{O}(\eta_0^{-10} N^{-2\omega}),$$

where $\mathfrak{m}_l(z) = \mathbb{E}[\rho_l(z)]$ and $\mathfrak{m}(z) = \sum_{l=1}^d \mathfrak{m}_l(z)$. Thus, we obtain that

$$(z + \mathfrak{m}(z) - \mathfrak{m}_s(z))\mathfrak{m}_s(z) = -\mathfrak{c}_s + \mathcal{O}(\eta_0^{-10}N^{-2\omega})$$

combining the fact $|\mathfrak{m}_s(z)| \geq \eta_0$ and Lemma B.2, we can conclude (G.7). Consequently, we obtain that

$$(z + g(z) - g_s(z))\mathbb{E}[Q_{i_s i_t}^{st}] = -\delta_{st}\delta_{i_s i_t} - \sum_{l \neq s}^{d} g_l(z) \sum_{r \neq s, l}^{d} a_{i_s}^{(s)} \mathbb{E}[Q_{i_t}^{tr}.\boldsymbol{a}^{(r)}] + \mathcal{O}(\eta_0^{-16}N^{-2\omega}),$$

For $\mathbb{E}[Q_{i_r}^{tr}.\boldsymbol{a}^{(r)}]$, by the previous trick, we can obtain that

$$z\mathbb{E}[Q_{i_t}^{tr}.\boldsymbol{a}^{(r)}] = -\sum_{l \neq t}^{d} \mathbb{E}[Q_{i_t}^{tr}.\boldsymbol{a}^{(r)}\rho_l(z)] - a_{i_t}^{(t)} \sum_{l \neq t}^{d} \sum_{w \neq t,l}^{d} \mathbb{E}[(\boldsymbol{a}^{(r)})'\boldsymbol{Q}^{rw}\boldsymbol{a}^{(w)}\rho_l(z)] + O(a_{i_t}^{(t)}\eta_0^{-3}N^{-1/2} + \eta_0^{-3}N^{-1}),$$

further by Lemma G.2 and (G.7), it yields that

$$(z+g(z)-g_t(z))\mathbb{E}[Q_{i_t}^{tr}.\boldsymbol{a}^{(r)}] = -a_{i_t}^{(t)} \sum_{l\neq t}^d g_l(z) \sum_{w\neq t,l}^d W_{rw,N}^{(d)} + \mathcal{O}(a_{i_t}^{(t)} \eta_0^{-3} N^{-1/2} + \eta_0^{-3} N^{-1} + \eta_0^{-16} N^{-2\omega}),$$

i.e.

$$a_{i_t}^{(t)} \mathbb{E}[Q_{i_t}^{tr}.\boldsymbol{a}^{(r)}] = (a_{i_t}^{(t)})^2 \mathfrak{c}_t^{-1} g_t(z) \sum_{l \neq t}^d g_l(z) \sum_{w \neq t, l}^d W_{rw, N}^{(d)} + a_{i_t}^{(t)} \mathcal{O}(a_{i_t}^{(t)} \eta_0^{-4} N^{-1/2} + \eta_0^{-4} N^{-1} + \eta_0^{-17} N^{-2\omega}).$$

Summing all $i_t = 1, \dots, n_t$ of above equations, we obtain

$$W_{tr,N}^{(d)} = \mathfrak{c}_t^{-1} g_t(z) \sum_{l \neq t}^d g_l(z) \sum_{w \neq t,l}^d W_{rw,N}^{(d)} + \mathcal{O}(\eta_0^{-17} N^{-2\omega + 1/2}),$$

so

$$\mathbb{E}[Q_{i_t}^{tr}.\boldsymbol{a}^{(r)}] = a_{i_t}^{(t)} W_{tr,N}^{(d)}(z) + \mathcal{O}(\eta_0^{-17} N^{-2\omega + 1/2}),$$

and

$$\mathbb{E}[Q_{i_s i_t}^{st}] = \mathfrak{c}_s^{-1} g_s(z) \left(\delta_{st} \delta_{i_s i_t} + a_{i_s}^{(s)} \sum_{l \neq s}^d g_l(z) \sum_{r \neq s}^d a_{i_t}^{(t)} W_{tr,N}^{(d)}(z) \right) + \mathcal{O}(\eta_0^{-19} N^{-2\omega + 1/2}).$$

Since $\omega \in (1/2 - \delta, 1/2)$, then $2\omega - 1/2 \in (1/2 - 2\delta, 1/2)$. Finally, combining Lemmas G.2 and (G.28), we complete our proof.

G.3 Mean and covariance functions

Before establishing the CLT for LSS of M for general $d \geq 3$, let's derive the general forms of the mean function $\mu_N^{(3)}(z)$ in (E.37) and covariance function $\mathcal{C}_N^{(3)}(z_1, z_2)$ in (E.5) as follows:

G.3.1 Covariance function

Theorem G.2. Under Assumptions A.1 and A.2, for any $z_1, z_2 \in \mathcal{S}_{\eta_0}$ in (G.1), let

$$C_{st,N}^{(d)}(z_1, z_2) := \text{Cov}(\text{Tr}(\boldsymbol{Q}^{ss}(z_1)), \text{Tr}(\boldsymbol{Q}^{tt}(z_2))) \quad \text{and} \quad C_N^{(d)}(z_1, z_2) := [C_{st,N}^{(d)}(z_1, z_2)]_{d \times d}, \quad (G.8)$$

where $s, t \in \{1, \dots, d\}$, then we have

$$\lim_{N \to \infty} \|\boldsymbol{C}_{N}^{(d)}(z_{1}, z_{2}) - \boldsymbol{\Pi}^{(d)}(z_{1}, z_{2})^{-1} \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1} \circ \boldsymbol{g}(z_{1})) \boldsymbol{F}_{N}^{(d)}(z_{1}, z_{2}) \| = 0, \tag{G.9}$$

where $\Pi^{(d)}(z_1, z_2)$ is defined in (B.11) and

$$\boldsymbol{F}_{N}^{(d)}(z_{1},z_{2}) = [\mathcal{F}_{st,N}^{(d)}(z_{1},z_{2})]_{d\times d} \quad \mathcal{F}_{st,N}^{(d)}(z_{1},z_{2}) := 2\mathcal{V}_{st}^{(d)}(z_{1},z_{2}) + \kappa_{4}\mathcal{U}_{st,N}^{(d)}(z_{1},z_{2}),$$

and the precise definitions of $\mathcal{V}_{st}^{(d)}(z_1, z_2)$ and $\mathcal{U}_{st,N}^{(d)}(z_1, z_2)$ are postponed to (G.33) and (G.36), respectively. Consequently, $\operatorname{Var}(\operatorname{Tr}(\boldsymbol{Q}(z)))$ are bounded by $C_{\eta_0,\mathfrak{c}}$ for any $z \in \mathcal{S}_{\eta_0}$ and

$$\lim_{N \to \infty} |\operatorname{Cov}(\operatorname{Tr}(\boldsymbol{Q}(z_1)), \operatorname{Tr}(\boldsymbol{Q}(z_2))) - \mathcal{C}_N^{(d)}(z_1, z_2)| = 0,$$

where

$$C_N^{(d)}(z_1, z_2) := \mathbf{1}_d' \mathbf{\Pi}^{(d)}(z_1, z_2)^{-1} \operatorname{diag}(\mathbf{c}^{-1} \circ \mathbf{g}(z_1)) \mathbf{F}_N^{(d)}(z_1, z_2) \mathbf{1}_d.$$
 (G.10)

Proof. Let's first show that $C_{k_1k_2,N}^{(d)}(z,z)$ is bounded by $C_{\eta_0,\mathfrak{c},d}$. Without loss of generality, we assume that $|C_{k_1k_2,N}^{(d)}(z,z)| > 1$, otherwise, they are already bounded. For convenience, we omit (z,z) behind $C_{k_1k_2,N}^{(d)}(z,z)$. By the cumulant expansion (D.4), we have

$$\begin{split} &z\mathcal{C}_{k_{1}k_{2},N}^{(d)} = z\operatorname{Cov}(\operatorname{Tr}(\boldsymbol{Q}^{k_{1}k_{1}}(z)),\operatorname{Tr}(\boldsymbol{Q}^{k_{2}k_{2}}(z))) \\ &= \frac{1}{\sqrt{N}} \sum_{l \neq k_{1}}^{d} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \mathbb{E}\left[X_{i_{1} \cdots i_{d}} \mathcal{A}_{i_{1} \cdots i_{d}}^{(k_{1},l)} Q_{i_{k_{1}}i_{l}}^{k_{1}l}(z) \operatorname{Tr}(\boldsymbol{Q}^{k_{2}k_{2}}(\bar{z}))^{c}\right] \\ &= \frac{1}{\sqrt{N}} \sum_{l \neq k_{1}}^{d} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \left(\sum_{\alpha = 1}^{3} \frac{\kappa_{\alpha + 1}}{\alpha !} \mathbb{E}\left[\mathcal{A}_{i_{1} \cdots i_{d}}^{(k_{1},l)} \partial_{i_{1} \cdots i_{d}}^{(\alpha)} \left\{Q_{i_{k_{1}}i_{l}}^{k_{1}l}(z) \operatorname{Tr}(\boldsymbol{Q}^{k_{2}k_{2}}(\bar{z}))^{c}\right\}\right] + \epsilon_{i_{1} \cdots i_{d}}^{(4)} \right), \end{split}$$

where the remainder satisfies that $|\epsilon_{i_1\cdots i_d}^{(4)}| \leq C_{\kappa_5} \sup_{z\in\mathcal{S}_{\eta_0}} |\partial_{i_1\cdots i_d}^{(4)} \left\{ Q_{i_{k_1}i_l}^{k_1l}(z) \operatorname{Tr}(\boldsymbol{Q}^{k_2k_2}(\bar{z}))^c \right\}|$. Similar as proofs of Theorem E.1, we claim that the major terms only appear in the first and third derivatives. Since the proofs are the same as those for Theorem E.1, here we only show that $N^{-1/2}|\sum_{i_1\cdots i_d}^{n_1\cdots n_d}\epsilon_{i_1\cdots i_d}^{(4)}| \to 0$ as an example. By Lemmas G.3 and G.4, it is enough to show that for each $l\neq k_1$ and $0\leq \gamma\leq 4$

$$N^{-1/2} \Big| \sum_{i_1 \dots i_d}^{n_1 \dots n_d} \mathcal{A}_{i_1 \dots i_d}^{(k_1, l)} \mathscr{D} \left(\partial_{i_1 \dots i_d}^{(\gamma)} \{ Q_{i_{k_1} i_l}^{k_1 l}(z) \} \right) \mathscr{D} \left(\partial_{i_1 \dots i_d}^{(4-\gamma)} \{ \operatorname{Tr} (\boldsymbol{Q}^{k_2 k_2}(\bar{z}))^c \} \right) \Big| \to 0.$$
 (G.11)

For $\gamma=0,$ it is easy to see $\mathscr{D}\big(\partial^{(0)}_{i_1\cdots i_d}\{Q^{k_1l}_{i_{k_1}i_l}(z)\}\big)=0.$ For $\gamma=3,$ since

$$\partial_{i_1\cdots i_d}^{(1)} \operatorname{Tr}(\boldsymbol{Q}^{k_2k_2}(\bar{z})) = \sum_{j=1}^{n_{k_2}} \partial_{i_1\cdots i_d}^{(1)} Q_{jj}^{k_2k_2}(\bar{z}) = -\frac{1}{\sqrt{N}} \sum_{t_1 \neq t_2}^{d,d} \mathcal{A}_{i_1\cdots i_d}^{(t_1,t_2)} Q_{i_1}^{t_1k_2}(\bar{z}) Q_{i_{t_2}}^{k_2t_2}(\bar{z}), \tag{G.12}$$

then $\mathscr{D}\left(\partial_{i_1\cdots i_d}^{(1)}\left\{\mathrm{Tr}(\boldsymbol{Q}^{k_2k_2}(\bar{z}))^c\right\}\right)=0$. Next, for $\gamma=4$, note that

$$\begin{split} &\mathcal{A}_{i_{1}\cdots i_{d}}^{(k_{1},l)}\mathcal{D}\left(\partial_{i_{1}\cdots i_{d}}^{(4)}\{Q_{i_{k_{1}}i_{l}}^{k_{1}l}(z)\}\right) = N^{-2}\mathcal{A}_{i_{1}\cdots i_{d}}^{(k_{1},l)}Q_{i_{k_{1}}i_{k_{1}}}^{k_{1}k_{1}}(z)Q_{i_{l}i_{l}}^{ll}(z)\times\\ &\sum_{s_{1}\neq k_{1}}^{d}\sum_{s_{2}\neq s_{1}}^{d}\sum_{s_{3}\neq s_{2},l}^{d}\mathcal{A}_{i_{1}\cdots i_{d}}^{(k_{1},s_{1})}Q_{i_{s_{1}}i_{s_{1}}}^{s_{1}s_{1}}(z)\mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{1},s_{2})}Q_{i_{s_{2}}i_{s_{2}}}^{s_{2}s_{2}}(z)\mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{2},s_{3})}Q_{i_{s_{3}}i_{s_{3}}}^{s_{3}s_{3}}(z)\mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{3},l)}, \end{split} \tag{G.13}$$

then (G.13) contains at least two different $Q_{i_{s_{l}}i_{s_{l}}}^{s_{l}s_{l}}$ coming from diagonal blocks, denote n_{k} to be the number $a_{i_{k}}^{(k)}$ appearing in (G.13), so $n_{r} \geq 1$ for $1 \leq r \leq d$. It is easy to see that $|\sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}}(G.13)| \leq O(N^{-2}\|\boldsymbol{Q}(z)\|^{5})$ if all $n_{r} \geq 2$, so that $(G.11) \leq O(N^{-3/2}\|\boldsymbol{Q}(z)\|^{6})$. Otherwise, there are at most two different $n_{r_{1}} = 1$ and $n_{r_{2}} = 1$. If there is only one $n_{r} = 1$, we can conclude that $|\sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}}(G.13)| \leq O(N^{-3/2}\|\boldsymbol{Q}(z)\|^{5})$, so that $(G.11) \leq O(N^{-1}\|\boldsymbol{Q}(z)\|^{6})$. If there are two different $n_{r_{1}} = 1$ and $n_{r_{2}} = 1$, then the only possible situation is $n_{k_{1}} = n_{l} = 1$, and we can conclude that $|\sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}}(G.13)| \leq O(N^{-1}\|\boldsymbol{Q}(z)\|^{5})$, so that $(G.11) \leq O(N^{-1/2}\|\boldsymbol{Q}(z)\|^{6})$. For $\gamma = 1$, we have $\mathcal{A}_{i_{1}\cdots i_{d}}^{(k_{l},l)}\mathcal{Q}\left(\partial_{i_{1}\cdots i_{d}}^{(k_{1},l)}\{Q_{i_{k_{1}}i_{l}}^{k_{1}}(z)\}\right) = N^{-1/2}(\mathcal{A}_{i_{1}\cdots i_{d}}^{(k_{1},l)})^{2}Q_{i_{k_{1}}i_{k_{1}}}^{k_{1}}(z)Q_{i_{1}i_{l}}^{ll}(z)$ and

$$\begin{split} &\mathcal{D} \big(\partial_{i_1 \cdots i_d}^{(3)} \operatorname{Tr} (\boldsymbol{Q}^{k_2 k_2}(z)) \big) \\ &= - N^{-3/2} \sum_{s_1 = 1}^d \sum_{s_2 \neq s_1}^d \sum_{s_3 \neq s_1, s_2}^d Q_{i_{s_1}}^{s_1 k_2}(z) Q_{i_{s_1}}^{k_2 s_1}(z) \mathcal{A}_{i_1 \cdots i_d}^{(s_1, s_2)} Q_{i_{s_2} i_{s_2}}^{s_2 s_2}(z) \mathcal{A}_{i_1 \cdots i_d}^{(s_2, s_3)} Q_{i_{s_3} i_{s_3}}^{s_3 s_3}(z) \mathcal{A}_{i_1 \cdots i_d}^{(s_3, s_1)}. \end{split}$$

Similar as previous arguments, if $\min_{1 \le r \le d} n_r = 2$ or 1, we can show that $(G.11) \le O(N^{-1} \| \mathbf{Q}(z) \|^6)$. If $\min_{1 \le r \le d} n_r = 0$, the only possible cases are that $s_1 = s_3 = k_1, s_2 = l$ and $s_1 = s_3 = l, s_2 = k_1$, then we can conclude that $(G.11) \le O(N^{-1/2} \| \mathbf{Q}(z) \|^6)$. For $\gamma = 3$, the proofs are the same as those for $\gamma = 2$, we omit details here to save space. Next, we only will present the detailed calculations for $\alpha = 1$ and 3.

First derivatives: When $\alpha = 1$, let

$$\mathcal{V}_{k_1 k_2, N}^{(d)}(z_1, z_2) = \frac{1}{N} \sum_{l \neq k}^{d} \mathbb{E}[\text{Tr}(\boldsymbol{Q}^{k_1 k_2}(\bar{z}_2) \boldsymbol{Q}^{k_2 l}(\bar{z}_2) \boldsymbol{Q}^{l k_1}(z_1))], \tag{G.14}$$

and readers can refer to §G.3.3 for proofs of $\mathcal{V}_{k_1k_2,N}^{(d)}(z_1,z_2) \to \mathcal{V}_{k_1k_2}^{(d)}(z_1,z_2)$ (G.33). By directly calculation as in the proof of Theorem E.1, we have

$$\begin{split} &\frac{1}{\sqrt{N}} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \mathcal{A}_{i_{1} \cdots i_{d}}^{(k_{1},l)} Q_{i_{k_{1}} i_{l}}^{k_{1} l}(z) \partial_{i_{1} \cdots i_{d}}^{(1)} \operatorname{Tr}(\boldsymbol{Q}^{k_{2} k_{2}}(\bar{z})) \\ &= -\frac{1}{N} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \sum_{t_{1} \neq t_{2}}^{d,d} \mathcal{A}_{i_{1} \cdots i_{d}}^{(k_{1},l)} Q_{i_{k_{1}} i_{l}}^{k_{1} l}(z) \mathcal{A}_{i_{1} \cdots i_{d}}^{(t_{1},t_{2})} Q_{i_{t_{1}}}^{t_{1} k_{2}}(\bar{z}) Q_{i_{t_{2}}}^{k_{2} t_{2}}(\bar{z}) \\ &= -\frac{2}{N} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \mathcal{A}_{i_{1} \cdots i_{d}}^{(k_{1},l)} Q_{i_{k_{1}} i_{l}}^{k_{1} l}(z) \mathcal{A}_{i_{1} \cdots i_{d}}^{(k_{1},l)} Q_{i_{k_{1}}}^{k_{1} k_{2}}(\bar{z}) Q_{i_{l}}^{k_{2} l}(\bar{z}) + \operatorname{O}(\eta_{0}^{-3} N^{-1/2}) \\ &= -\frac{2}{N} \operatorname{Tr}\left(\boldsymbol{Q}^{k_{1} k_{2}}(\bar{z}) \boldsymbol{Q}^{k_{2} l}(\bar{z}) \boldsymbol{Q}^{l k_{1}}(z)\right) + \operatorname{O}(\eta_{0}^{-3} N^{-1/2}), \end{split}$$

and

$$\frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \mathcal{A}_{i_1 \cdots i_d}^{(k_1, l)} \partial_{i_1 \cdots i_d}^{(1)} Q_{i_{k_1} i_l}^{k_1 l}(z) = -\left(N \rho_{k_1}(z) \rho_l(z) + N^{-1} \operatorname{Tr} \left(\boldsymbol{Q}^{k_1 l}(z) \boldsymbol{Q}^{l k_1}(z)\right) + \rho_{k_1}(z) \sum_{j \neq k, l} (\boldsymbol{a}^{(j)})' \boldsymbol{Q}^{j l}(z) \boldsymbol{a}^{(l)} + \rho_l(z) \sum_{j \neq k, l} (\boldsymbol{a}^{(j)})' \boldsymbol{Q}^{j k_1}(z) \boldsymbol{a}^{(k_1)}\right) + \operatorname{O}(\eta_0^{-2} N^{-1/2}),$$

where $\rho_l(z) = N^{-1} \operatorname{Tr}(\mathbf{Q}^{ll}(z))$. By Lemma G.2

$$\operatorname{Cov}(N^{-1}\operatorname{Tr}(\boldsymbol{Q}^{k_1l}(z)\boldsymbol{Q}^{lk_1}(z)),\operatorname{Tr}(\boldsymbol{Q}^{k_2k_2}(z))) \leq \operatorname{O}(C_{\eta_0}N^{-\omega})\mathcal{C}_{k_2k_2,N},$$

so does others like $\rho_{k_1}(z)(\boldsymbol{a}^{(j)})'\boldsymbol{Q}^{jl}(z)\boldsymbol{a}^{(l)}$, then we have

$$\frac{1}{\sqrt{N}} \sum_{l \neq k}^{d} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \mathbb{E} \left[\mathcal{A}_{i_{1} \cdots i_{d}}^{(k_{1},l)} \partial_{i_{1} \cdots i_{d}}^{(1)} \left\{ Q_{i_{k_{1}} i_{l}}^{k_{1} l}(z) \operatorname{Tr}(\boldsymbol{Q}^{k_{2} k_{2}}(\bar{z}))^{c} \right\} \right]$$

$$= -\sum_{l \neq k_{1}}^{d} \operatorname{Cov}(N \rho_{k_{1}}(z) \rho_{l}(z), \operatorname{Tr}(\boldsymbol{Q}^{k_{2} k_{2}}(z))) - 2 \mathcal{V}_{k_{1} k_{2}, N}^{(3)}(z, z) + \operatorname{O}(C_{\eta_{0}} N^{-\omega}) \mathcal{C}_{k_{2} k_{2}, N}.$$

Next, we can repeat the trick in (E.7) to obtain that

$$\begin{aligned} &\operatorname{Cov}(N\rho_{k_{1}}(z)\rho_{l}(z),\operatorname{Tr}(\boldsymbol{Q}^{k_{2}k_{2}}(z))) \\ &= \frac{1}{N}\mathbb{E}\left[\left(\operatorname{Tr}(\boldsymbol{Q}^{k_{1}k_{1}}(z))\operatorname{Tr}(\boldsymbol{Q}^{ll}(z)) - \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{k_{1}k_{1}}(z))]\operatorname{Tr}(\boldsymbol{Q}^{ll}(z)) + \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{k_{1}k_{1}}(z))]\operatorname{Tr}(\boldsymbol{Q}^{ll}(z)) \\ &- \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{k_{1}k_{1}}(z))]\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{ll}(z))] + \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{k_{1}k_{1}}(z))]\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{ll}(z))] - \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{k_{1}k_{1}}(z))\operatorname{Tr}(\boldsymbol{Q}^{ll}(z))]\right) \\ &\times \left(\operatorname{Tr}(\boldsymbol{Q}^{k_{2}k_{2}}(\bar{z})) - \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{k_{2}k_{2}}(\bar{z}))]\right)\right] \\ &= \mathfrak{m}_{l}(z)\operatorname{Cov}(\operatorname{Tr}(\boldsymbol{Q}^{k_{1}k_{1}}(z)), \operatorname{Tr}(\boldsymbol{Q}^{k_{2}k_{2}}(z))) + \mathfrak{m}_{k_{1}}(z)\operatorname{Cov}(\operatorname{Tr}(\boldsymbol{Q}^{ll}(z)), \operatorname{Tr}(\boldsymbol{Q}^{k_{2}k_{2}}(z))) + \operatorname{O}(C_{\eta_{0}}N^{-\omega})\mathcal{C}_{k_{2}k_{2},N}) \end{aligned}$$

As a result, we obtain

$$\frac{1}{\sqrt{N}} \sum_{l \neq k_1}^{d} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \mathbb{E} \left[\mathcal{A}_{i_1 \cdots i_d}^{(k_1, l)} \partial_{i_1 \cdots i_d}^{(1)} \left\{ Q_{i_{k_1} i_l}^{k_1 l}(z) \operatorname{Tr}(\boldsymbol{Q}^{k_2 k_2}(\bar{z}))^c \right\} \right] \\
= -\mathcal{C}_{k_1 k_2, N}^{(d)} \sum_{l \neq k_1}^{d} \mathfrak{m}_l(z) - \mathfrak{m}_{k_1}(z) \sum_{l \neq k_1}^{d} \mathcal{C}_{lk_2, N}^{(d)} - 2\mathcal{V}_{k_1 k_2, N}^{(d)}(z, z) + \mathcal{O}(C_{\eta_0} N^{-\omega}) \mathcal{C}_{k_2 k_2, N}.$$

Third derivatives: When $\alpha = 3$, let's consider

$$\frac{1}{\sqrt{N}} \sum_{l \neq k_1}^{d} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \mathbb{E} \left[\mathcal{A}_{i_1 \cdots i_d}^{(k_1, l)} \partial_{i_1 \cdots i_d}^{(1)} Q_{i_{k_1} i_l}^{k_1 l}(z) \partial_{i_1 \cdots i_d}^{(2)} \operatorname{Tr}(\boldsymbol{Q}^{k_2 k_2}(\bar{z})) \right],$$

where

$$\partial_{i_1\cdots i_d}^{(2)} \operatorname{Tr} \boldsymbol{Q}^{k_2k_2}(\bar{z}) = \frac{2}{N} \sum_{t_1 \neq t_2, t_3 \neq t_4} \mathcal{A}_{i_1\cdots i_d}^{(t_1,t_2)} \mathcal{A}_{i_1\cdots i_d}^{(t_3,t_4)} Q_{i_{t_2}i_{t_3}}^{t_2t_3}(\bar{z}) Q_{i_{t_4}}^{t_4k_2}(\bar{z}) Q_{\cdot i_{t_1}}^{k_2t_1}(\bar{z}),$$

then by Lemma G.3 and (A.5), we have

$$\begin{split} &\frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \mathbb{E} \left[\mathcal{A}_{i_1 \cdots i_d}^{(k_1,l)} \partial_{i_1 \cdots i_d}^{(1)} Q_{i_{k_1} i_l}^{k_1 l}(z) \partial_{i_1 \cdots i_d}^{(2)} \operatorname{Tr}(\boldsymbol{Q}^{k_2 k_2}(\bar{z})) \right] \\ &= -\frac{2}{N^2} \sum_{t_1 \neq t_2}^{d} \sum_{s_1 \neq s_2}^{d} \sum_{i_1 \cdots i_d}^{d} \mathbb{E} \left[\mathcal{A}_{i_1 \cdots i_d}^{(k_1,l)} Q_{i_{k_1} i_{s_1}}^{k_1 i_{s_1}}(z) \mathcal{A}_{i_1 \cdots i_d}^{(s_1,s_2)} Q_{i_{s_2} i_l}^{s_2 l}(z) \mathcal{A}_{i_1 \cdots i_d}^{(t_1,t_2)} \mathcal{A}_{i_1 \cdots i_d}^{(t_3,t_4)} Q_{i_{t_2} i_{t_3}}^{t_2 t_3}(\bar{z}) Q_{i_{t_4}}^{k_2 t_1}(\bar{z}) Q_{i_{t_1}}^{k_2 t_1}(\bar{z}) \right] \\ &= -\frac{2}{N^2} \sum_{t_1 \neq t_2}^{d} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \mathbb{E} \left[\left(\mathcal{A}_{i_1 \cdots i_d}^{(k_1,l)} \right)^2 Q_{i_{k_1} i_{k_1}}^{k_1 k_1}(z) Q_{i_l i_l}^{l l}(z) (\mathcal{A}_{i_1 \cdots i_d}^{(t_1,t_2)})^2 Q_{i_{t_2} i_{t_2}}^{t_2 t_2}(\bar{z}_2) Q_{i_{t_1}}^{t_1 k_2}(\bar{z}) Q_{i_{t_1}}^{k_2 t_1}(\bar{z}) \right] + \mathcal{O}(\eta_0^{-5} N^{-1/2}) \\ &= -\frac{2}{N^2} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \mathbb{E} \left[\left(\mathcal{A}_{i_1 \cdots i_d}^{(k_1,l)} \right)^4 Q_{i_{k_1} i_{k_1}}^{k_1 k_1}(z) Q_{i_l i_l}^{l l}(z) Q_{i_{k_1} i_{k_1}}^{k_1 k_1}(\bar{z}) Q_{i_{k_1}}^{l k_2}(\bar{z}) Q_{i_{k_1}}^{k_2 l}(\bar{z}) \right] \\ &- \frac{2}{N^2} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \mathbb{E} \left[\left(\mathcal{A}_{i_1 \cdots i_d}^{(k_1,l)} \right)^4 Q_{i_{k_1} i_{k_1}}^{k_1 k_1}(z) Q_{i_l i_l}^{l l}(z) Q_{i_{k_1} i_{k_1}}^{k_1 k_2}(\bar{z}) Q_{i_{k_1} i_{k_2}}^{k_1 k_2}(\bar{z}) Q_{i_{k_1} i_{k_2}}^{k_2 l}(\bar{z}) \right] + \mathcal{O}(\eta_0^{-5} N^{-1/2}) \\ &= -\frac{2\mathcal{B}_{(4)}^{(k_1,l)}}{N^2} \mathbb{E} \left[\operatorname{Tr} \left(\mathbf{Q}^{k_1 k_1}(z) \circ \mathbf{Q}^{k_1 k_1}(\bar{z}) \right) \cdot \operatorname{Tr} \left(\mathbf{Q}^{l l}(z) \circ \left(\mathbf{Q}^{l k_2}(\bar{z}) \mathbf{Q}^{k_2 l}(\bar{z}) \right) \right) \right] + \mathcal{O}(\eta_0^{-5} N^{-1/2}), \end{split}$$

where $\mathcal{B}_{(4)}^{(k,l)}$ is defined in (A.5). For simplicity, denote

$$\widetilde{\mathcal{U}}_{k_{1}k_{2},N}^{(d)}(z_{1},z_{2}) := N^{-2} \sum_{l \neq k_{1}}^{d} \mathcal{B}_{(4)}^{(k_{1},l)} \mathbb{E}[\text{Tr}(\boldsymbol{Q}^{k_{1}k_{1}}(z_{1}) \circ \boldsymbol{Q}^{k_{1}k_{1}}(\bar{z}_{2})) \cdot \text{Tr}(\boldsymbol{Q}^{ll}(z_{1}) \circ (\boldsymbol{Q}^{lk_{2}}(\bar{z}_{2})\boldsymbol{Q}^{k_{2}l}(\bar{z}_{2})))]
+ N^{-2} \sum_{l \neq k_{1}}^{d} \mathcal{B}_{(4)}^{(k_{1},l)} \mathbb{E}[\text{Tr}(\boldsymbol{Q}^{ll}(z_{1}) \circ \boldsymbol{Q}^{ll}(\bar{z}_{2})) \cdot \text{Tr}(\boldsymbol{Q}^{k_{1}k_{1}}(z_{1}) \circ (\boldsymbol{Q}^{k_{1}k_{2}}(\bar{z}_{2})\boldsymbol{Q}^{k_{2}k_{1}}(\bar{z}_{2})))], \tag{G.15}$$

and readers can refer to §G.3.3 for proofs of $\widetilde{\mathcal{U}}_{k_1k_2,N}^{(d)}(z_1,z_2) \to \mathcal{U}_{k_1k_2,N}^{(d)}(z_1,z_2)$ (G.36). As a result, we obtain

$$\frac{1}{\sqrt{N}} \sum_{l \neq k_1}^{d} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \frac{\kappa_4}{2} \mathbb{E} \left[\mathcal{A}_{i_1 \cdots i_d}^{(k_1, l)} \partial_{i_1 \cdots i_d}^{(1)} Q_{i_{k_1} i_l}^{k_1 l}(z) \partial_{i_1 \cdots i_d}^{(2)} \operatorname{Tr}(\boldsymbol{Q}^{k_2 k_2}(\bar{z})) \right] = -\kappa_4 \mathcal{U}_{k_1 k_2, N}^{(d)}(z, z) + \mathcal{O}(\eta_0^{-5} N^{-1/2}).$$

In summary, we obtain that

$$z\mathcal{C}_{k_{1}k_{2},N}^{(d)} = -\mathcal{C}_{k_{1}k_{2},N}^{(d)} \left(\sum_{l \neq k_{1}}^{d} \mathfrak{m}_{l}(z) + \mathcal{O}(N^{-\omega}) \right) - \mathfrak{m}_{k_{1}}(z) \sum_{l \neq k_{1}}^{d} \mathcal{C}_{lk_{2},N}^{(d)} - 2\mathcal{V}_{k_{1}k_{2},N}^{(d)}(z,z) - \kappa_{4}\mathcal{U}_{k_{1}k_{2},N}^{(d)}(z,z) + \mathcal{O}(C_{\eta_{0}}N^{-\omega}) + \mathcal{O}(C_{\eta_{0}}N^{-\omega})\mathcal{C}_{k_{2}k_{2},N}^{(d)},$$

i.e.

$$(z + \mathfrak{m}(z) - \mathfrak{m}_{k_1}(z))\mathcal{C}_{k_1k_2,N}^{(d)} = -\mathfrak{m}_{k_1}(z)\sum_{l \neq k_1}^{d} \mathcal{C}_{lk_2,N}^{(d)} - \mathcal{F}_{k_1k_2,N}^{(d)}(z,z) + \mathcal{O}(C_{\eta_0}N^{-\omega})\mathcal{C}_{k_2k_2,N}^{(d)} + \mathcal{O}(C_{\eta_0}N^{-\omega}),$$

where

$$\mathcal{F}_{k_1k_2,N}^{(d)}(z_1,z_2) := 2\mathcal{V}_{k_1k_2,N}^{(d)}(z_1,z_2) + \kappa_4 \mathcal{U}_{k_1k_2,N}^{(d)}(z_1,z_2). \tag{G.16}$$

Now, in matrix notations, we obtain that

$$\mathbf{\Theta}_{N}^{(d)}(z,z)\mathbf{C}_{N}^{(d)} = -\mathbf{F}_{N}^{(d)} + O(C_{\eta_{0}}N^{-\omega})\mathbf{1}_{d\times d} + O(C_{\eta_{0}}N^{-\omega})\mathbf{1}_{d\times d}\operatorname{diag}(\mathbf{C}_{N}^{(d)}).$$
(G.17)

Similar as (E.20), define

$$\boldsymbol{\Theta}_{N}^{(d)}(z,z) := (z + \mathfrak{m}(z))\boldsymbol{I}_{d} - \operatorname{diag}(\boldsymbol{m}(z)) + \operatorname{diag}(\boldsymbol{m}(z))\boldsymbol{S}_{d}, \tag{G.18}$$

where S_d is defined in (B.2). According to (G.7), we have

$$\|\boldsymbol{\Theta}_{N}^{(d)}(z,z) + \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1} \circ \boldsymbol{g}(z))^{-1} \boldsymbol{\Pi}^{(d)}(z,z)\|_{\infty} \leq \operatorname{O}(C_{\eta_0} N^{-\omega}),$$

which implies that $\Pi_N^{(d)}(z,z)$ is invertible and $|||\Theta_N^{(d)}(z,z)^{-1} - \Pi^{(d)}(z,z)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z))||| \le O(C_{\eta_0}N^{-\omega})$, so it gives that

$$\lim_{N\to\infty} \|\boldsymbol{C}_N^{(d)}(z,z) - \boldsymbol{\Pi}^{(d)}(z,z)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z)) \boldsymbol{F}_N^{(d)}(z,z) \| = 0.$$

Moreover, by the definitions of $\mathcal{V}_{st,N}^{(d)}(z_1, z_2)$ and $\mathcal{U}_{st,N}^{(d)}(z_1, z_2)$ in (G.14) and (G.15), we know that $|\mathcal{F}_{st,N}^{(d)}(z_1, z_2)| \leq C_{\eta_0}$, so

$$C_N^{(d)} = \Pi^{(d)}(z, z)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ g(z)) F_N^{(d)} + \operatorname{o}(\mathbf{1}_{d \times d}) + \operatorname{o}(\mathbf{1}_{d \times d}) \operatorname{diag}(C_N^{(d)})$$

$$\Rightarrow \|C_N^{(d)}\| \le \|\Pi^{(d)}(z, z)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ g(z)) F_N^{(d)}\| + \operatorname{o}(1) + \operatorname{o}(1) \|C_N^{(d)}\|,$$

which ensures that $\|C_N^{(d)}\|$ is bounded by $C_{\eta_0,\mathfrak{c},d}$. For $z_1 \neq z_2 \in \mathcal{S}_{\eta_0}$, by the previous arguments, we can still derive the following system equation for $C_{k_1k_2,N}^{(d)}(z_1,z_2)$:

$$(z_1 + \mathfrak{m}(z_1) - \mathfrak{m}_{k_1}(z_1))\mathcal{C}_{k_1k_2,N}^{(d)}(z_1, z_2) = -\mathfrak{m}_{k_1}(z_2) \sum_{l \neq k_1}^{d} \mathcal{C}_{lk_2,N}^{(d)}(z_1, z_2) - \mathcal{F}_{k_1k_2,N}^{(d)}(z_1, z_2) + \mathcal{O}(C_{\eta_0} N^{-\omega}),$$

since we have shown that $C_{k_2k_2,N}^{(d)}(z_2,z_2)$ is bounded by $C_{\eta_0,\mathfrak{c},d}$, then the above equation can be transformed into the following matrix forms:

$$\lim_{N\to\infty} \|\boldsymbol{C}_N^{(d)}(z_1,z_2) - \boldsymbol{\Pi}^{(d)}(z_1,z_2)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z_1)) \boldsymbol{F}_N^{(d)}(z_1,z_2) \| = 0,$$

which completes our proof.

G.3.2 Mean function

Theorem G.3. Under Assumptions A.1 and A.2, for any $z \in S_{\eta_0}$ in (G.1), let

$$\overrightarrow{M}_{N}^{(d)}(z) = (M_{1 N}^{(d)}(z), \cdots, M_{d N}^{(d)}(z))'$$

such that

$$M_{i,N}^{(d)}(z) := g_i(z) \sum_{r \neq i}^{d} \sum_{w \neq i,r}^{d} W_{rw}^{(d)}(z) - 2\kappa_3 G_{i,N}^{(d)}(z) + \kappa_4 H_{i,N}^{(d)}(z,z)$$

$$+ \sum_{l \neq i}^{d} \left[(g(z) - g_i(z) - g_l(z)) W_{il}^{(d)}(z) + V_{il}^{(d)}(z,z) \right], \tag{G.19}$$

where $W_{jk}^{(d)}(z)$, $V_{ij}^{(d)}(z,z)$, $G_{i,N}^{(d)}(z)$, $H_{i,N}^{(d)}(z,z)$ are defined in (G.28), (G.29), (G.21), (G.22). Then we have

$$\lim_{N \to \infty} |\mathbb{E}[\text{Tr}(\boldsymbol{Q}(z))] - Ng(z) - \mu_N^{(d)}(z)| = 0,$$

where

$$\mu_N^{(d)}(z) := \mathbf{1}_d' \mathbf{\Pi}^{(d)}(z, z)^{-1} \operatorname{diag}(\mathbf{c}^{-1} \circ \mathbf{g}(z)) \overrightarrow{M}_N^{(d)}(z), \tag{G.20}$$

and $\Pi^{(d)}(z,z)$ is defined in (B.11).

Proof. For simplicity, we will omit (z) behind $\mathbf{Q}(z)$, so does $\rho_k = N^{-1} \operatorname{Tr}(\mathbf{Q}^{kk})$, $\mathfrak{m}_k = \mathbb{E}[\rho_k]$, $W_{kl,N}^{(d)} = \mathbb{E}[(\mathbf{a}^{(k)})'\mathbf{Q}^{kl}\mathbf{a}^{(l)}]$ and $V_{kl,N}^{(d)} = V_{kl,N}^{(d)}(z,z) = \mathbb{E}[\operatorname{Tr}(\mathbf{Q}^{kl}(z)\mathbf{Q}^{lk}(z))]$. Moreover, for proofs of $W_{kl,N}^{(d)}(z) \to W_{kl}(z)$ and $V_{kl,N}^{(d)}(z_1,z_2) \to V_{kl}^{(d)}(z_1,z_2)$, readers can refer to §G.3.3. Note that $\mathbf{M}\mathbf{Q} - \mathbf{I} = z\mathbf{Q}$, we have

$$z\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{kk})] = \frac{1}{\sqrt{N}} \sum_{l \neq k}^{d} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \mathbb{E}[X_{i_1 \cdots i_d} \mathcal{A}_{i_1 \cdots i_d}^{(k,l)} Q_{i_k i_l}^{kl}] - n_k,$$

where $\mathcal{A}_{i_1\cdots i_d}^{(k,l)}=\prod_{j\neq k,l}^d a_{i_j}^{(j)}$. By the cumulant expansion, we have

$$\sum_{l\neq k}^d \mathbb{E}[X_{i_1\cdots i_d}\mathcal{A}^{(k,l)}_{i_1\cdots i_d}Q^{kl}_{i_ki_l}] = \sum_{\alpha=1}^3 \sum_{l\neq k}^d \frac{\kappa_{\alpha+1}}{\alpha!} \mathbb{E}[\mathcal{A}^{(k,l)}_{i_1\cdots i_d}\partial^{(\alpha)}_{i_1\cdots i_d}Q^{kl}_{i_ki_l}] + \epsilon^{(4)}_{i_1\cdots i_d}.$$

First derivatives: When $\alpha = 1$, since

$$\partial^{(1)}_{i_1\cdots i_d}Q^{kl}_{i_ki_l} = -\frac{1}{\sqrt{N}}\sum_{t_1\neq t_2}^d Q^{kt_1}_{i_ki_1}\mathcal{A}^{(t_1,t_2)}_{i_1\cdots i_d}Q^{t_2l}_{i_{t_2}i_l}$$

then by direct calculation, we have

$$\begin{split} &\frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{l \neq k}^{d} \mathbb{E}[\mathcal{A}_{i_1 \cdots i_d}^{(k,l)} \partial_{i_1 \cdots i_d}^{(1)} Q_{i_k i_l}^{kl}] = -\frac{1}{N} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{l \neq k}^{d} \sum_{t_1 \neq t_2}^{d} \mathbb{E}[\mathcal{A}_{i_1 \cdots i_d}^{(k,l)} Q_{i_k i_1}^{kt_1} \mathcal{A}_{i_1 \cdots i_d}^{(t_1,t_2)} Q_{i_{t_2} i_l}^{t_2 l}] \\ &= -\sum_{l \neq k}^{d} \left(N \mathfrak{m}_k \mathfrak{m}_l + V_{kl,N}^{(d)} + \mathfrak{m}_k \sum_{j \neq k,l} W_{jl,N}^{(d)} + \mathfrak{m}_l \sum_{j \neq k,l} W_{jk,N}^{(d)} \right) + \mathcal{O}(C_{\eta_0} N^{-\omega}), \end{split}$$

where we use Lemma G.2 and Theorem G.2 to conclude that $Cov(\rho_k, W_{kl,N}) \leq O(C_{\eta_0} N^{-\omega})$ and $Var(N\rho_k) \leq C_{\eta_0 \mathfrak{c},d}$, respectively.

Second derivatives: When $\alpha = 2$, by Lemma G.3 and (A.5), we have

$$\begin{split} &\frac{1}{\sqrt{N}} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \sum_{l \neq k}^{d} \mathbb{E} \left[\mathcal{A}_{i_{1} \cdots i_{d}}^{(k,l)} \partial_{i_{1} \cdots i_{d}}^{(2)} Q_{i_{k}i_{l}}^{kl} \right] \\ &= \frac{2}{N^{3/2}} \sum_{l \neq k}^{d} \sum_{t \neq k, l}^{d} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \mathbb{E} \left[\mathcal{A}_{i_{1} \cdots i_{d}}^{(k,l)} Q_{i_{k}i_{k}}^{kk} \mathcal{A}_{i_{1} \cdots i_{d}}^{(k,t)} Q_{i_{t}i_{t}}^{tt} \mathcal{A}_{i_{1} \cdots i_{d}}^{(t,l)} Q_{i_{l}i_{l}}^{ll} \right] + \mathcal{O}(\eta_{0}^{-3} N^{-1/2}) \\ &= 2 \sum_{l \neq k}^{d} \sum_{t \neq k, l}^{d} \mathcal{B}_{(3)}^{(k,l,t)} \mathbb{E} \left[\mathbf{1}' \operatorname{diag}(\mathbf{Q}^{kk}) \mathbf{a}^{(k)} \cdot \mathbf{1}' \operatorname{diag}(\mathbf{Q}^{tt}) \mathbf{a}^{(t)} \cdot \mathbf{1}' \operatorname{diag}(\mathbf{Q}^{ll}) \mathbf{a}^{(l)} \right] + \mathcal{O}(\eta_{0}^{-3} N^{-1/2}), \end{split}$$

where $\mathcal{B}_{(3)}^{(k,l,t)} = \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} (\mathcal{A}_{i_1 \cdots i_d}^{(k,l,t)})^3$. Similar as (E.32), we can further imply that

$$\frac{1}{\sqrt{N}} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \sum_{l \neq k}^{d} \mathbb{E} \left[\mathcal{A}_{i_{1} \cdots i_{d}}^{(k,l)} \partial_{i_{1} \cdots i_{d}}^{(2)} Q_{i_{k} i_{l}}^{kl} \right]
= 2 \sum_{l \neq k}^{d} \sum_{t \neq k, l}^{d} \mathcal{B}_{(3)}^{(k,l,t)} (\mathfrak{c}_{k} \mathfrak{c}_{t} \mathfrak{c}_{l})^{-1} g_{k}(z) g_{t}(z) g_{l}(z) \mathfrak{b}_{k}^{(1)} \mathfrak{b}_{t}^{(1)} \mathfrak{b}_{l}^{(1)} + \mathcal{O}(C_{\eta_{0}} N^{-\omega})
: = 2 G_{k,N}^{(d)}(z) + \mathcal{O}(C_{\eta_{0}} N^{-\omega}).$$
(G.21)

Third derivatives: When $\alpha = 3$, similar as (E.33), by Lemmas G.2 and G.3, we have

$$\frac{1}{\sqrt{N}} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \sum_{l \neq k}^{d} \mathbb{E} \left[\mathcal{A}_{i_{1} \cdots i_{d}}^{(k,l)} \partial_{i_{1} \cdots i_{d}}^{(3)} Q_{i_{k} i_{l}}^{kl} \right] = -\frac{6}{N^{2}} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \sum_{l \neq k}^{d} \mathbb{E} \left[(\mathcal{A}_{i_{1} \cdots i_{d}}^{(k,l)})^{4} (Q_{i_{k} i_{k}}^{kk} Q_{i_{l} i_{l}}^{ll})^{2} \right] + \mathcal{O}(\eta_{0}^{-4} N^{-1/2})$$

$$= -6N^{-2} \sum_{l \neq k}^{d} \mathcal{B}_{(4)}^{(k,l)} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{kk} \circ \boldsymbol{Q}^{kk}) \operatorname{Tr}(\boldsymbol{Q}^{ll} \circ \boldsymbol{Q}^{ll}) \right] + \mathcal{O}(C_{\eta_{0}} N^{-\omega})$$

$$= -6\mathfrak{c}_{k}^{-1} g_{k}(z) g_{k}(z) \sum_{l \neq k}^{d} \mathcal{B}_{(4)}^{(k,l)} \mathfrak{c}_{l}^{-1} g_{l}(z) g_{l}(z) + \mathcal{O}(C_{\eta_{0}} N^{-\omega}) := -6H_{3,k}^{(d)}(z,z) + \mathcal{O}(C_{\eta_{0}} N^{-\omega}),$$

where $\mathcal{B}_{(4)}^{(k,l)}$ is defined in (A.5) and

$$H_{k,N}^{(d)}(z_1, z_2) := \mathfrak{c}_k^{-1} g_k(z_1) g_k(z_2) \sum_{l \neq k}^d \mathcal{B}_{(4)}^{(k,l)} \mathfrak{c}_l^{-1} g_l(z_1) g_l(z_2). \tag{G.22}$$

Remainders: When $\alpha = 4$, similar as what we have done in §E.2 for l = 4, by Lemma G.3, it is enough to consider

$$\begin{split} &\frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{l \neq k}^{d} \mathbb{E} \left[\mathcal{A}_{i_1 \cdots i_d}^{(k,l)} \mathcal{D} \{ \partial_{i_1 \cdots i_d}^{(4)} Q_{i_k i_l}^{kl} \} \right] = \frac{4}{N^{5/2}} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{l \neq k}^{d} \sum_{s_1 \neq k}^{d} \sum_{s_2 \neq s_1}^{d} \sum_{s_3 \neq s_2, l}^{d} \\ &\mathbb{E} \left[\mathcal{A}_{i_1 \cdots i_d}^{(k,l)} Q_{i_k i_k}^{kk} \mathcal{A}_{i_1 \cdots i_d}^{(k,s_1)} Q_{i_{s_1} i_{s_1}}^{s_1 s_1} \mathcal{A}_{i_1 \cdots i_d}^{(s_1,s_2)} Q_{i_{s_2} i_{s_2}}^{s_2 s_2} \mathcal{A}_{i_1 \cdots i_d}^{(s_2,s_3)} Q_{i_{s_3} i_{s_3}}^{s_3 s_3} \mathcal{A}_{i_1 \cdots i_d}^{(s_1,l)} Q_{i_l i_l}^{ll} \right], \end{split}$$

where \mathscr{D} is defined in (D.33). The above equation contains at least three different types of diagonal terms, so that $\min_{1 \leq r \leq d} n_r \geq 1$, where n_r is the number of $\mathfrak{a}_r^{(r)}$ appears in the above equation, then we can show that $N^{-1/2}|\sum_{i_1\cdots i_d}^{n_1\cdots n_d} \epsilon_{i_1\cdots i_d}^{(4)}| = O(\eta_0^{-5}N^{-1/2})$ by the same arguments as those for (G.11) later, here we omit details for convenience.

As a result, we obtain

$$\begin{split} zN\mathfrak{m}_k &= -\sum_{l\neq k}^d \left(N\mathfrak{m}_k \mathfrak{m}_l + V_{kl,N}^{(d)} + \mathfrak{m}_k \sum_{j\neq k,l} W_{jl,N}^{(d)} + \mathfrak{m}_l \sum_{j\neq k,l} W_{jk,N}^{(d)} \right) \\ &+ 2\kappa_3 H_{2,k}^{(d)}(z) - \kappa_4 H_{3,k}^{(d)}(z) - n_k + \mathcal{O}(C_{\eta_0} N^{-\omega}) := -N\mathfrak{m}_k \sum_{l\neq k}^d \mathfrak{m}_l - n_k - M_{k,N}^{(d)} + \mathcal{O}(C_{\eta_0} N^{-\omega}), \end{split}$$
 i.e. $\left(z + \sum_{l\neq k}^d \mathfrak{m}_l \right) N\mathfrak{m}_k = -\mathfrak{c}_k N - M_{k,N}^{(d)} + \mathcal{O}(C_{\eta_0} N^{-\omega}). \text{ Let } h_k := N(\mathfrak{m}_k - g_k) \text{ and } h = \sum_{k=1}^d h_k, \end{split}$

recall that $g_k = -\frac{\mathfrak{c}_k}{z+q-q_k}$, then

$$\begin{aligned}
\left(z + \sum_{l \neq k}^{d} \mathfrak{m}_{l}\right) h_{k} &= -\mathfrak{c}_{k} N + M_{k,N}^{(d)} - \left(z + \sum_{l \neq k}^{d} \mathfrak{m}_{l}\right) g_{k} + \mathcal{O}(C_{\eta_{0}} N^{-\omega}) \\
&= \frac{\mathfrak{c}_{k} (h - h_{k})}{z + g - g_{k}} - M_{k,N}^{(d)} + \mathcal{O}(C_{\eta_{0}} N^{-\omega}) \\
&= -g_{k} (h - h_{k}) - M_{k,N}^{(d)} + \mathcal{O}(C_{\eta_{0}} N^{-\omega}).
\end{aligned}$$

Therefore, we obtain

$$N\boldsymbol{\Theta}_{N}^{(d)}(z,z)(\boldsymbol{g}(z)-\boldsymbol{m}(z)) = -\overrightarrow{M}_{N}^{(d)} + \mathcal{O}(C_{\eta_0}N^{-\omega}),$$

where $\Theta_N^{(d)}(z,z)$ is defined in (G.17) and we have shown that

$$\lim_{N\to\infty} \|\boldsymbol{\Theta}_N^{(d)}(z,z)^{-1} + \boldsymbol{\Pi}^{(d)}(z,z)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z))\| = 0.$$

Consequently, we conclude that

$$\lim_{N\to\infty} |\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}(z))] - Ng(z) - \mathbf{1}'_d \boldsymbol{\Pi}^{(d)}(z,z)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z)) \overrightarrow{M}_N^{(d)}(z)| = 0,$$

which completes our proof.

G.3.3 System equations of major terms in mean function $\mu_N^{(d)}(z)$ and variance function $\mathcal{C}_N^{(d)}(z_1,z_2)$

We will extend all system equations in §E.2 for general $d \geq 3$. The key method is to use the cumulant expansion (D.4). In fact, we can use the same method as in Theorem D.1 to show that only the first derivatives will generate major terms, so we only present the detailed calculation procedures of the first derivatives and omit others to save space.

System equations for $W_{kl,N}^{(d)}(z) = \mathbb{E}[(\boldsymbol{a}^{(k)})'\boldsymbol{Q}(z)\boldsymbol{a}^{(l)}]$:

By the cumulant expansion (D.4) and directly calculations, we can obtain

$$\begin{split} zW_{kl,N}^{(d)} &= \frac{1}{\sqrt{N}} \sum_{t \neq k}^{d} \sum_{i_0 \cdots i_d}^{n_1 \cdots n_d} \mathbb{E} \big[X_{i_1 \cdots i_d} a_{i_k}^{(k)} a_{i_0}^{(l)} \mathcal{A}_{i_1 \cdots i_d}^{(k,t)} Q_{i_t i_0}^{tl} \big] - \delta_{kl} \\ &= -\frac{1}{N} \sum_{t \neq k}^{d} \sum_{s \neq r}^{d} \sum_{i_0 \cdots i_d}^{n_1 \cdots n_d} \mathbb{E} \big[a_{i_0}^{(l)} a_{i_k}^{(k)} \mathcal{A}_{i_1 \cdots i_d}^{(t,k)} Q_{i_t i_s}^{ts} \mathcal{A}_{i_1 \cdots i_d}^{(s,r)} Q_{i_r i_0}^{rl} \big] - \delta_{kl} + \mathcal{O}(C_{\eta_0} N^{-1/2}) \\ &= -\frac{1}{N} \sum_{t \neq k}^{d} \sum_{r \neq t}^{d} \sum_{i_0 \cdots i_d}^{n_1 \cdots n_d} \mathbb{E} \big[a_{i_0}^{(l)} a_{i_k}^{(k)} \mathcal{A}_{i_1 \cdots i_d}^{(t,k)} Q_{i_t i_t}^{tt} \mathcal{A}_{i_1 \cdots i_d}^{(t,r)} Q_{i_r i_0}^{rl} \big] - \delta_{kl} + \mathcal{O}(C_{\eta_0} N^{-1/2}) \\ &= -W_{kl,N}^{(d)} \sum_{t \neq k}^{d} \mathfrak{m}_t - \sum_{t \neq k}^{d} \sum_{r \neq k,t}^{d} \mathfrak{m}_t W_{rl,N}^{(d)} - \delta_{kl} + \mathcal{O}(\eta_0^{-6} N^{-\omega}), \end{split}$$

where we use Lemma G.2 in the last equation. According to (G.7), we can further obtain

$$(z+g-g_k)W_{kl,N}^{(d)} = -\sum_{t \neq k} (g-g_k - g_t)W_{tl,N}^{(d)} - \delta_{kl} + \mathcal{O}(\eta_0^{-16}N^{-\omega}).$$
 (G.23)

Next, we will show that

Lemma G.5. Given g(z) and S_d in (B.1) and (B.2), define

$$\mathbf{\Gamma}^{(d)}(z) := (z + g(z))\mathbf{I}_d - \operatorname{diag}(\mathbf{g}(z)) + g(z)\mathbf{S}_d - \operatorname{diag}(\mathbf{g}(z))\mathbf{S}_d - \mathbf{S}_d \operatorname{diag}(\mathbf{g}(z)), \tag{G.24}$$

then $\Gamma^{(d)}(z)$ is invertible and $\|\Gamma^{(d)}(z)^{-1}\| \leq O(\eta_0^{-1})$ for any $z \in \mathcal{S}_{\eta_0}$ in (G.1).

Proof. By (G.23), we have

$$\Gamma^{(d)}(z)\mathbf{W}_{N}^{(d)}(z) = -\mathbf{I}_{d} + \mathcal{O}(\eta_{0}^{-16}N^{-\omega}), \tag{G.25}$$

where $\boldsymbol{W}_{N}^{(d)}(z) := [W_{kl,N}^{(d)}(z)]_{d\times d}$. For simplicity, let

$$\overrightarrow{W}_{d,N} := \overrightarrow{W}_{d,N}(z) := \left((\boldsymbol{a}^{(1)})' \boldsymbol{Q}^{1d}(z) \boldsymbol{a}^{(d)}, \cdots, (\boldsymbol{a}^{(d)})' \boldsymbol{Q}^{dd}(z) \boldsymbol{a}^{(d)} \right)'$$

be the *d*-th column of $W_N^{(d)}(z)$. Suppose $\Gamma^{(d)}$ is not invertible, then there exists a nonzero vector $\mathbf{r} := \mathbf{r}(z) = (r_1(z), \dots, r_d(z))'$ such that $\Gamma^{(d)}\mathbf{r} = \mathbf{0}_{d\times 1}$, so $\mathbf{r}'\Gamma^{(d)} = \mathbf{0}_{1\times d}$ due to $\Gamma(z)$ is symmetric. Note that

$$\mathbf{\Gamma}^{(d)}\overrightarrow{W}_{d,N} = -\boldsymbol{\delta}^{(d)} + \mathcal{O}(\eta_0^{-16}N^{-\omega})\mathbf{1}_{d\times 1} \quad \Rightarrow \quad 0 = \boldsymbol{r}'\mathbf{\Gamma}^{(d)}\overrightarrow{W}_{d,N} = -r_d + \mathcal{O}(\eta_0^{-16}N^{-\omega}),$$

where δ_d is the *d*-th column of I_d and *d* is a fixed integer, it implies that $|r_d| = O(\eta_0^{-16} N^{-\omega})$. By $\Gamma^{(d)} \mathbf{r} = \mathbf{0}$, it gives that $\Gamma_{k}^{(d)} \mathbf{r} = 0$, where $\Gamma_{k}^{(d)}$ is the *k*-th row of $\Gamma^{(d)}$, then we have $(z + g - g_k)r_k + \sum_{l \neq k}^d (g - g_l - g_k)r_l = 0$, i.e.

$$(z+g_k)r_k = (g_k - g)\sum_{l=1}^d r_l + \langle \boldsymbol{g}, \boldsymbol{r} \rangle, \tag{G.26}$$

where $1 \le k \le d$. In particular, when d = k, since $|r_d| = O(\eta_0^{-16} N^{-\omega})$ and $|z + g_k| \le O(\eta_0^{-1})$ for $z \in \mathcal{S}_{\eta_0}$ in (G.1), it gives that

$$(g-g_d)\sum_{l=1}^d r_l = \langle \boldsymbol{g}, \boldsymbol{r} \rangle + \mathrm{O}(\eta_0^{-17}N^{-\omega}).$$

Replacing $\langle \boldsymbol{g}, \boldsymbol{r} \rangle = (g - g_d) \sum_{l=1}^d r_l + \mathcal{O}(\eta_0^{-17} N^{-\omega})$ in (G.26), we have

$$(z+g_k)r_k = (g_k - g_d)\sum_{l=1}^d r_l + \mathcal{O}(\eta_0^{-17}N^{-\omega}), \quad 1 \le k \le d.$$
 (G.27)

Summing all d above equations (d is a fixed integer), it yields that

$$z\sum_{l=1}^{d} r_l + \langle \boldsymbol{g}, \boldsymbol{r} \rangle = (g - dg_d) \sum_{l=1}^{d} r_l + \mathcal{O}(\eta_0^{-17} N^{-\omega}),$$

replacing $\langle \boldsymbol{g}, \boldsymbol{r} \rangle = (g-g_d) \sum_{l=1}^d r_l + \mathcal{O}(\eta_0^{-17} N^{-\omega})$ again, we have

$$z\sum_{l=1}^{d} r_l + (g - g_d)\sum_{l=1}^{d} r_l = (g - dg_d)\sum_{l=1}^{d} r_l + O(\eta_0^{-17}N^{-\omega})$$

i.e. $(z + (d-1)g_d) \sum_{l=1}^d r_l = O(\eta_0^{-17} N^{-\omega})$. Since $\Im(z + (d-1)g_d) \ge \eta_0$ for all $z \in \mathcal{S}_{\eta_0}$, it implies that $\sum_{l=1}^d r_l = O(\eta_0^{-18} N^{-\omega})$. Since $\|\mathbf{r}\|_2 = 1$ and d is a fixed integer, there exists $1 \le k_0 \le d$ such that $r_{k_0} \ne 0$, so (G.27) deduces that $|z + g_k| = O(\eta_0^{-19} N^{-\omega})$, which is contradiction as $N \to \infty$ since $\Im(z + g_k) > \eta_0$ for any $z \in \mathcal{S}_{\eta_0}$. Therefore, $\Gamma^{(d)}$ must be invertible for all $z \in \mathcal{S}_{\eta_0}$. Finally, by (G.23) again, note that

$$\boldsymbol{\Gamma}^{(d)}(z)^{-1}(\boldsymbol{I}_d + \mathcal{O}(\eta_0^{-16}N^{-\omega})\mathbf{1}_{d\times d}) = \boldsymbol{W}_N^{(d)}(z) \Longrightarrow \boldsymbol{\Gamma}^{(d)}(z)^{-1} = \boldsymbol{W}_N^{(d)}(z)(\boldsymbol{I}_d + \mathcal{O}(\eta_0^{-16}N^{-\omega})\mathbf{1}_{d\times d})^{-1},$$

where $I_d + O(\eta_0^{-16} N^{-\omega}) \mathbf{1}_{d \times d}$ is invertible for sufficiently large N, so it gives that

$$\|\mathbf{\Gamma}^{(d)}(z)^{-1}\| \le \mathrm{O}(\|\mathbf{W}_{N}^{(d)}(z)\|) \le \mathrm{O}(\eta_{0}^{-1}),$$

where we use the fact that $|W_{st,N}^{(d)}(z)| = |\mathbb{E}[(\boldsymbol{a}^{(s)})'\boldsymbol{Q}(z)\boldsymbol{a}^{(t)}]| \leq \eta_0^{-1}$.

Based on (G.25), there exists a $W^{(d)}(z)$ such that

$$\boldsymbol{W}^{(d)}(z) = [W_{st}^{(d)}(z)]_{d \times d} = -\boldsymbol{\Gamma}^{(d)}(z)^{-1}, \quad \|\boldsymbol{W}_{N}^{(d)}(z) - \boldsymbol{W}^{(d)}(z)\|_{\infty} \le O(\eta_{0}^{-17}N^{-\omega}). \tag{G.28}$$

System equations for $V_{kl,N}^{(d)}(z_1,z_2)=N^{-1}\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{kl}(z_1)\boldsymbol{Q}^{lk}(z_2))]$:

Define $V_N^{(d)}(z_1, z_2) = [V_{kl,N}^{(d)}(z_1, z_2)]_{d \times d}$, where $z_1, z_2 \in \mathcal{S}_{\eta_0}$. Since

$$z_1 V_{kl,N}(z_1, z_2) = N^{-3/2} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{t \neq k}^{d} \mathbb{E} \left[X_{i_1 \cdots i_d} \mathcal{A}_{i_1 \cdots i_d}^{(k,t)} Q_{i_t i_l}^{tl}(z_1) Q_{i_k i_l}^{kl}(z_2) \right] - \delta_{kl} \mathfrak{m}_k(z_2),$$

by the cumulant expansion (D.4) and Lemma G.2, we have

$$\begin{split} N^{-3/2} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{t \neq k}^{d} \mathbb{E} \left[\partial_{i_1 \cdots i_d}^{(1)} \{ \mathcal{A}_{i_1 \cdots i_d}^{(k,t)} Q_{i_t i_l}^{tl}(z_1) Q_{i_k i_l}^{kl}(z_2) \} \right] \\ &= -N^{-2} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{t \neq k}^{d} \sum_{s_1 \neq s_2}^{d} \mathbb{E} \left[\mathcal{A}_{i_1 \cdots i_d}^{(k,t)} Q_{i_t i_{s_1}}^{ts_1}(z_1) \mathcal{A}_{i_1 \cdots i_d}^{(s_1, s_2)} Q_{i_{s_2} i_l}^{s_2 l}(z_1) Q_{i_k i_l}^{kl}(z_2) \right] \\ &- N^{-2} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{t \neq k}^{d} \sum_{s_1 \neq s_2}^{d} \mathbb{E} \left[\mathcal{A}_{i_1 \cdots i_d}^{(k,t)} Q_{i_t i_l}^{tl}(z_1) Q_{i_k i_{s_1}}^{ks_1}(z_2) \mathcal{A}_{i_1 \cdots i_d}^{(s_1, s_2)} Q_{i_{s_2} i_l}^{s_2 l}(z_2) \right] + \mathcal{O}(\eta_0^{-4} N^{-1/2}) \\ &= -N^{-2} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{t \neq k}^{d} \mathbb{E} \left[(\mathcal{A}_{i_1 \cdots i_d}^{(k,t)})^2 \left(Q_{i_t i_t}^{tt}(z_1) Q_{i_k i_l}^{kl}(z_1) Q_{i_k i_l}^{kl}(z_2) + Q_{i_k i_k}^{kk}(z_2) Q_{i_t i_l}^{tl}(z_1) Q_{i_t i_l}^{tl}(z_2) \right) \right] + \mathcal{O}(\eta_0^{-4} N^{-1/2}) \\ &= -V_{kl,N}^{(d)}(z_1, z_2) \sum_{t \neq k}^{d} \mathfrak{m}_t(z_1) - \mathfrak{m}_k(z_2) \sum_{t \neq k}^{d} V_{tl,N}^{(d)}(z_1, z_2) + \mathcal{O}(C_{\eta_0} N^{-\omega}) \\ &= -V_{kl,N}^{(d)}(z_1, z_2) \sum_{t \neq k}^{d} g_t(z_1) - g_k(z_2) \sum_{t \neq k}^{d} V_{tl,N}^{(d)}(z_1, z_2) + \mathcal{O}(C_{\eta_0} N^{-\omega}), \end{split}$$

where we use Theorem (G.7) in the last step. Now, we obtain that

$$(z_1 + g(z_1) - g_k(z_1))V_{kl,N}^{(d)}(z_1, z_2) = -g_k(z_2) \left(\delta_{kl} + \sum_{t \neq k}^d V_{tl,N}^{(d)}(z_1, z_2)\right) + \mathcal{O}(C_{\eta_0} N^{-\omega}),$$

which implies that

$$\Pi^{(d)}(z_1, z_2) V_N^{(d)}(z_1, z_2) = \operatorname{diag}(\mathfrak{c}^{-1} \circ g(z_1) \circ g(z_2)) + \operatorname{o}(\mathbf{1}_{d \times d})$$

Since we have shown that $\Pi^{(d)}(z_1, z_2)$ is invertible in Remark B.2, then we can derive that

$$\mathbf{V}^{(d)}(z_1, z_2) := \lim_{N \to \infty} \mathbf{V}_N(z_1, z_2) = \mathbf{\Pi}^{(d)}(z_1, z_2)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \mathbf{g}(z_1) \circ \mathbf{g}(z_2)).$$
(G.29)

System equations for $\mathcal{V}_{k_1k_2,N}^{(d)}(z_1,z_2) = N^{-1} \sum_{l \neq k_1}^d \mathbb{E}[\mathrm{Tr}(\boldsymbol{Q}^{k_1k_2}(\bar{z}_2)\boldsymbol{Q}^{k_2l}(\bar{z}_1)\boldsymbol{Q}^{lk_1}(z_1))]$:

It is enough to find the limiting value of the following terms:

$$V_{klr,N}^{(d)}(z_1, z_2) := \frac{1}{N} \mathbb{E}[\text{Tr}\,\boldsymbol{Q}^{kl}(z_1)\boldsymbol{Q}^{lr}(z_1)\boldsymbol{Q}^{rk}(z_2)], \tag{G.30}$$

where $z_1, z_2 \in \mathcal{S}_{\eta_0}$ and $k, l, r \in \{1, \dots, d\}$. Similarly, for any fixed r, define

$$\mathbf{V}_{r,N}^{(d)}(z_1, z_2) := [V_{klr,N}^{(d)}(z_1, z_2)]_{d \times d}, \tag{G.31}$$

By the cumulant expansion (D.4), since

$$\begin{split} z_1 V_{klr,N}^{(d)}(z_1, z_2) &= \frac{z_1}{N} \sum_{i_1 = 1}^{n_1} \mathbb{E}[Q_{i_1}^{kl}(z_1) \boldsymbol{Q}^{lr}(z_1) Q_{\cdot i_1}^{rk}(z_2)] \\ &= \frac{1}{N^{3/2}} \sum_{j \neq k}^{d} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \mathbb{E}[X_{i_1 \cdots i_d} \mathcal{A}_{i_1 \cdots i_d}^{(k,j)} Q_{i_j}^{jl}(z_1) \boldsymbol{Q}^{lr}(z_1) Q_{\cdot i_1}^{rk}(z_2)] - \delta_{kl} V_{kr}(z_1, z_2) \\ &= \frac{1}{N^{3/2}} \sum_{i \neq k}^{d} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \mathbb{E}[\mathcal{A}_{i_1 \cdots i_d}^{(k,j)} \partial_{i_1 \cdots i_d}^{(1)} \{Q_{i_j}^{jl}(z_1) \boldsymbol{Q}^{lr}(z_1) Q_{\cdot i_1}^{rk}(z_2)\}] - \delta_{kl} V_{kr}(z_1, z_2) + \mathcal{O}(C_{\eta_0} N^{-1/2}), \end{split}$$

where

$$\begin{split} &\frac{1}{N^{3/2}} \sum_{j \neq k}^{d} \sum_{s,t}^{n_l,n_r} \sum_{i_1 \cdots i_d}^{n_l,n_r} \mathbb{E}[\mathcal{A}_{i_1 \cdots i_d}^{(k,j)} \partial_{i_1 \cdots i_d}^{(1)} \{Q_{i_j s}^{jl}(z_1)\} Q_{st}^{lr}(z_1) Q_{ti_k}^{rk}(z_2)] \\ &= -\frac{1}{N^2} \sum_{j \neq k}^{d} \sum_{s,t}^{n_l,n_r} \sum_{i_1 \cdots i_d}^{n_l,n_r} \sum_{p \neq q}^{d} \mathbb{E}[\mathcal{A}_{i_1 \cdots i_d}^{(k,j)} Q_{i_j i_p}^{jp}(z_1) \mathcal{A}_{i_1 \cdots i_d}^{(p,q)} Q_{i_q s}^{ql}(z_1) Q_{st}^{lr}(z_1) Q_{ti_k}^{rk}(z_2)] \\ &= -\frac{1}{N^2} \sum_{j \neq k}^{d} \sum_{s,t}^{n_l,n_r} \sum_{i_1 \cdots i_d}^{n_l \cdots n_d} \sum_{q \neq j}^{d} \mathbb{E}[\mathcal{A}_{i_1 \cdots i_d}^{(k,j)} Q_{i_j i_j}^{jj}(z_1) \mathcal{A}_{i_1 \cdots i_d}^{(j,q)} Q_{i_q s}^{ql}(z_1) Q_{st}^{lr}(z_1) Q_{ti_k}^{rk}(z_2)] \\ &= -V_{klr,N}^{(d)}(z_1,z_2) \sum_{j \neq k}^{d} \mathfrak{m}_j(z_1) + \mathcal{O}(C_{\eta_0} N^{-\omega}), \end{split}$$

and

$$\begin{split} &\frac{1}{N^{3/2}} \sum_{j \neq k}^{d} \sum_{s,t}^{n_{l},n_{r}} \sum_{i_{1} \cdots i_{d}}^{n_{l},n_{r}} \mathbb{E}[\mathcal{A}_{i_{1} \cdots i_{d}}^{(k,j)} Q_{i_{j}s}^{jl}(z_{1}) \partial_{i_{1} \cdots i_{d}}^{(1)} \{Q_{st}^{lr}(z_{1})\} Q_{ti_{k}}^{rk}(z_{2})] \\ &= -\frac{1}{N^{2}} \sum_{j \neq k}^{d} \sum_{s,t}^{n_{l},n_{r}} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \sum_{p \neq q}^{d} \mathbb{E}[\mathcal{A}_{i_{1} \cdots i_{d}}^{(k,j)} Q_{i_{j}s}^{jl}(z_{1}) Q_{si_{p}}^{lp}(z_{1}) \mathcal{A}_{i_{1} \cdots i_{d}}^{(p,q)} Q_{i_{q}t}^{qr}(z_{1}) Q_{ti_{k}}^{rk}(z_{2})] \\ &= -V_{kr,N}^{(d)}(z_{1},z_{2}) \sum_{j \neq k}^{d} V_{jl,N}^{(d)}(z_{1},z_{1}) + \mathcal{O}(C_{\eta_{0}}N^{-\omega}), \end{split}$$

and

$$\begin{split} &\frac{1}{N^{3/2}} \sum_{j \neq k}^{d} \sum_{s,t}^{n_{l},n_{r}} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \mathbb{E}[\mathcal{A}_{i_{1} \cdots i_{d}}^{(k,j)} Q_{i_{j}s}^{jl}(z_{1}) Q_{st}^{lr}(z_{1}) \partial_{i_{1} \cdots i_{d}}^{(1)} \left\{ Q_{ti_{k}}^{rk}(z_{2}) \right\}] \\ &= -\frac{1}{N^{2}} \sum_{j \neq k}^{d} \sum_{s,t}^{n_{l},n_{r}} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \sum_{p \neq q}^{d} \mathbb{E}[\mathcal{A}_{i_{1} \cdots i_{d}}^{(k,j)} Q_{i_{j}s}^{jl}(z_{1}) Q_{st}^{lr}(z_{1}) Q_{ti_{p}}^{rp}(z_{2}) \mathcal{A}_{i_{1} \cdots i_{d}}^{(p,q)} Q_{i_{q}i_{k}}^{qk}(z_{2})] \\ &= -\mathfrak{m}_{k}(z_{2}) \sum_{j \neq k}^{d} V_{jlr,N}^{(d)}(z_{1},z_{2}) + \mathcal{O}(C_{\eta_{0}}N^{-\omega}). \end{split}$$

In summary, we can conclude that

$$V_{klr,N}^{(d)}(z_1,z_2) = \mathfrak{c}_k^{-1} g_k(z_1) \Big(\delta_{kl} V_{kr}^{(d)}(z_1,z_2) + V_{kr}^{(d)}(z_1,z_2) \sum_{j\neq k}^d V_{jl}^{(d)}(z_1,z_2) + g_k(z_2) \sum_{j\neq k}^d V_{jlr,N}^{(d)}(z_1,z_2) \Big) + \mathcal{O}(C_{\eta_0} N^{-\omega}).$$

i.e.

$$\lim_{N\to\infty} \|\boldsymbol{V}_{r,N}^{(d)}(z_1,z_2) - \boldsymbol{\Pi}^{(d)}(z_1,z_2)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z_1)) \big(\operatorname{diag}(\boldsymbol{V}_{\cdot r}^{(d)}(z_1,z_2)) + \operatorname{diag}(\boldsymbol{V}_{\cdot r}^{(d)}(z_1,z_2)) \boldsymbol{S}_d \boldsymbol{V}^{(d)}(z_1,z_2) \big) \| = 0,$$
where $\boldsymbol{V}_{\cdot r}^{(d)}(z_1,z_2)$ is the r-th column of $\boldsymbol{V}^{(d)}(z_1,z_2)$. Thus, the limit value $\boldsymbol{V}_{r,N}^{(d)}(z_1,z_2)$ is given as

$$\boldsymbol{V}_{r}^{(d)}(z_{1}, z_{2}) := \boldsymbol{\Pi}^{(d)}(z_{1}, z_{2})^{-1} \operatorname{diag}(\boldsymbol{\epsilon}^{-1} \circ \boldsymbol{g}(z_{1})) [\operatorname{diag}(\boldsymbol{V}^{(d)}(z_{2}, z_{2})) + \operatorname{diag}(\boldsymbol{S}_{d} \boldsymbol{V}_{\cdot r}^{(d)}(z_{1}, z_{2})) \boldsymbol{V}^{(d)}(z_{1}, z_{2})], \tag{G.32}$$

Once we solve $V_{klr,N}^{(d)}(z_1,z_2)$, by (G.14), the limiting expression of $\mathcal{V}_{k_1k_2,N}^{(d)}(z_1,z_2)$ is given as

$$\lim_{N \to \infty} \mathcal{V}_{k_1 k_2, N}^{(d)}(z_1, z_2) = \mathcal{V}_{k_1 k_2}^{(d)}(z_1, z_2) := \sum_{l \neq k_1}^{d} V_{k_1 k_2 l}^{(d)}(z_1, z_2). \tag{G.33}$$

System equations for $\widetilde{\mathcal{U}}_{k_1k_2,N}^{(d)}(z_1,z_2)$ in (G.15): By Theorem G.2, we can show that

$$Cov(N^{-1}\operatorname{Tr}(\boldsymbol{Q}^{k_1k_1}(z_1)\circ\boldsymbol{Q}^{k_1k_1}(\bar{z}_2)),N^{-1}\operatorname{Tr}(\boldsymbol{Q}^{k_1k_1}(z_1)\circ(\boldsymbol{Q}^{k_1k_2}(\bar{z}_2)\boldsymbol{Q}^{k_2k_1}(\bar{z}_2))))=O(C_{\eta_0}N^{-2\omega}).$$

Consequently, by (G.15), we only need to compute the limiting values of $N^{-1}\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{k_1k_1}(z_1) \circ \boldsymbol{Q}^{k_1k_1}(\bar{z}_2))]$ and $N^{-1}\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}^{k_1k_1}(z_1) \circ (\boldsymbol{Q}^{k_1k_2}(\bar{z}_2)\boldsymbol{Q}^{k_2k_1}(\bar{z}_2)))]$ respectively. For the first term, by Theorem G.1, we can obtain

$$\lim_{N \to \infty} N^{-1} \mathbb{E}[\text{Tr}(\boldsymbol{Q}^{k_1 k_1}(z_1) \circ \boldsymbol{Q}^{k_1 k_1}(\bar{z}_2))] = \mathfrak{c}_{k_1}^{-1} g_{k_1}(z_1) g_{k_1}(\bar{z}_2). \tag{G.34}$$

For the second term, we define

$$\mathring{V}_{kl,N}^{(d)}(z_1,z_2) := \frac{1}{N} \mathbb{E}[\mathrm{Tr}(\boldsymbol{Q}^{kk}(z_1) \circ (\boldsymbol{Q}^{kl}(z_2)\boldsymbol{Q}^{lk}(z_2)))].$$

by the cumulant expansion (D.4) again, we have

$$\begin{split} &z_1\mathring{V}_{kl,N}^{(d)}(z_1,z_2) = \frac{z_1}{N}\sum_{i_k=1}^{n_k}\mathbb{E}[Q_{i_ki_k}^{kk}(z_1)Q_{i_k}^{kl}.(z_2)Q_{\cdot i_k}^{lk}(z_2)]\\ &= \frac{1}{N^{3/2}}\sum_{t\neq k}^{d}\sum_{i_1\cdots i_d}^{n_1\cdots n_d}\mathbb{E}\big[X_{i_1\cdots i_d}\mathcal{A}_{i_1\cdots i_d}^{(k,t)}Q_{i_ti_k}^{tk}(z_1)Q_{i_k}^{kl}.(z_2)Q_{\cdot i_k}^{lk}(z_2)\big] - V_{kl,N}^{(d)}(z_2,z_2)\\ &= \frac{1}{N^{3/2}}\sum_{t\neq k}^{d}\sum_{i_1\cdots i_d}^{n_1\cdots n_d}\mathbb{E}\big[\mathcal{A}_{i_1\cdots i_d}^{(k,t)}\partial_{i_1\cdots i_d}^{(1)}\big\{Q_{i_ti_k}^{tk}(z_1)Q_{i_k}^{kl}.(z_2)Q_{\cdot i_k}^{lk}(z_2)\big\}\big] - V_{kl,N}^{(d)}(z_2,z_2) \end{split}$$

where

$$\begin{split} &\frac{1}{N^{3/2}} \sum_{t \neq k}^{d} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \sum_{s=1}^{n_{l}} \mathbb{E} \left[\mathcal{A}_{i_{1} \cdots i_{d}}^{(k,t)} \partial_{i_{1} \cdots i_{d}}^{(1)} \{Q_{i_{t}i_{k}}^{tk}(z_{1})\} Q_{i_{k}s}^{kl}(z_{2}) Q_{si_{k}}^{lk}(z_{2}) \right] \\ &= -\frac{1}{N^{2}} \sum_{t \neq k}^{d} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \sum_{s=1}^{n_{l}} \sum_{p \neq q}^{d} \mathbb{E} \left[\mathcal{A}_{i_{1} \cdots i_{d}}^{(k,t)} Q_{i_{t}i_{p}}^{tp}(z_{1}) \mathcal{A}_{i_{1} \cdots i_{d}}^{(p,q)} Q_{i_{q}i_{k}}^{qk}(z_{1}) Q_{i_{k}s}^{kl}(z_{2}) Q_{si_{k}}^{lk}(z_{2}) \right] \\ &= -\mathring{V}_{kl,N}^{(d)}(z_{1},z_{2}) \sum_{t \neq k}^{d} \mathfrak{m}_{t}(z_{1}) + \mathcal{O}(C_{\eta_{0}}N^{-\omega}) \end{split}$$

and

$$\begin{split} &\frac{1}{N^{3/2}} \sum_{t \neq k}^{d} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \sum_{s=1}^{n_{l}} \mathbb{E} \left[\mathcal{A}_{i_{1} \cdots i_{d}}^{(k,t)} Q_{i_{t}i_{k}}^{tk}(z_{1}) \partial_{i_{1} \cdots i_{d}}^{(1)} \left\{ Q_{i_{k}s}^{kl}(z_{2}) Q_{si_{k}}^{lk}(z_{2}) \right\} \right] \\ &= -\frac{2}{N^{2}} \sum_{t \neq k}^{d} \sum_{n \neq q}^{d} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \sum_{s=1}^{n_{l}} \mathbb{E} \left[\mathcal{A}_{i_{1} \cdots i_{d}}^{(k,t)} Q_{i_{t}i_{k}}^{tk}(z_{1}) Q_{i_{k}s}^{kl}(z_{2}) Q_{i_{k}i_{p}}^{kp}(z_{2}) \mathcal{A}_{i_{1} \cdots i_{d}}^{(p,q)} Q_{i_{q}s}^{ql}(z_{2}) \right] = \mathcal{O}(C_{\eta_{0}} N^{-\omega}). \end{split}$$

Hence, we obtain that

$$(z_1 + \mathfrak{m}(z_1) - \mathfrak{m}_k(z_1))\mathring{V}_{kl,N}^{(d)}(z_1, z_2) = V_{kl,N}^{(d)}(z_2, z_2) + \mathcal{O}(C_{\eta_0}N^{-\omega})$$

in matrix notations

$$\mathring{\boldsymbol{V}}_{N}^{(d)}(z_{1}, z_{2}) = \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z_{1})) \boldsymbol{V}^{(d)}(z_{2}, z_{2}) + \operatorname{o}(\mathbf{1}_{d \times d}),$$

where $\mathring{V}_{N}^{(d)}(z_{1}, z_{2}) = [\mathring{V}_{kl,N}^{(d)}(z_{1}, z_{2})]_{d \times d}$. So it concludes that

$$\mathring{\boldsymbol{V}}^{(d)}(z_1, z_2) := [\mathring{V}_{st}^{(d)}(z_1, z_2)]_{d \times d} := \lim_{N \to \infty} \mathring{\boldsymbol{V}}_N^{(d)}(z_1, z_2) = \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z_1)) \boldsymbol{V}^{(d)}(z_2, z_2).$$
(G.35)

Now, by (G.15), we obtain that

$$\widetilde{\mathcal{U}}_{k_1k_2}^{(3)}(z_1, z_2) = \mathcal{U}_{k_1k_2}^{(d)}(z_1, z_2) + \mathcal{O}(C_{n_0}N^{-\omega}).$$

where

$$\mathcal{U}_{k_{1}k_{2},N}^{(d)}(z_{1},z_{2}) := \mathfrak{c}_{k_{1}}^{-1}g_{k_{1}}(z_{1})g_{k_{1}}(\bar{z}_{2}) \sum_{l \neq k_{1}}^{d} \mathcal{B}_{(4)}^{(k_{1},l)}\mathring{V}_{lk_{2}}^{(d)}(z_{1},z_{2}) + \mathring{V}_{k_{1}k_{2}}^{(d)}(z_{1},z_{2}) \sum_{l \neq k_{1}}^{d} \mathcal{B}_{(4)}^{(k_{1},l)}\mathfrak{c}_{l}^{-1}g_{l}(z_{1})g_{l}(\bar{z}_{2}). \tag{G.36}$$

G.4 CLT for the LSS

Let's consider the family of functions as follows:

$$\mathfrak{F}_d := \{ f(z) : f \text{ is analytic on an open set containing the interval } [-\max\{\zeta, \mathfrak{v}_d\}, \max\{\zeta, \mathfrak{v}_d\}] \},$$
(G.37)

where ζ (C.17) is the boundary of LSD ν and \mathfrak{v}_d is defined in Theorem C.1. For any $f \in \mathfrak{F}_d$, the LSS of M is given as

$$\mathcal{L}_{\boldsymbol{M}}(f) := \frac{1}{N} \sum_{l=1}^{N} f(\lambda_l).$$

where $\lambda_1 \geq \cdots \geq \lambda_N$ be are eigenvalues of M. Similar as Theorem F.1, we will establish the CLT of

$$G_N(f) := N \int_{-\infty}^{\infty} f(x)(\nu_N(dx) - \nu(dx)) = N \Big(\mathcal{L}_{\boldsymbol{M}}(f) - \int_{-\infty}^{\infty} f(x)\nu(dx) \Big), \tag{G.38}$$

where ν_N and ν are the ESD and LSD of M respectively. Precisely, we will show that

Theorem G.4. Under Assumptions A.1 and A.2, let \mathfrak{C}_1 and \mathfrak{C}_2 be two disjoint rectangular contours with vertexes of $\pm E_1 \pm \eta_1$ and $\pm E_2 \pm \eta_2$ such that $E_1, E_2 \geq \max\{\zeta, \mathfrak{v}_d\} + t$ for any t > 0, where ζ and \mathfrak{v}_d are defined in (C.17) and (C.15), then we have

$$(G_N(f) - \xi_N^{(d)})/\sigma_N^{(d)} \stackrel{d}{\longrightarrow} \mathcal{N}(0,1)$$

where

$$\begin{split} \xi_N^{(d)} &:= -\frac{1}{2\pi \mathrm{i}} \oint_{\mathfrak{C}_1} f(z) \mu_N^{(d)}(z) dz, \\ (\sigma_N^{(d)})^2 &:= -\frac{1}{4\pi^2} \oint_{\mathfrak{C}_1} \oint_{\mathfrak{C}_2} f(z_1) f(z_2) \mathcal{C}_N^{(d)}(z_1, z_2) dz_1 dz_2. \end{split}$$

and the mean function $\mu_N^{(d)}(z)$ and covariance function $\mathcal{C}_N^{(d)}(z_1, z_2)$ are defined in (G.20) and (G.10), respectively.

The basic outlines are the same as those in \S F.

G.4.1 Tightness

Theorem G.5. Under Assumptions A.1 and A.2, $\text{Tr}(\mathbf{Q}(z)) - \mathbb{E}[\text{Tr}(\mathbf{Q}(z))]$ is a tight sequence in S_{η_0} in (G.1), i.e.

$$\sup_{\substack{z_1, z_2 \in \mathcal{S}_{\eta_0} \\ z_1 \neq z_2}} \frac{\mathbb{E}\left[|\operatorname{Tr}(\boldsymbol{Q}(z_1) - \boldsymbol{Q}(z_2)) - \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}(z_1) - \boldsymbol{Q}(z_2))|^2\right]}{|z_1 - z_2|^2} < C_{\eta_0}.$$

Proof. For any $z \in \mathcal{S}_{\eta_0}$, the tightness of process $\text{Tr}(\mathbf{Q}(z)) - \mathbb{E}[\text{Tr}(\mathbf{Q}(z))]$ is equivalent to

$$\operatorname{Var}\left(\operatorname{Tr}(\boldsymbol{Q}^{kl}(z_1)\boldsymbol{Q}^{lk}(z_2))\right) \leq C_{\eta_0,d,\mathfrak{c}}$$

where $z_1, z_2 \in \mathcal{S}_{\eta_0}$ and $k, l \in \{1, \dots, d\}$. Define

$$C_{k_1 l_1, k_2 l_2, N}^{(d)}(z_1, z_2) = \operatorname{Cov}\left(\operatorname{Tr}(\boldsymbol{Q}^{k_1 l_1}(z_1) \boldsymbol{Q}^{l_1 k_1}(z_2)), \operatorname{Tr}(\boldsymbol{Q}^{k_2 l_2}(z_1) \boldsymbol{Q}^{l_2 k_2}(z_2))\right),$$
(G.39)

it is enough to show that $|\mathcal{C}_{k_1l_1,k_2l_2,N}^{(d)}(z_1,z_2)| \leq C_{\eta_0,d,\mathfrak{c}}$ for any $k_1,k_2,l_1,l_2 \in \{1,\cdots,d\}$. Similar as what we have done in §F.1, let's derive a system equation for all $\mathcal{C}_{k_1l_1,k_2l_2,N}^{(d)}(z_1,z_2)$. We omit (z_1,z_2) behind $\mathcal{C}_{k_1l_1,k_2l_2,N}^{(d)}(z_1,z_2)$, then

$$z_{1}\mathcal{C}_{k_{1}l_{1},k_{2}l_{2},N}^{(d)} = \frac{1}{\sqrt{N}} \sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}} \sum_{s\neq k_{1}}^{d} \mathbb{E}\left[X_{i_{1}\cdots i_{d}}\mathcal{A}_{i_{1}\cdots i_{d}}^{(k_{1},s)}Q_{i_{s}}^{sl_{1}}(z_{1})Q_{i_{k}}^{l_{1}k_{1}}(z_{2})\operatorname{Tr}(\boldsymbol{Q}^{k_{2}l_{2}}(\bar{z}_{1})\boldsymbol{Q}^{l_{2}k_{2}}(\bar{z}_{2}))^{c}\right]$$
(G.40)

$$-\delta_{k_1 l_1} \operatorname{Cov} \left(\operatorname{Tr}(\boldsymbol{Q}^{k_1 k_1}(z_1)), \operatorname{Tr}(\boldsymbol{Q}^{k_2 l_2}(z_1) \boldsymbol{Q}^{l_2 k_2}(z_2)) \right), \tag{G.41}$$

and we only need to show both of above two terms are bounded by C_{η_0} .

Calculations of (G.41): Define

$$C_{k_1 l_1, k_2, N}^{(d)}(z_1, z_2) := \operatorname{Cov}\left(\operatorname{Tr}(\boldsymbol{Q}^{k_1 l_1}(z_1) \boldsymbol{Q}^{l_1 k_1}(z_2), \operatorname{Tr}(\boldsymbol{Q}^{k_2 k_2}(z_1)))\right), \tag{G.42}$$

here, we still omit the (z_1, z_2) behind $C_{k_1 l_1, k_2, N}^{(d)}(z_1, z_2)$. By the cumulant expansion (D.4), we have

$$z_{1}C_{k_{1}l_{1},k_{2},N}^{(d)} = \frac{1}{\sqrt{N}} \sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}} \sum_{s\neq k_{1}}^{d} \mathbb{E}\left[X_{i_{1}\cdots i_{d}}\mathcal{A}_{i_{1}\cdots i_{d}}^{(k_{1},s)}Q_{i_{s}}^{sl_{1}}(z_{1})Q_{\cdot i_{k_{1}}}^{l_{1}k_{1}}(z_{2})\operatorname{Tr}(\boldsymbol{Q}^{k_{2}k_{2}}(\bar{z}_{1}))^{c}\right]$$

$$= \frac{1}{\sqrt{N}} \sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}} \left(\sum_{\alpha=0}^{3} \sum_{s\neq k}^{d} \mathbb{E}\left[\partial_{i_{1}\cdots i_{d}}^{(\alpha)} \left\{\mathcal{A}_{i_{1}\cdots i_{d}}^{(k_{1},s)}Q_{i_{s}}^{sl_{1}}(z_{1})Q_{\cdot i_{k_{1}}}^{l_{1}k_{1}}(z_{2})\operatorname{Tr}(\boldsymbol{Q}^{k_{2}k_{2}}(\bar{z}_{1}))^{c}\right\}\right] + \epsilon_{i_{1}\cdots i_{d}}^{(4)}\right).$$

For convenience, we omit the detailed calculation for minor terms since the proofs are the same as those in Theorems F.2, G.3 and G.2. Actually, only $\alpha = 1, 3$ will have the major terms:

First derivatives: When $\alpha = 1$, by (G.12), we have

$$\partial_{i_1 \cdots i_d}^{(1)} \operatorname{Tr}(\boldsymbol{Q}^{k_2 k_2}(\bar{z})) = -N^{-1/2} \sum_{t_1 \neq t_2}^{d,d} \mathcal{A}_{i_1 \cdots i_d}^{(t_1, t_2)} Q_{i_1}^{t_1 k_2}(\bar{z}) Q_{i_{t_2}}^{k_2 t_2}(\bar{z}),$$

and by Lemma G.3,

$$\begin{split} &\frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_{l_1}} \sum_{i_t}^{n_{l_1}} \mathcal{A}_{i_1 \cdots i_d}^{(k_1,s)} \partial_{i_1 \cdots i_d}^{(1)} \{Q_{i_s i_t}^{sl_1}(z_1) Q_{i_{k_1} i_t}^{k_1 l_1}(z_2)\} \\ &= -N^{-1} \sum_{i_1 \cdots i_d}^{n_{l_1} \cdots n_d} \mathcal{A}_{i_1 \cdots i_d}^{(k_1,s)} \big[Q_{i_s i_s}^{ss_1}(z_1) \mathcal{A}_{i_1 \cdots i_d}^{(s_1,s_2)} Q_{i_{s_2}}^{s_2 l_1}(z_1) Q_{i_{k_1}}^{l_1 k_1}(z_2) + Q_{i_{k_1} i_{s_1}}^{k_1 s_1}(z_2) \mathcal{A}_{i_1 \cdots i_d}^{(s_1,s_2)} Q_{i_{s_2}}^{s_2 l_1}(z_2) Q_{i_s}^{l_1 s}(z_1) \big] \\ &= -N^{-1} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} (\mathcal{A}_{i_1 \cdots i_d}^{(k_1,s)})^2 [Q_{i_s i_s}^{ss}(z_1) Q_{i_{k_1}}^{k_1 l_1}(z_1) Q_{i_{k_1}}^{l_1 k_1}(z_2) + Q_{i_{k_1} i_{k_1}}^{k_1 l_1}(z_2) Q_{i_s}^{sl_1}(z_2) Q_{i_s}^{l_1 s}(z_1)] + \mathcal{O}(\eta_0^{-3} N^{-1/2}) \\ &= -N^{-1} [\text{Tr}(\mathbf{Q}^{ss}(z_1)) \, \text{Tr}(\mathbf{Q}^{k_1 l_1}(z_1) \mathbf{Q}^{l_1 k_1}(z_2)) + \text{Tr}(\mathbf{Q}^{k_1 k_1}(z_2)) \, \text{Tr}(\mathbf{Q}^{sl_1}(z_1) \mathbf{Q}^{l_1 s}(z_2))] + \mathcal{O}(\eta_0^{-3} N^{-1/2}) \\ &= -N^{-1} [\text{Tr}(\mathbf{Q}^{ss}(z_1)) \, \text{Tr}(\mathbf{Q}^{k_1 l_1}(z_1) \mathbf{Q}^{l_1 k_1}(z_2)) + \text{Tr}(\mathbf{Q}^{k_1 k_1}(z_2)) \, \text{Tr}(\mathbf{Q}^{sl_1}(z_1) \mathbf{Q}^{l_1 s}(z_2))] + \mathcal{O}(\eta_0^{-3} N^{-1/2}) \\ &= -N^{-1} [\text{Tr}(\mathbf{Q}^{ss}(z_1)) \, \text{Tr}(\mathbf{Q}^{k_1 l_1}(z_1) \mathbf{Q}^{l_1 k_1}(z_2)) + \text{Tr}(\mathbf{Q}^{k_1 k_1}(z_2)) \, \text{Tr}(\mathbf{Q}^{sl_1}(z_1) \mathbf{Q}^{l_1 s}(z_2))] + \mathcal{O}(\eta_0^{-3} N^{-1/2}) \\ &= -N^{-1} [\text{Tr}(\mathbf{Q}^{ss}(z_1)) \, \text{Tr}(\mathbf{Q}^{sl_1 l_1}(z_1) \mathbf{Q}^{l_1 k_1}(z_2)) + \text{Tr}(\mathbf{Q}^{sl_1 k_1}(z_2)) \, \text{Tr}(\mathbf{Q}^{sl_1}(z_1) \mathbf{Q}^{l_1 s}(z_2))] + \mathcal{O}(\eta_0^{-3} N^{-1/2}) \\ &= -N^{-1} [\text{Tr}(\mathbf{Q}^{ss}(z_1)) \, \text{Tr}(\mathbf{Q}^{sl_1 l_1}(z_1) \mathbf{Q}^{l_1 l_1}(z_2)) + \text{Tr}(\mathbf{Q}^{sl_1 l_1}(z_2)) \, \text{Tr}(\mathbf{Q}^{sl_1 l_1}(z_1) \mathbf{Q}^{l_1 l_2}(z_2))] \\ &= -N^{-1} [\text{Tr}(\mathbf{Q}^{ss}(z_1)) \, \text{Tr}(\mathbf{Q}^{sl_1 l_1}(z_1) \mathbf{Q}^{l_1 l_1}(z_2)) + \text{Tr}(\mathbf{Q}^{sl_1 l_1}(z_2)) \, \text{Tr}(\mathbf{Q}^{sl_1 l_2}(z_2))] \\ &= -N^{-1} [\text{Tr}(\mathbf{Q}^{sl_1 l_2}(z_2)) \, \text{Tr}(\mathbf{Q}^{sl_1 l_2}(z_2)) \, \text{Tr}(\mathbf{Q}^{sl_1 l_2}(z_2)) + \mathcal{O}(\mathbf{Q}^{sl_1 l_2}(z_2)) \\ &= -N^{-1} [\text{Tr}(\mathbf{Q}^{sl_1 l_2}(z_2)) \, \text{Tr}(\mathbf{Q}^{sl_1 l_2}(z_2)) \, \text{Tr}(\mathbf{Q}^{sl_1 l_2}(z_2)) \\ &= -N^{-1} [\text{Tr}(\mathbf{Q}^{sl_1 l_2}(z_2)) \, \text{$$

then by direct calculation, we can obtain that

$$\begin{split} &\frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{s \neq k_1}^{d} \mathbb{E} \left[\mathcal{A}_{i_1 \cdots i_d}^{(k_1,s)} Q_{i_s}^{sl_1}(z_1) Q_{\cdot i_{k_1}}^{l_1 k_1}(z_2) \partial_{i_1 \cdots i_d}^{(1)} \left\{ \operatorname{Tr}(\boldsymbol{Q}^{k_2 k_2}(\bar{z}_1)) \right\} \right] \\ &= -\frac{1}{N} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{s \neq k_1}^{d} \sum_{t_1 \neq t_2}^{d} \mathbb{E} \left[\mathcal{A}_{i_1 \cdots i_d}^{(k_1,s)} Q_{i_s}^{sl_1}(z_1) Q_{\cdot i_{k_1}}^{l_1 k_1}(z_2) \mathcal{A}_{i_1 \cdots i_d}^{(t_1,t_2)} Q_{i_1}^{t_1 k_2}(\bar{z}_1) Q_{\cdot i_{t_2}}^{k_2 t_2}(\bar{z}_1) \right] \\ &= -\frac{2}{N} \sum_{s \neq k_1}^{d} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{sl_1}(z_1) \boldsymbol{Q}^{l_1 k_1}(z_2) \boldsymbol{Q}^{k_1 k_2}(\bar{z}_1) \boldsymbol{Q}^{k_2 s}(\bar{z}_1)) \right] + \mathcal{O}(C_{\eta_0} N^{-1/2}), \end{split}$$

and

$$\begin{split} &\frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{s \neq k_1}^{d} \mathbb{E} \left[\partial_{i_1 \cdots i_d}^{(1)} \{ \mathcal{A}_{i_1 \cdots i_d}^{(k_1, s)} Q_{i_s}^{sl_1}(z_1) Q_{i_{k_1}}^{l_1 k_1}(z_2) \} \operatorname{Tr}(\boldsymbol{Q}^{k_2 k_2}(\bar{z}_1))^c \right] \\ &= -N^{-1} \sum_{s \neq k_1}^{d} \operatorname{Cov}(\operatorname{Tr}(\boldsymbol{Q}^{ss}(z_1)) \operatorname{Tr}(\boldsymbol{Q}^{k_1 l_1}(z_1) \boldsymbol{Q}^{l_1 k_1}(z_2)), \operatorname{Tr}(\boldsymbol{Q}^{k_2 k_2}(z_1))) \\ &- N^{-1} \sum_{s \neq k_1}^{d} \operatorname{Cov}(\operatorname{Tr}(\boldsymbol{Q}^{k_1 k_1}(z_2)) \operatorname{Tr}(\boldsymbol{Q}^{sl_1}(z_1) \boldsymbol{Q}^{l_1 s}(z_2)), \operatorname{Tr}(\boldsymbol{Q}^{k_2 k_2}(z_1))) + \operatorname{O}(C_{\eta_0} N^{-\omega}), \end{split}$$

similar as (E.7), we can show that

$$N^{-1}\operatorname{Cov}(\operatorname{Tr}(\boldsymbol{Q}^{ss}(z_1))\operatorname{Tr}(\boldsymbol{Q}^{k_1l_1}(z_1)\boldsymbol{Q}^{l_1k_1}(z_2)),\operatorname{Tr}(\boldsymbol{Q}^{k_2k_2}(z_1)))$$

$$=\mathfrak{m}_s(z_1)\mathcal{C}_{k_1l_1,k_2,N}^{(d)}+V_{k_1l_1,N}^{(d)}(z_1,z_2)\mathcal{C}_{sk_2,N}^{(d)}(z_1,z_1)+\operatorname{O}(C_{\eta_0}N^{-\omega}),$$

where $V_{k_1 l_1, N}^{(d)}(z_1, z_2) = N^{-1} \mathbb{E}[\text{Tr}(\boldsymbol{Q}^{k_1 l_1}(z_1) \boldsymbol{Q}^{l_1 k_1}(z_2))]$ and $C_{sk_2, N}^{(d)}(z_1, z_2)$ is defined in (G.8). For simplicity, we define

$$\mathcal{V}_{k_1 l_1, k_2, N}^{(d)}(z_1, z_2) := \frac{1}{N} \sum_{s \neq k_1}^{d} \mathbb{E}[\text{Tr}(\boldsymbol{Q}^{s l_1}(z_1) \boldsymbol{Q}^{l_1 k_1}(z_2) \boldsymbol{Q}^{k_1 k_2}(\bar{z}_1) \boldsymbol{Q}^{k_2 s}(\bar{z}_1))] + \mathcal{O}(C_{\eta_0} N^{-1/2}),$$

then we obtain

$$\frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{s \neq k_1}^{d} \mathbb{E} \left[\partial_{i_1 \cdots i_d}^{(1)} \left\{ \mathcal{A}_{i_1 \cdots i_d}^{(k_1, s)} Q_{i_s}^{sl_1}(z_1) Q_{i_{k_1}}^{l_1 k_1}(z_2) \operatorname{Tr} (\boldsymbol{Q}^{k_2 k_2}(\bar{z}_1))^c \right\} \right] \\
= -C_{k_1 l_1, k_2, N}^{(d)} \sum_{s \neq k_1}^{d} \mathfrak{m}_s(z_1) - V_{k_1 l_1, N}^{(d)}(z_1, z_2) \sum_{s \neq k_1}^{d} C_{sk_2, N}^{(d)}(z_1, z_2) - \mathfrak{m}_{k_1}(z_2) \sum_{s \neq k_1}^{d} C_{sl_1, k_2, N}^{(d)} \\
- C_{k_1 k_2, N}^{(d)}(z_2, z_1) \sum_{s \neq k_1}^{d} V_{sl_1, N}^{(d)}(z_1, z_2) - 2V_{k_1 l_1, k_2, N}^{(d)}(z_1, z_2) + \operatorname{O}(C_{\eta_0} N^{-\omega}). \tag{G.43}$$

Third derivatives: When $\alpha = 3$, similar as proofs in Theorem F.2 for $\alpha = 3$, only the following case contains the major terms:

$$\frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{s \neq k_1}^{d} \mathbb{E} \left[\partial_{i_1 \cdots i_d}^{(2)} \{ \operatorname{Tr}(\boldsymbol{Q}^{k_2 k_2}(\bar{z}_1))^c \} \partial_{i_1 \cdots i_d}^{(1)} \{ \mathcal{A}_{i_1 \cdots i_d}^{(k_1, s)} Q_{i_s}^{sl_1}(z_1) Q_{i_{k_1}}^{l_1 k_1}(z_2) \} \right],$$

where

$$\partial_{i_1\cdots i_d}^{(2)} \operatorname{Tr} \boldsymbol{Q}^{k_2k_2}(\bar{z}) = \frac{2}{N} \sum_{t_1 \neq t_2, t_3 \neq t_4}^{d} \mathcal{A}_{i_1\cdots i_d}^{(t_1,t_2)} \mathcal{A}_{i_1\cdots i_d}^{(t_3,t_4)} Q_{i_{t_2}i_{t_3}}^{t_2t_3}(\bar{z}) Q_{i_{t_4}}^{t_4k_2}(\bar{z}) Q_{\cdot i_{t_1}}^{k_2t_1}(\bar{z}),$$

then by Lemmas G.3, G.4 and (A.5), we have

$$\frac{1}{\sqrt{N}} \sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}} \sum_{s\neq k_{1}}^{d} \mathbb{E}\left[\partial_{i_{1}\cdots i_{d}}^{(2)} \left\{ \operatorname{Tr}(\boldsymbol{Q}^{k_{2}k_{2}}(\bar{z}_{1}))^{c} \right\} \partial_{i_{1}\cdots i_{d}}^{(1)} \left\{ \mathcal{A}_{i_{1}\cdots i_{d}}^{(k_{1},s)} Q_{i_{s}}^{sl_{1}}(z_{1}) Q_{\cdot i_{k_{1}}}^{l_{1}k_{1}}(z_{2}) \right\} \right] = \mathcal{O}(C_{\eta_{0}} N^{-1/2})$$

$$-\frac{2}{N^{2}} \sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}} \sum_{s\neq k_{1}}^{d} \sum_{t_{1},t_{2}}^{(s,k_{1})} \mathbb{E}\left[(\mathcal{A}_{i_{1}\cdots i_{d}}^{(t_{1},t_{2})})^{2} Q_{i_{2}i_{2}}^{t_{2}t_{2}}(\bar{z}_{1}) Q_{i_{1}}^{t_{1}k_{2}}(\bar{z}_{1}) Q_{\cdot i_{t_{1}}}^{k_{2}t_{1}}(\bar{z}_{1}) (\mathcal{A}_{i_{1}\cdots i_{d}}^{(k_{1},s)})^{2} Q_{i_{s}i_{s}}^{ss}(z_{1}) Q_{\cdot i_{k_{1}}}^{k_{1}l_{1}}(z_{2}) \right]$$

$$-\frac{2}{N^{2}} \sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}} \sum_{s\neq k_{1}}^{d} \sum_{t_{1},t_{2}}^{(s,k_{1})} \mathbb{E}\left[(\mathcal{A}_{i_{1}\cdots i_{d}}^{(t_{1},t_{2})})^{2} Q_{i_{2}i_{2}}^{t_{2}t_{2}}(\bar{z}_{1}) Q_{i_{t_{1}}}^{t_{1}k_{2}}(\bar{z}_{1}) Q_{\cdot i_{t_{1}}}^{k_{2}t_{1}}(\bar{z}_{1}) (\mathcal{A}_{i_{1}\cdots i_{d}}^{(k_{1},s)})^{2} Q_{i_{s}\cdot}^{sl_{1}}(z_{1}) Q_{\cdot i_{s}}^{k_{1}k_{1}}(z_{2}) \right]$$

where the notation $\sum_{t_1,t_2}^{(s,k_1)}$ means that the summation of t_1 and t_2 are over $\{1,\cdots,d\}\setminus\{s,k_1\}$. For simplicity, we define

$$\begin{split} &\mathcal{U}_{k_{1}l_{1},k_{2},N}^{(d)}(z_{1},z_{2}) \\ &:= \frac{1}{N^{2}} \sum_{s\neq k_{1}}^{d} \mathcal{B}_{(4)}^{(k_{1},s)} \mathbb{E} \big[\operatorname{Tr}(\boldsymbol{Q}^{ss}(z_{1}) \circ \boldsymbol{Q}^{ss}(\bar{z}_{1})) \cdot \operatorname{Tr}((\boldsymbol{Q}^{k_{1}l_{1}}(z_{1})\boldsymbol{Q}^{l_{1}k_{1}}(z_{2})) \circ (\boldsymbol{Q}^{k_{1}k_{2}}(\bar{z}_{1})\boldsymbol{Q}^{k_{2}k_{1}}(\bar{z}_{1}))) \big] \\ &+ \frac{1}{N^{2}} \sum_{s\neq k_{1}}^{d} \mathcal{B}_{(4)}^{(k_{1},s)} \mathbb{E} \big[\operatorname{Tr}(\boldsymbol{Q}^{ss}(z_{1}) \circ (\boldsymbol{Q}^{sk_{2}}(\bar{z}_{1})\boldsymbol{Q}^{k_{2}s}(\bar{z}_{1}))) \cdot \operatorname{Tr}((\boldsymbol{Q}^{k_{1}l_{1}}(z_{1})\boldsymbol{Q}^{l_{1}k_{1}}(z_{2})) \circ \boldsymbol{Q}^{k_{1}k_{1}}(\bar{z}_{1})) \big] \\ &+ \frac{1}{N^{2}} \sum_{s\neq k_{1}}^{d} \mathcal{B}_{(4)}^{(k_{1},s)} \mathbb{E} \big[\operatorname{Tr}((\boldsymbol{Q}^{sl_{1}}(z_{1})\boldsymbol{Q}^{l_{1}s}(z_{2})) \circ \boldsymbol{Q}^{ss}(\bar{z}_{1})) \cdot \operatorname{Tr}(\boldsymbol{Q}^{k_{1}k_{1}}(z_{1}) \circ (\boldsymbol{Q}^{k_{1}k_{2}}(\bar{z}_{1})\boldsymbol{Q}^{k_{2}k_{1}}(\bar{z}_{1}))) \big] \\ &+ \frac{1}{N^{2}} \sum_{s\neq k_{1}}^{d} \mathcal{B}_{(4)}^{(k_{1},s)} \mathbb{E} \big[\operatorname{Tr}((\boldsymbol{Q}^{sl_{1}}(z_{1})\boldsymbol{Q}^{l_{1}s}(z_{1})) \circ (\boldsymbol{Q}^{sk_{2}}(\bar{z}_{1})\boldsymbol{Q}^{k_{2}s}(\bar{z}_{1}))) \cdot \operatorname{Tr}(\boldsymbol{Q}^{k_{1}k_{1}}(z_{2}) \circ \boldsymbol{Q}^{k_{1}k_{1}}(\bar{z}_{1})) \big], \end{split}$$

where $\mathcal{B}_{(4)}^{(k_1,s)}$ is defined in (A.5). Then combining (G.43) and (G.44), we obtain

$$\begin{split} &(z_{1}+\mathfrak{m}(z_{1})-\mathfrak{m}_{k_{1}}(z_{1}))\mathcal{C}^{(d)}_{k_{1}l_{1},k_{2},N}=-V^{(d)}_{k_{1}l_{1},N}(z_{1},z_{2})\sum_{s\neq k_{1}}^{d}\mathcal{C}^{(d)}_{sk_{2},N}(z_{1},z_{2})-\mathfrak{m}_{k_{1}}(z_{2})\sum_{s\neq k_{1}}^{d}\mathcal{C}^{(d)}_{sl_{1},k_{2},N}(z_{1},z_{2})-\mathcal{C}^{(d)}_{k_{1}l_{2},N}(z_{1},z_{2})-\kappa_{4}\mathcal{U}^{(d)}_{k_{1}l_{1},k_{2},N}(z_{1},z_{2})+\mathcal{O}(C_{\eta_{0}}N^{-\omega})\\ &:=-\mathfrak{m}_{k_{1}}(z_{2})\sum_{s\neq k_{1}}^{d}\mathcal{C}^{(d)}_{sl_{1},k_{2},N}-\mathcal{F}^{(d)}_{k_{1}l_{1},k_{2},N}(z_{1},z_{2})+\mathcal{O}(C_{\eta_{0}}N^{-\omega}). \end{split}$$

Hence, for any **fixed** $k_2 \in \{1, \dots, d\}$, define

$$\boldsymbol{C}_{k_2,N}^{(d)}(z_1,z_2) = [\mathcal{C}_{kl,k_2,N}^{(d)}(z_1,z_2)]_{d\times d} \quad \text{and} \quad \boldsymbol{F}_{k_2,N}^{(d)}(z_1,z_2) = [\mathcal{F}_{kl,k_2,N}^{(d)}(z_1,z_1)]_{d\times d}, \tag{G.44}$$

then we obtain that

$$\mathbf{\Theta}_{N}^{(d)}(z_1, z_2) \mathbf{C}_{k_2, N}^{(d)}(z_1, z_2) = -\mathbf{F}_{k_2, N}^{(d)}(z_1, z_2) + \mathrm{o}(\mathbf{1}_{d \times d}),$$

where $\Theta_N^{(d)}(z_1, z_2)$ is defined in (G.18) and it is invertible, so we can further derive

$$\lim_{N \to \infty} \| \boldsymbol{C}_{k_2,N}^{(d)}(z_1, z_2) - \boldsymbol{\Pi}^{(d)}(z_1, z_2)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z_1)) \boldsymbol{F}_{k_2,N}^{(d)}(z_1, z_2) \| = 0, \tag{G.45}$$

which suggests that all entries of $C_{k_2,N}^{(d)}(z_1,z_2)$ are bounded by $C_{\eta_0,\mathfrak{c},d}$.

Calculations of (G.40): By the cumulant expansion (D.4) again, we have

$$\begin{split} &\frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{s \neq k_1}^{d} \mathbb{E} \left[X_{i_1 \cdots i_d} \mathcal{A}_{i_1 \cdots i_d}^{(k_1, s)} Q_{i_s}^{sl_1}(z_1) Q_{\cdot i_{k_1}}^{l_1 k_1}(z_2) \operatorname{Tr}(\boldsymbol{Q}^{k_2 l_2}(\bar{z}_1) \boldsymbol{Q}^{l_2 k_2}(\bar{z}_2))^c \right] \\ &= \frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \left(\sum_{s \neq k_1}^{d} \sum_{\alpha = 0}^{3} \frac{\kappa_{\alpha + 1}}{\alpha!} \mathbb{E} \left[\mathcal{A}_{i_1 \cdots i_d}^{(k_1, s)} \partial_{i_1 \cdots i_d}^{(\alpha)} \left\{ Q_{i_s}^{sl}(z_1) Q_{\cdot i_{k_1}}^{l_1 k_1}(z_2) \operatorname{Tr}(\boldsymbol{Q}^{k_2 l_2}(\bar{z}_1) \boldsymbol{Q}^{l_2 k_2}(\bar{z}_2))^c \right\} \right] + \epsilon_{i_1 \cdots i_d}^{(4)} \right). \end{split}$$

Here, we still omit the details for calculating minors.

First derivatives: When $\alpha = 1$, since

$$\partial_{i_1\cdots i_d}^{(1)}\operatorname{Tr}(\boldsymbol{Q}^{kl}(z_1)\boldsymbol{Q}^{lk}(z_2)) = -N^{-1/2}\sum_{s_1\neq s_2}^d\sum_{j=1}^2\mathcal{A}^{(s_1,s_2)}_{i_1\cdots i_d}Q^{s_1k}_{i_{s_1}}(z_j)\boldsymbol{Q}^{kl}(z_{3-j})Q^{ls_2}_{\cdot i_{s_2}}(z_j),$$

and

$$\begin{split} &\frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_{l_1}} \sum_{i_t}^{n_{l_1}} \mathcal{A}_{i_1 \cdots i_d}^{(k_1,s)} \partial_{i_1 \cdots i_d}^{(1)} \left\{ Q_{i_s i_t}^{sl_1}(z_1) Q_{i_{k_1} i_t}^{k_1 l_1}(z_2) \right\} \\ &= -N^{-1} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \mathcal{A}_{i_1 \cdots i_d}^{(k_1,s)} \mathcal{A}_{i_1 \cdots i_d}^{(s_1,s_2)} \left[Q_{i_s i_s}^{ss_1}(z_1) Q_{i_{s_2}}^{s_2 l_1}(z_1) Q_{i_{k_1}}^{l_1 k_1}(z_2) + Q_{i_{k_1} i_{s_1}}^{k_1 s_1}(z_2) Q_{i_{s_2}}^{s_2 l_1}(z_2) Q_{i_s}^{l_1 s}(z_1) \right] \\ &= -N^{-1} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} (\mathcal{A}_{i_1 \cdots i_d}^{(k_1,s)})^2 \left[Q_{i_s i_s}^{ss}(z_1) Q_{i_{k_1}}^{k_1 l_1}(z_1) Q_{i_{k_1}}^{l_1 k_1}(z_2) + Q_{i_{k_1} i_{k_1}}^{k_1 l_1}(z_2) Q_{i_s}^{sl_1}(z_2) Q_{i_s}^{l_1 s}(z_1) \right] + \mathcal{O}(\eta_0^{-3} N^{-1/2}) \\ &= -N^{-1} \left[\mathrm{Tr}(\mathbf{Q}^{ss}(z_1)) \, \mathrm{Tr}(\mathbf{Q}^{k_1 l_1}(z_1) \mathbf{Q}^{l_1 k_1}(z_2)) + \mathrm{Tr}(\mathbf{Q}^{k_1 k_1}(z_2)) \, \mathrm{Tr}(\mathbf{Q}^{sl_1}(z_1) \mathbf{Q}^{l_1 s}(z_2)) \right] + \mathcal{O}(\eta_0^{-3} N^{-1/2}) \end{split}$$

For simplicity, we define

$$\mathcal{V}_{k_{1}l_{1},k_{2}l_{2},N}^{(d)}(z_{1},z_{2}) = \frac{1}{N} \sum_{\substack{s=1\\s=1}}^{d} \sum_{\substack{i=1\\s=1}}^{2} \mathbb{E} \left[\operatorname{Tr} \left(\boldsymbol{Q}^{sl_{1}}(z_{1}) \boldsymbol{Q}^{l_{1}k_{1}}(z_{2}) [\boldsymbol{Q}^{k_{1}k_{2}}(\bar{z}_{j}) \boldsymbol{Q}^{k_{2}l_{2}}(\bar{z}_{3-j}) \boldsymbol{Q}^{l_{2}s}(\bar{z}_{j}) + \boldsymbol{Q}^{k_{1}l_{2}}(\bar{z}_{j}) \boldsymbol{Q}^{l_{2}k_{2}}(\bar{z}_{3-j}) \boldsymbol{Q}^{k_{2}s}(\bar{z}_{j})] \right) \right],$$

then by direct calculations, we have

$$\frac{1}{\sqrt{N}} \sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}} \sum_{s\neq k_{1}}^{d} \mathbb{E}\left[A_{i_{1}\cdots i_{d}}^{(k_{1},s)}Q_{i_{s}\cdot}^{sl_{1}}(z_{1})Q_{\cdot i_{k_{1}}}^{l_{1}k_{1}}(z_{2})\partial_{i_{1}\cdots i_{d}}^{(1)}\left\{\operatorname{Tr}(\boldsymbol{Q}^{k_{2}l_{2}}(\bar{z}_{1})\boldsymbol{Q}^{l_{2}k_{2}}(\bar{z}_{2}))^{c}\right\}\right]$$

$$= -\frac{2}{N} \sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}} \sum_{s\neq k_{1}}^{d} \sum_{s_{1}\neq s_{2}}^{d} \sum_{j=1}^{2} \mathbb{E}\left[A_{i_{1}\cdots i_{d}}^{(k_{1},s)}Q_{i_{s}\cdot}^{sl_{1}}(z_{1})Q_{\cdot i_{k_{1}}}^{l_{1}k_{1}}(z_{2})A_{i_{1}\cdots i_{d}}^{(s_{1},s_{2})}Q_{i_{s_{1}\cdot}}^{s_{1}k_{2}}(\bar{z}_{j})\boldsymbol{Q}^{k_{2}l_{2}}(\bar{z}_{3-j})Q_{\cdot i_{s_{2}}}^{l_{2}s_{2}}(\bar{z}_{j})\right]$$

$$= -\frac{2}{N} \sum_{s\neq k_{1}}^{d} \sum_{j=1}^{2} \mathbb{E}\left[\operatorname{Tr}\left(\boldsymbol{Q}^{sl_{1}}(z_{1})\boldsymbol{Q}^{l_{1}k_{1}}(z_{2})[\boldsymbol{Q}^{k_{1}k_{2}}(\bar{z}_{j})\boldsymbol{Q}^{k_{2}l_{2}}(\bar{z}_{3-j})\boldsymbol{Q}^{l_{2}s}(\bar{z}_{j})\right]$$

$$+ \boldsymbol{Q}^{k_{1}l_{2}}(\bar{z}_{j})\boldsymbol{Q}^{l_{2}k_{2}}(\bar{z}_{3-j})\boldsymbol{Q}^{k_{2}s}(\bar{z}_{j})\right]\right] + \operatorname{O}(C_{\eta_{0}}N^{-1/2}) = -2\mathcal{V}_{k_{1}l_{1},k_{2}l_{2},N}^{(d)}(z_{1},z_{2}) + \operatorname{O}(C_{\eta_{0}}N^{-1/2})$$
(G.46)

and

$$\frac{1}{\sqrt{N}} \sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}} \sum_{s\neq k_{1}}^{d} \mathbb{E}\left[\partial_{i_{1}\cdots i_{d}}^{(1)} \left\{\mathcal{A}_{i_{1}\cdots i_{d}}^{(k_{1},s)} Q_{i_{s}}^{sl_{1}}(z_{1}) Q_{\cdot i_{k_{1}}}^{l_{1}k_{1}}(z_{2})\right\} \operatorname{Tr}(\boldsymbol{Q}^{k_{2}l_{2}}(\bar{z}_{1}) \boldsymbol{Q}^{l_{2}k_{2}}(\bar{z}_{2}))^{c}\right] \\
= -\frac{1}{N} \sum_{s\neq k_{1}}^{d} \operatorname{Cov}\left(\operatorname{Tr}(\boldsymbol{Q}^{ss}(z_{1})) \operatorname{Tr}(\boldsymbol{Q}^{k_{1}l_{1}}(z_{1}) \boldsymbol{Q}^{l_{1}k_{1}}(z_{2})), \operatorname{Tr}(\boldsymbol{Q}^{k_{2}l_{2}}(z_{1}) \boldsymbol{Q}^{l_{2}k_{2}}(z_{2}))\right) \\
-\frac{1}{N} \sum_{s\neq k_{1}}^{d} \operatorname{Cov}\left(\operatorname{Tr}(\boldsymbol{Q}^{k_{1}k_{1}}(z_{2})) \operatorname{Tr}(\boldsymbol{Q}^{sl_{1}}(z_{1}) \boldsymbol{Q}^{l_{1}s}(z_{2})), \operatorname{Tr}(\boldsymbol{Q}^{k_{2}l_{2}}(z_{1}) \boldsymbol{Q}^{l_{2}k_{2}}(z_{2})) + \operatorname{O}(C_{\eta_{0}} N^{-\omega})\right) \\
= -\mathcal{C}_{k_{1}l_{1},k_{2}l_{2},N}^{(d)} \sum_{s\neq k_{1}}^{d} \mathfrak{m}_{s}(z_{1}) - V_{k_{1}l_{1},N}^{(d)}(z_{1},z_{2}) \sum_{s\neq k_{1}}^{d} \mathcal{C}_{s,k_{2}l_{2},N}^{(d)} \\
-\mathfrak{m}_{k_{1}}(z_{2}) \sum_{s\neq k_{1}}^{d} \mathcal{C}_{sl_{1},k_{2}l_{2},N}^{(d)} - \mathcal{C}_{k_{1},k_{2}l_{2},N}^{(d)} \sum_{s\neq k_{1}}^{d} V_{sl_{1},N}^{(d)}(z_{1},z_{2}) + \operatorname{O}(C_{\eta_{0}} N^{-\omega}) \mathcal{C}_{k_{2}l_{2},k_{2}l_{2},N}^{(d)}$$
(G.47)

where we use the same trick as (E.7) and $V_{sl_1,N}^{(d)}(z_1,z_2) = N^{-1}\mathbb{E}[\text{Tr}(\boldsymbol{Q}^{sl_1}(z_1)\boldsymbol{Q}^{l_1s}(z_2))].$

Third derivatives: When $\alpha = 3$, similar as proofs for $\alpha = 3$ in Theorem F.2, the only one contains major terms is

$$\frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{s \neq k_1}^{d} \mathbb{E} \left[\partial_{i_1 \cdots i_d}^{(1)} \left\{ \mathcal{A}_{i_1 \cdots i_d}^{(k_1, s)} Q_{i_s}^{sl_1}(z_1) Q_{i_{k_1}}^{l_1 k_1}(z_2) \right\} \partial_{i_1 \cdots i_d}^{(2)} \left\{ \operatorname{Tr} (\boldsymbol{Q}^{k_2 l_2}(\bar{z}_1) \boldsymbol{Q}^{l_2 k_2}(\bar{z}_2))^c \right\} \right] \\
= -2\mathcal{U}_{k_1 l_1, k_2 l_2, N}^{(d)}(z_1, z_2) + \mathcal{O}(C_{\eta_0} N^{-\omega}), \tag{G.48}$$

where

$$\mathcal{U}_{k_1 l_1, k_2 l_2, N}^{(d)}(z_1, z_2) := \mathcal{U}_{k_1 l_1, k_2 l_2, N}^{(1,d)}(z, \bar{z}) + \mathcal{U}_{k_1 l_1, k_2 l_2, N}^{(2,d)}(z, \bar{z}) + \mathcal{U}_{k_1 l_1, k_2 l_2, N}^{(3,d)}(z, \bar{z})$$

and $\mathcal{U}_{k_1 l_1, k_2 l_2, N}^{(1,d)}(z, \bar{z}), \mathcal{U}_{k_1 l_1, k_2 l_2, N}^{(2,d)}(z, \bar{z}), \mathcal{U}_{k_1 l_1, k_2 l_2, N}^{(3,d)}(z, \bar{z})$ will be defined in (G.52), (G.53) and (G.54), respectively. Notice that

$$\partial_{i_{1}\cdots i_{d}}^{(2)} \left\{ \operatorname{Tr}(\boldsymbol{Q}^{k_{2}l_{2}}(\bar{z}_{1})\boldsymbol{Q}^{l_{2}k_{2}}(\bar{z}_{2})) \right\} \\
= \frac{2}{N} \sum_{\substack{t_{1} \neq t_{2} \\ t_{2} \neq t_{d}}}^{d} \mathcal{A}_{i_{1}\cdots i_{d}}^{(t_{1},t_{2})} Q_{i_{t_{2}}i_{t_{3}}}^{t_{2}t_{3}}(\bar{z}_{1}) \mathcal{A}_{i_{1}\cdots i_{d}}^{(t_{3},t_{4})} Q_{i_{t_{4}}}^{t_{4}l_{2}}(\bar{z}_{1}) \boldsymbol{Q}^{l_{2}k_{2}}(\bar{z}_{2}) Q_{\cdot i_{t_{1}}}^{k_{2}t_{1}}(\bar{z}_{1}) \tag{G.49}$$

$$+\frac{2}{N}\sum_{\substack{t_1\neq t_2\\t_3\neq t_4}}^{d} Q_{i_{t_4}}^{t_4k_2}(\bar{z}) \boldsymbol{Q}^{k_2l_2}(\bar{z}) Q_{i_{t_1}}^{l_2t_1}(\bar{z}) \mathcal{A}_{i_1\cdots i_d}^{(t_1,t_2)} Q_{i_{t_2}i_{t_3}}^{t_2t_3}(\bar{z}) \mathcal{A}_{i_1\cdots i_d}^{(t_3,t_4)}$$
(G.50)

$$+\frac{2}{N} \sum_{\substack{t_1 \neq t_2 \\ t_3 \neq t_4}}^{d} \mathcal{A}_{i_1 \cdots i_d}^{(t_1, t_2)} Q_{i_{t_2}}^{t_2 l_2}(\bar{z}_1) Q_{\cdot i_{t_3}}^{l_2 t_3}(\bar{z}_1) \mathcal{A}_{i_1 \cdots i_d}^{(t_3, t_4)} Q_{i_{t_4}}^{t_4 k_2}(\bar{z}_2) Q_{\cdot i_{t_1}}^{k_2 t_1}(\bar{z}_2), \tag{G.51}$$

then we combining (G.49) with $\partial_{i_1\cdots i_d}^{(1)}\{\mathcal{A}_{i_1\cdots i_d}^{(k_1,s)}Q_{i_s}^{sl_1}(z_1)Q_{\cdot i_{k_1}}^{l_1k_1}(z_2)\}$, by Lemmas G.3, G.4 and (A.5),

it gives that

$$\begin{split} &\frac{1}{\sqrt{N}} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \sum_{s \neq k_{1}}^{d} \mathbb{E} \left[\partial_{i_{1} \cdots i_{d}}^{(1)} \left\{ A_{i_{1} \cdots i_{d}}^{(k_{1},s)} Q_{i_{s}}^{l_{1}}(z_{1}) Q_{i_{k_{1}}}^{l_{1}k_{1}}(z_{2}) \right\} A_{i_{1} \cdots i_{d}}^{(l_{1},l_{2})} Q_{i_{2}i_{3}}^{l_{2}i_{3}}(\bar{z}_{1}) A_{i_{1} \cdots i_{d}}^{(l_{2},l_{1})} Q_{i_{k_{1}}}^{l_{2}l_{2}}(\bar{z}_{2}) Q_{i_{k_{1}}}^{k_{2}l_{1}}(\bar{z}_{1}) \right] \\ &= -\frac{1}{N^{2}} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \sum_{s \neq k_{1}}^{d} \mathbb{E} \left[\left(A_{i_{1} \cdots i_{d}}^{(k_{1},s)} \right)^{2} Q_{i_{s}i_{s}}^{s_{1}s}(z_{1}) Q_{i_{k_{1}}}^{l_{1}l_{1}}(z_{1}) Q_{i_{k_{1}}}^{l_{1}l_{1}}(z_{2}) (A_{i_{1} \cdots i_{d}}^{(l_{1},l_{2})})^{2} Q_{i_{k_{2}}i_{2}}^{t_{2}l_{2}}(\bar{z}_{2}) Q_{i_{k_{1}}}^{k_{2}l_{1}}(\bar{z}_{1}) \right] \\ &- \frac{1}{N^{2}} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \sum_{s \neq k_{1}}^{d} \mathbb{E} \left[\left(A_{i_{1} \cdots i_{d}}^{(k_{1},s)} \right)^{2} Q_{i_{s}}^{t_{1}l_{1}}(z_{1}) Q_{i_{1}k_{1}}^{l_{1}l_{1}}(z_{2}) (A_{i_{1} \cdots i_{d}}^{(l_{1},l_{2})})^{2} Q_{i_{2}i_{2}}^{t_{2}l_{2}}(\bar{z}_{1}) Q_{i_{1}l_{1}}^{t_{2}l_{2}}(\bar{z}_{2}) Q_{i_{k_{1}}l_{1}}^{k_{2}l_{1}}(\bar{z}_{1}) \right] \\ &- \frac{1}{N^{2}} \sum_{s \neq k_{1}}^{d} \mathcal{B} \left\{ B_{i_{1} \cdots i_{d}}^{(k_{1},s)} \mathbb{E} \left[\operatorname{Tr}(Q^{ss}(z_{1}) \circ Q^{ss}(\bar{z}_{2})) \operatorname{Tr}((Q^{k_{1}l_{1}}(z_{1}) Q^{l_{1}k_{1}}(z_{2})) \circ (Q^{k_{1}l_{2}}(\bar{z}_{1}) Q^{l_{2}k_{2}}(\bar{z}_{2}) Q^{k_{2}k_{1}}(\bar{z}_{1})) \right] \\ &- \frac{1}{N^{2}} \sum_{s \neq k_{1}}^{d} \mathcal{B} \left\{ B_{i_{1} \cdots s}^{(k_{1},s)} \mathbb{E} \left[\operatorname{Tr}(Q^{ss}(z_{1}) \circ (Q^{sl_{2}}(\bar{z}_{1}) Q^{l_{2}k_{2}}(\bar{z}_{2}) Q^{k_{2}s}(\bar{z}_{1})) \right] \operatorname{Tr}(Q^{k_{1}l_{1}}(z_{2}) \circ (Q^{k_{1}l_{2}}(z_{1}) Q^{l_{2}k_{2}}(\bar{z}_{2}) Q^{k_{2}k_{1}}(\bar{z}_{1})) \right] \\ &- \frac{1}{N^{2}} \sum_{s \neq k_{1}}^{d} \mathcal{B} \left\{ B_{i_{1} \cdots s}^{(k_{1},s)} \mathbb{E} \left[\operatorname{Tr}(Q^{sl_{1}}(z_{1}) Q^{l_{1}s}(z_{2})) \circ Q^{ss}(\bar{z}_{1})) \operatorname{Tr}(Q^{k_{1}l_{1}}(z_{2}) \circ (Q^{k_{1}l_{2}}(\bar{z}_{1}) Q^{l_{2}k_{2}}(\bar{z}_{2}) Q^{k_{2}k_{1}}(\bar{z}_{1})) \right] \\ &- \frac{1}{N^{2}} \sum_{s \neq k_{1}}^{d} \mathcal{B} \left\{ B_{i_{1} \cdots s}^{(k_{1},s)} \mathbb{E} \left[\operatorname{Tr}(Q^{sl_{1}}(z_{1}) Q^{l_{1}s}(z_{2})) \circ (Q^{sl_{2}}(\bar{z}_{1}) Q^{l_{2}k_{2}}(\bar{z}_{2}) Q^{k_{2}s}(\bar{z}_{1})) \right] \right\} + O(C_$$

Similarly, combining (G.50) with $\partial_{i_1\cdots i_d}^{(1)}\{\mathcal{A}_{i_1\cdots i_d}^{(k_1,s)}Q_{i_s}^{sl_1}(z_1)Q_{i_{k_1}}^{l_1k_1}(z_2)\}$ will obtain the same result, just replace all \bar{z}_2, \bar{z}_1 by \bar{z}_1, \bar{z}_2 respectively, i.e.

$$\mathcal{U}_{k_{1}l_{1},k_{2}l_{2},N}^{(2,d)}(z_{1},z_{2}) \qquad (G.53)$$

$$:= \frac{1}{N^{2}} \sum_{s \neq k_{1}}^{d} \mathcal{B}_{(4)}^{(k_{1},s)} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{ss}(z_{1}) \circ \boldsymbol{Q}^{ss}(\bar{z}_{2})) \operatorname{Tr}((\boldsymbol{Q}^{k_{1}l_{1}}(z_{1})\boldsymbol{Q}^{l_{1}k_{1}}(z_{2})) \circ (\boldsymbol{Q}^{k_{1}l_{2}}(\bar{z}_{2})\boldsymbol{Q}^{l_{2}k_{2}}(\bar{z}_{1})\boldsymbol{Q}^{k_{2}k_{1}}(\bar{z}_{2}))) \right]$$

$$+ \frac{1}{N^{2}} \sum_{s \neq k_{1}}^{d} \mathcal{B}_{(4)}^{(k_{1},s)} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{ss}(z_{1}) \circ (\boldsymbol{Q}^{sl_{2}}(\bar{z}_{2})\boldsymbol{Q}^{l_{2}k_{2}}(\bar{z}_{1})\boldsymbol{Q}^{k_{2}s}(\bar{z}_{2}))) \operatorname{Tr}((\boldsymbol{Q}^{k_{1}l_{1}}(z_{1})\boldsymbol{Q}^{l_{1}k_{1}}(z_{2})) \circ \boldsymbol{Q}^{k_{1}k_{1}}(\bar{z}_{2})) \right]$$

$$+ \frac{1}{N^{2}} \sum_{s \neq k_{1}}^{d} \mathcal{B}_{(4)}^{(k_{1},s)} \mathbb{E} \left[\operatorname{Tr}((\boldsymbol{Q}^{sl_{1}}(z_{1})\boldsymbol{Q}^{l_{1}s}(z_{2})) \circ \boldsymbol{Q}^{ss}(\bar{z}_{2})) \operatorname{Tr}(\boldsymbol{Q}^{k_{1}k_{1}}(z_{2}) \circ (\boldsymbol{Q}^{k_{1}l_{2}}(\bar{z}_{2})\boldsymbol{Q}^{l_{2}k_{2}}(\bar{z}_{1})\boldsymbol{Q}^{k_{2}k_{1}}(\bar{z}_{2}))) \right]$$

$$+ \frac{1}{N^{2}} \sum_{s \neq k_{1}}^{d} \mathcal{B}_{(4)}^{(k_{1},s)} \mathbb{E} \left[\operatorname{Tr}((\boldsymbol{Q}^{sl_{1}}(z_{1})\boldsymbol{Q}^{l_{1}s}(z_{2})) \circ (\boldsymbol{Q}^{sl_{2}}(\bar{z}_{1})\boldsymbol{Q}^{l_{2}k_{2}}(\bar{z}_{1})\boldsymbol{Q}^{k_{2}s}(\bar{z}_{2}))) \operatorname{Tr}(\boldsymbol{Q}^{k_{1}k_{1}}(z_{1}) \circ \boldsymbol{Q}^{k_{1}k_{1}}(z_{2})) \right]$$

For (G.51), we directly list it as follows:

$$\mathcal{U}_{k_{1}l_{1},k_{2}l_{2},N}^{(3,d)}(z_{1},z_{2}) \qquad (G.54)$$

$$: = \frac{1}{N^{2}} \sum_{s \neq k_{1}}^{d} \mathcal{B}_{(4)}^{(k_{1},s)} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{ss}(z_{1}) \circ (\boldsymbol{Q}^{sl_{2}}(\bar{z}_{1})\boldsymbol{Q}^{l_{2}s}(\bar{z}_{1}))) \operatorname{Tr}((\boldsymbol{Q}^{k_{1}l_{1}}(z_{1})\boldsymbol{Q}^{l_{1}k_{1}}(z_{2})) \circ (\boldsymbol{Q}^{k_{1}k_{2}}(\bar{z}_{2})\boldsymbol{Q}^{k_{2}k_{1}}(\bar{z}_{2}))) \right] \\
+ \frac{1}{N^{2}} \sum_{s \neq k_{1}}^{d} \mathcal{B}_{(4)}^{(k_{1},s)} \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{ss}(z_{1}) \circ (\boldsymbol{Q}^{sk_{2}}(\bar{z}_{2})\boldsymbol{Q}^{k_{2}s}(\bar{z}_{2}))) \operatorname{Tr}((\boldsymbol{Q}^{k_{1}l_{1}}(z_{1})\boldsymbol{Q}^{l_{1}k_{1}}(z_{2})) \circ (\boldsymbol{Q}^{k_{1}l_{2}}(\bar{z}_{1})\boldsymbol{Q}^{l_{2}k_{1}}(\bar{z}_{1}))) \right] \\
+ \frac{1}{N^{2}} \sum_{s \neq k_{1}}^{d} \mathcal{B}_{(4)}^{(k_{1},s)} \mathbb{E} \left[\operatorname{Tr}((\boldsymbol{Q}^{sl_{1}}(z_{1})\boldsymbol{Q}^{l_{1}s}(z_{2})) \circ (\boldsymbol{Q}^{sl_{2}}(\bar{z}_{1})\boldsymbol{Q}^{l_{2}s}(\bar{z}_{1})) \operatorname{Tr}(\boldsymbol{Q}^{k_{1}k_{1}}(z_{2}) \circ (\boldsymbol{Q}^{k_{1}k_{2}}(\bar{z}_{2})\boldsymbol{Q}^{k_{2}k_{1}}(\bar{z}_{2}))) \right] \\
+ \frac{1}{N^{2}} \sum_{s \neq k_{1}}^{d} \mathcal{B}_{(4)}^{(k_{1},s)} \mathbb{E} \left[\operatorname{Tr}((\boldsymbol{Q}^{sl_{1}}(z_{1})\boldsymbol{Q}^{l_{1}s}(z_{2})) \circ (\boldsymbol{Q}^{sk_{2}}(\bar{z}_{2})\boldsymbol{Q}^{k_{2}s}(\bar{z}_{2})) \operatorname{Tr}(\boldsymbol{Q}^{k_{1}k_{1}}(z_{2}) \circ (\boldsymbol{Q}^{k_{1}l_{2}}(\bar{z}_{1})\boldsymbol{Q}^{l_{2}k_{1}}(\bar{z}_{1}))) \right].$$

As a result, combining (G.46), (G.47) and (G.48), we obtain that

$$\begin{split} &(z_{1}+\mathfrak{m}(z_{1})-\mathfrak{m}_{k_{1}}(z_{1}))\mathcal{C}^{(d)}_{k_{1}l_{1},k_{2}l_{2},N}=-\Big(\delta_{k_{1}l_{1}}+\sum_{s\neq k_{1}}^{d}V^{(d)}_{sl_{1},N}(z_{1},z_{2})\Big)\mathcal{C}^{(d)}_{k_{1},k_{2}l_{2},N}-2\mathcal{V}^{(d)}_{k_{1}l_{1},k_{2}l_{2},N}(z_{1},z_{2})+\mathrm{O}(C_{\eta_{0}}N^{-\omega})\\ &-\kappa_{4}\mathcal{U}^{(d)}_{k_{1}l_{1},k_{2}l_{2},N}(z_{1},z_{2})-V^{(d)}_{k_{1}l_{1},N}(z_{1},z_{2})\sum_{s\neq k_{1}}^{d}\mathcal{C}^{(d)}_{s,k_{2}l_{2},N}-\mathfrak{m}_{k_{1}}(z_{2})\sum_{s\neq k_{1}}^{d}\mathcal{C}^{(d)}_{sl_{1},k_{2}l_{2},N}+\mathrm{O}(C_{\eta_{0}}N^{-\omega})\mathcal{C}^{(d)}_{k_{2}l_{2},k_{2}l_{2},N}\\ &:=-\mathfrak{m}_{k_{1}}(z_{2})\sum_{s\neq k_{1}}^{d}\mathcal{C}^{(d)}_{sl_{1},k_{2}l_{2},N}-\mathcal{F}^{(d)}_{k_{1}l_{1},k_{2}l_{2},N}(z_{1},z_{2})+\mathrm{O}(C_{\eta_{0}}N^{-\omega})\mathcal{C}^{(d)}_{k_{2}l_{2},k_{2}l_{2},N}+\mathrm{O}(C_{\eta_{0}}N^{-\omega}). \end{split}$$

Hence, for any $k_2, l_2 \in \{1, \dots, d\}$, define

$$\boldsymbol{C}_{k_{2}l_{2},N}^{(d)}(z_{1},z_{2}):=[\mathcal{C}_{k_{1}l_{1},k_{2}l_{2},N}^{(d)}(z_{1},z_{2})]_{d\times d}\quad\text{and}\quad \boldsymbol{F}_{k_{2}l_{2},N}^{(d)}(z,\bar{z}):=[\mathcal{F}_{k_{1}l_{1},k_{2}l_{2}}^{N}(z,\bar{z})]_{d\times d},\quad (G.55)$$

we have

$$\boldsymbol{\Theta}_{N}^{(d)}(z_{1},z_{2})\boldsymbol{C}_{k_{2}l_{2},N}^{(d)}(z_{1},z_{2}) = -\boldsymbol{F}_{k_{2}l_{2},N}^{(d)}(z_{1},z_{2}) + \boldsymbol{1}_{d\times d}\mathrm{O}(C_{\eta_{0}}N^{-\omega})\mathcal{C}_{k_{2}l_{2},k_{2}l_{2},N}^{(d)},$$

where $\Theta_N^{(d)}$ is defined in (G.18). Notice that

$$\|\mathbf{1}_{d\times d} \mathcal{O}(C_{\eta_0} N^{-\omega}) \mathcal{C}_{k_2 l_2 k_2 l_2 N}^{(d)} \| \le \sqrt{d} C_{\eta_0} N^{-\omega} \| C_{k_2 l_2, N}(z_1, z_2) \|,$$

so we can use the same argument as those in Theorem G.2 to derive that

$$\lim_{N\to\infty} \|\boldsymbol{C}_{k_2 l_2,N}^{(d)}(z_1,z_2)\| \leq \lim_{N\to\infty} \|\boldsymbol{\Pi}^{(d)}(z_1,z_2)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z_1))\| \cdot \|\boldsymbol{F}_{k_2 l_2,N}^{(d)}(z_1,z_2)\| \leq C_{\eta_0,\mathfrak{c},d},$$

which suggests that all entries of $C_{k_2l_2,N}^{(d)}(z_1,z_2)$ are bounded by $C_{\eta_0,\epsilon,d}$.

G.4.2 Characteristic function

Theorem G.6. Under Assumptions A.1 and A.2, $\operatorname{Tr}(\boldsymbol{Q}(z)) - \mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}(z))]$ weakly converges to a Gaussian random process on $z \in \mathcal{S}_{\eta_0}$ in (G.1).

Proof. Recall the following notations in Theorem F.3:

$$\gamma(z) := \sum_{l=1}^{d} \gamma_l(z) := \sum_{l=1}^{d} \text{Tr}(\mathbf{Q}^{ll}(z))^c, \quad (\mathfrak{a}(\tau), \mathfrak{b}(\tau)) := \left\{ \begin{array}{ll} (1/2, 1/2) & \tau = 1 \\ (1/2\mathrm{i}, -1/2\mathrm{i}) & \tau = \mathrm{i} \end{array} \right.,$$

where $l \in \{1, \dots, d\}$. Given $q \in \mathbb{N}^+$, let $\mathbf{z}_q := (z_1, \dots, z_q)', \mathbf{\tau}_q := (\tau_1, \dots, \tau_q)'$ and $\mathbf{t}_q := (t_1, \dots, t_q)'$, where $z_s \in \mathcal{S}_{\eta_0}, \tau_s \in \{1, i\}$ and $t_s \in \mathbb{R}$ respectively, define

$$e_q := e_q(\boldsymbol{t}_q, \boldsymbol{\tau}_q, \boldsymbol{z}_q) := \exp\left(i \sum_{s=1}^q t_s[\mathfrak{a}(\tau_s)\gamma(z_s) + \mathfrak{b}(\tau_s)\gamma(\bar{z}_s)]\right), \tag{G.56}$$

so the characteristic function is $\mathbb{E}[e_q]$. Notice that

$$\frac{\partial}{\partial t_s} \mathbb{E}[e_q] = i \mathbb{E}\left[e_q\left(\mathfrak{a}(\tau_s)\gamma(z_s) + \mathfrak{b}(\tau_s)\gamma(\bar{z}_s)\right)\right],$$

and we will show that there exists a set of covariance coefficients A_{rw} such that for each fixed t_q

$$\lim_{N\to\infty} \left| \mathbb{E}\left[e_q \left(\mathfrak{a}(\zeta_s) \gamma(z_s) + \mathfrak{b}(\zeta_s) \gamma(\bar{z}_s) \right) \right] + \mathbb{E}[e_q] \sum_{r=1}^q t_r A_{rs,N} \right| = 0.$$

For any $z \in \mathcal{S}_{\eta_0}$, by the cumulant expansion (D.4), we have

$$z\mathbb{E}[e_{q}\gamma_{l}(z)] = z\operatorname{Cov}(\gamma_{l}(z), e_{q}) = \frac{1}{\sqrt{N}} \sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}} \sum_{r\neq l}^{d} \mathbb{E}[X_{i_{1}\cdots i_{d}}\mathcal{A}_{i_{1}\cdots i_{d}}^{(l,r)}Q_{i_{r}i_{l}}^{rl}(z)e_{q}^{c}]$$

$$= \frac{1}{\sqrt{N}} \sum_{i_{1}\cdots i_{d}}^{n_{1}\cdots n_{d}} \left(\sum_{r\neq l}^{d} \sum_{\alpha=0}^{3} \frac{\kappa_{\alpha+1}}{\alpha!} \mathbb{E}[\partial_{i_{1}\cdots i_{d}}^{(\alpha)} \{\mathcal{A}_{i_{1}\cdots i_{d}}^{(l,r)}Q_{i_{r}i_{l}}^{rl}(z)e_{q}^{c}\}] + \epsilon_{i_{1}\cdots i_{d}}^{(4)}\right).$$

Similar as proofs of Theorem F.3, only the cases of $\alpha = 1, 3$ contain the major terms:

First derivatives: When $\alpha = 1$, since

$$\begin{split} &\frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{r \neq l}^{d} \mathbb{E} \big[\partial_{i_1 \cdots i_d}^{(1)} \big\{ \mathcal{A}_{i_1 \cdots i_d}^{(l,r)} Q_{i_r i_l}^{rl}(z) \big\} e_q^c \big] \\ &= -\frac{1}{N} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{r \neq l}^{d} \sum_{s_1 \neq s_2}^{d} \mathbb{E} \big[\mathcal{A}_{i_1 \cdots i_d}^{(l,r)} Q_{i_r i_{s_1}}^{rs_1}(z) \mathcal{A}_{i_1 \cdots i_d}^{(s_1,s_2)} Q_{i_{s_2} i_l}^{s_2 l}(z) e_q^c \big] \\ &= -\frac{1}{N} \sum_{r \neq l}^{d} \operatorname{Cov}(\operatorname{Tr}(\boldsymbol{Q}^{rr}(z)) \operatorname{Tr}(\boldsymbol{Q}^{ll}(z)), e_q) + \operatorname{O}(C_{\eta_0} N^{-1/2}) \\ &= -\operatorname{Cov}(\gamma_l(z), e_q) \sum_{r \neq l}^{d} \mathfrak{m}_r(z) - \mathfrak{m}_l(z) \sum_{r \neq l}^{d} \operatorname{Cov}(\gamma_r(z), e_q) + \operatorname{O}(C_{\eta_0} N^{-\omega}), \end{split}$$

where we use the fact that $|e_q| \leq 1$. And

$$\partial_{i_1\cdots i_d}^{(1)}\{e_q\} = -\frac{\mathrm{i} e_q}{\sqrt{N}} \sum_{s=1}^q \sum_{w=1}^d \sum_{s,\neq s_2}^d t_s \mathcal{A}_{i_1\cdots i_d}^{(s_1,s_2)} \left[\mathfrak{a}(\tau_s)Q_{i_{s_1}}^{s_1w}(z_s)Q_{i_{s_2}}^{ws_2}(z_s) + \mathfrak{b}(\tau_s)Q_{i_{s_1}}^{s_1w}(\bar{z}_s)Q_{i_{s_2}}^{ws_2}(\bar{z}_s)\right],$$

then

$$\frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{r \neq l}^{d} \mathbb{E} \left[\mathcal{A}_{i_1 \cdots i_d}^{(l,r)} Q_{i_r i_l}^{rl}(z) \partial_{i_1 \cdots i_d}^{(1)} \left\{ e_q \right\} \right] \\
= -\frac{2\mathbf{i}}{N} \sum_{s=1}^{q} \sum_{v=1}^{d} \sum_{z=1}^{d} t_s \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{rl}(z)[\mathfrak{a}(\tau_s) \boldsymbol{Q}^{lw}(z_s) \boldsymbol{Q}^{wr}(z_s) + \mathfrak{b}(\tau_s) \boldsymbol{Q}^{lw}(\bar{z}_s) \boldsymbol{Q}^{wr}(\bar{z}_s)]) e_q \right] + \mathcal{O}(C_{\eta_0} N^{-1/2}).$$

Moreover, by Theorem G.2, we can obtain that

$$\operatorname{Cov}(N^{-1}\operatorname{Tr}(\boldsymbol{Q}^{rw}(z)\boldsymbol{Q}^{wl}(z_s)\boldsymbol{Q}^{lr}(z_s)), e_q) = \operatorname{O}(C_{\eta_0}N^{-\omega}),$$

so it implies that

$$\frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{r \neq l}^{d} \mathbb{E} \left[\partial_{i_1 \cdots i_d}^{(1)} \left\{ \mathcal{A}_{i_1 \cdots i_d}^{(l,r)} Q_{i_r i_l}^{rl}(z) e_q^c \right\} \right]$$

$$= -\operatorname{Cov}(\gamma_l(z), e_q) \sum_{r \neq l}^{d} \mathfrak{m}_r(z) - \mathfrak{m}_l(z) \sum_{r \neq l}^{d} \operatorname{Cov}(\gamma_r(z), e_q)$$

$$- \frac{2i\mathbb{E}[e_q]}{N} \sum_{s=1}^{q} \sum_{w=1}^{d} \sum_{r \neq l}^{d} t_s \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{rl}(z)[\mathfrak{a}(\tau_s)\boldsymbol{Q}^{lw}(z_s)\boldsymbol{Q}^{wr}(z_s) + \mathfrak{b}(\tau_s)\boldsymbol{Q}^{lw}(\bar{z}_s)\boldsymbol{Q}^{wr}(\bar{z}_s)]) \right] + \operatorname{O}(C_{\eta_0} N^{-\omega})$$

$$: = -\operatorname{Cov}(\gamma_l(z), e_q) \sum_{r \neq l}^{d} \mathfrak{m}_r(z) - \mathfrak{m}_l(z) \sum_{r \neq l}^{d} \operatorname{Cov}(\gamma_r(z), e_q)$$

$$- 2i\mathbb{E}[e_q] \sum_{r \neq l}^{q} t_s \left[\mathfrak{a}(\tau_s) \mathcal{V}_{l,e,N}^{(d)}(z, z_s) + \mathfrak{b}(\tau_s) \mathcal{V}_{l,e,N}^{(d)}(z, \bar{z}_s) \right] + \operatorname{O}(C_{\eta_0} N^{-\omega}).$$

Third derivatives: When $\alpha = 3$, the only case contains major terms is

$$\frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{r \neq l}^{d} \mathbb{E} \left[\partial_{i_1 \cdots i_d}^{(1)} \{\mathcal{A}_{i_1 \cdots i_d}^{(l,r)} Q_{i_r i_l}^{rl}(z)\} \partial_{i_1 \cdots i_d}^{(2)} \{e_q\} \right],$$

since

$$\begin{split} \partial_{i_{1}\cdots i_{d}}^{(2)}\{e_{q}\} &= -\frac{e_{q}}{N} \Big(\sum_{s=1}^{q} \sum_{w=1}^{d} \sum_{s_{1} \neq s_{2}}^{d} t_{s} \mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{1},s_{2})} [\mathfrak{a}(\tau_{s})Q_{i_{s_{1}}}^{s_{1}w}(z_{s})Q_{\cdot i_{s_{2}}}^{ws_{2}}(z_{s}) + \mathfrak{b}(\tau_{s})Q_{i_{s_{1}}}^{s_{1}w}(\bar{z}_{s})Q_{\cdot i_{s_{2}}}^{ws_{2}}(\bar{z}_{s})]\Big)^{2} + \frac{2\mathrm{i}e_{q}}{N} \\ &\times \sum_{s=1}^{q} \sum_{w=1}^{d} \sum_{\substack{s_{1} \neq s_{2} \\ s_{3} \neq s_{4}}}^{d} t_{s} \mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{1},s_{2})} \mathcal{A}_{i_{1}\cdots i_{d}}^{(s_{3},s_{4})} [\mathfrak{a}(\tau_{s})Q_{i_{s_{1}}i_{s_{3}}}^{s_{1}s_{3}}(z_{s})Q_{i_{s_{4}}}^{s_{4}w}(z_{s})Q_{\cdot i_{s_{2}}}^{ws_{2}}(z_{s}) + \mathfrak{b}(\tau_{s})Q_{i_{s_{1}}i_{s_{3}}}^{s_{1}s_{3}}(\bar{z}_{s})Q_{i_{s_{4}}}^{s_{4}w}(\bar{z}_{s})Q_{\cdot i_{s_{2}}}^{ws_{2}}(\bar{z}_{s})], \end{split}$$

for the previous term, since it only contains the off-diagonal terms, by Lemma G.4, if it associate with $\partial_{i_1\cdots i_d}^{(1)}\{\mathcal{A}_{i_1\cdots i_d}^{(l,r)}Q_{i_ri_l}^{rl}(z)\}$, the summation over all $i_1\cdots i_d$ will be minor. For the later one, by

Lemma G.3 and (A.5), we have

$$\begin{split} &\frac{1}{N^{3/2}} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \sum_{w=1}^{d} \sum_{r \neq l}^{d} \sum_{\substack{s_{1} \neq s_{2} \\ s_{3} \neq s_{4}}}^{d} \mathbb{E}\left[e_{q} \partial_{i_{1} \cdots i_{d}}^{(1)} \left\{\mathcal{A}_{i_{1} \cdots i_{d}}^{(l,r)} Q_{i_{r}i_{l}}^{rl}(z)\right\} \mathcal{A}_{i_{1} \cdots i_{d}}^{(s_{1},s_{2})} \mathcal{A}_{i_{1} \cdots i_{d}}^{(s_{3},s_{4})} Q_{i_{s_{1}}i_{s_{3}}}^{s_{1}s_{3}}(z_{s}) Q_{i_{s_{4}}}^{s_{4}w}(z_{s}) Q_{i_{s_{2}}}^{ws_{2}}(z_{s})\right] \\ &= -\frac{1}{N^{2}} \sum_{i_{1} \cdots i_{d}}^{n_{1} \cdots n_{d}} \sum_{w=1}^{d} \sum_{r \neq l}^{d} \sum_{\substack{s_{1} \neq s_{2} \\ s_{3} \neq s_{4} \\ s_{5} \neq s_{6}}}^{d} \mathbb{E}\left[e_{q} \mathcal{A}_{i_{1} \cdots i_{d}}^{(l,r)} Q_{i_{r}i_{s_{5}}}^{rs_{5}}(z) \mathcal{A}_{i_{1} \cdots i_{d}}^{(s_{5},s_{6})} Q_{i_{s_{6}}i_{l}}^{s_{6}l}(z) \mathcal{A}_{i_{1} \cdots i_{d}}^{(s_{1},s_{2})} \mathcal{A}_{i_{1} \cdots i_{d}}^{(s_{3},s_{4})} Q_{i_{s_{1}}i_{s_{3}}}^{s_{1}s_{3}}(z_{s}) Q_{i_{s_{4}}}^{ws_{2}}(z_{s})\right] \\ &= -\frac{1}{N^{2}} \sum_{w=1}^{d} \sum_{r \neq l}^{d} \mathcal{B}_{(4)}^{(l,r)} \mathbb{E}\left[e_{q} \operatorname{Tr}(\boldsymbol{Q}^{rr}(z) \circ \boldsymbol{Q}^{rr}(z_{s})) \operatorname{Tr}(\boldsymbol{Q}^{ll}(z) \circ (\boldsymbol{Q}^{lw}(z_{s}) \boldsymbol{Q}^{wl}(z_{s})))\right] \\ &- \frac{1}{N^{2}} \sum_{w=1}^{d} \sum_{r \neq l}^{d} \mathcal{B}_{(4)}^{(l,r)} \mathbb{E}\left[e_{q} \operatorname{Tr}(\boldsymbol{Q}^{rr}(z) \circ (\boldsymbol{Q}^{rw}(z_{s}) \boldsymbol{Q}^{wr}(z_{s}))) \operatorname{Tr}(\boldsymbol{Q}^{ll}(z) \circ \boldsymbol{Q}^{ll}(z_{s}))\right] + \operatorname{O}(C_{\eta_{0}} N^{-1/2}). \end{split}$$

Similarly, by Theorem G.2, we have

$$\operatorname{Cov}(N^{-1}\operatorname{Tr}(\boldsymbol{Q}^{rr}(z)\circ\boldsymbol{Q}^{rr}(z_s))N^{-1}\operatorname{Tr}(\boldsymbol{Q}^{ll}(z)\circ(\boldsymbol{Q}^{lw}(z_s)\boldsymbol{Q}^{wl}(z_s))),e_q)=\operatorname{O}(C_{\eta_0}N^{-\omega}),$$

and so does the other one. For simplicity, denote

$$\frac{1}{N^{2}} \sum_{s=1}^{q} t_{s} \sum_{w=1}^{d} \sum_{r\neq l}^{d} \mathcal{B}_{(4)}^{(l,r)} \left(\mathfrak{a}(\tau_{s}) \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{rr}(z) \circ \boldsymbol{Q}^{rr}(z_{s})) \operatorname{Tr}(\boldsymbol{Q}^{ll}(z) \circ (\boldsymbol{Q}^{lw}(z_{s}) \boldsymbol{Q}^{wl}(z_{s}))) \right] \right] \\
+ \mathfrak{b}(\tau_{s}) \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{rr}(z) \circ \boldsymbol{Q}^{rr}(\bar{z}_{s})) \operatorname{Tr}(\boldsymbol{Q}^{ll}(z) \circ (\boldsymbol{Q}^{lw}(\bar{z}_{s}) \boldsymbol{Q}^{wl}(\bar{z}_{s}))) \right] \\
+ \mathfrak{a}(\tau_{s}) \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{rr}(z) \circ (\boldsymbol{Q}^{rw}(z_{s}) \boldsymbol{Q}^{wr}(z_{s}))) \operatorname{Tr}(\boldsymbol{Q}^{ll}(z) \circ \boldsymbol{Q}^{ll}(z_{s})) \right] \\
+ \mathfrak{b}(\tau_{s}) \mathbb{E} \left[\operatorname{Tr}(\boldsymbol{Q}^{rr}(z) \circ (\boldsymbol{Q}^{rw}(\bar{z}_{s}) \boldsymbol{Q}^{wr}(\bar{z}_{s}))) \operatorname{Tr}(\boldsymbol{Q}^{ll}(z) \circ \boldsymbol{Q}^{ll}(\bar{z}_{s})) \right] \right) \\
:= \sum_{s=1}^{q} t_{s} \left[\mathfrak{a}(\tau_{s}) \mathcal{U}_{l,e,N}^{(d)}(z,z_{s}) + \mathfrak{b}(\tau_{s}) \mathcal{U}_{l,e,N}^{(d)}(z,\bar{z}_{s}) \right],$$

then we obtain that

$$\frac{1}{\sqrt{N}} \sum_{i_1 \cdots i_d}^{n_1 \cdots n_d} \sum_{r \neq l}^{d} \mathbb{E} \left[\partial_{i_1 \cdots i_d}^{(1)} \{ \mathcal{A}_{i_1 \cdots i_d}^{(l,r)} Q_{i_r i_l}^{rl}(z) \} \partial_{i_1 \cdots i_d}^{(2)} \{ e_q \} \right]
= -2i \mathbb{E} \left[e_q \right] \sum_{s=1}^{q} t_s \left[\mathfrak{a}(\tau_s) \mathcal{U}_{l,e,N}^{(d)}(z, z_s) + \mathfrak{b}(\tau_s) \mathcal{U}_{l,e,N}^{(d)}(z, \bar{z}_s) \right] + \mathcal{O}(C_{\eta_0} N^{-\omega}).$$
(G.58)

Now, define

$$\mathcal{C}_{l,e,N}^{(d)}(z) := \mathrm{Cov}(\gamma_l(z), e_q) \quad \text{and} \quad \mathcal{F}_{l,e,N}^{(d)}(z, z_s) := 2\mathcal{V}_{l,e,N}^{(d)}(z, z_s) + \kappa_4 \mathcal{U}_{l,e,N}^{(d)}(z, z_s)$$

and

$$\boldsymbol{C}_{e,N}^{(d)}(z) := (\mathcal{C}_{1,e,N}^{(d)}(z), \cdots, \mathcal{C}_{d,e,N}^{(d)}(z))', \quad \boldsymbol{F}_{e,N}^{(d)}(z,z_s) := (\mathcal{F}_{1,e,N}^{(d)}(z,z_s), \cdots, \mathcal{F}_{d,e,N}^{(d)}(z,z_s))'.$$

Combining (G.57) and (G.58), we obtain that

$$(z + \mathfrak{m}(z) - \mathfrak{m}_{l}(z))\mathcal{C}_{l,e,N}^{(d)}(z) = -\mathfrak{m}_{l}(z)\sum_{r \neq l}^{d} \mathcal{C}_{r,e,N}^{(d)}(z)$$
$$-i\mathbb{E}[e_{q}]\sum_{s=1}^{q} t_{s} \left[\mathfrak{a}(\tau_{s})\mathcal{F}_{l,e,N}^{(d)}(z,z_{s}) + \mathfrak{b}(\tau_{s})\mathcal{F}_{l,e,N}^{(d)}(z,\bar{z}_{s})\right] + \mathcal{O}(C_{\eta_{0}}N^{-\omega}),$$

then we obtain that

$$\boldsymbol{\Theta}_{N}^{(d)}(z,z)\boldsymbol{C}_{e,N}^{(d)}(z) = -\mathrm{i}\mathbb{E}[e_q]\sum_{s=1}^{q}t_s\big[\mathfrak{a}(\tau_s)\boldsymbol{F}_{e,N}^{(d)}(z,z_s) + \mathfrak{b}(\tau_s)\boldsymbol{F}_{e,N}^{(d)}(z,\bar{z}_s)\big] + \mathrm{o}(\boldsymbol{1}_d),$$

where $\Theta_N^{(d)}(z,z)$ is defined in (G.18) and it is invertible such that

$$\lim_{N\to\infty} \|\boldsymbol{\Theta}_N^{(d)}(z,z)^{-1} + \boldsymbol{\Pi}^{(d)}(z,z)^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z))\| = 0.$$

Hence, we obtain that

$$\boldsymbol{C}_{e,N}^{(d)}(z) = \mathrm{i}\mathbb{E}[e_q] \sum_{s=1}^q t_s \boldsymbol{\Pi}^{(d)}(z,z)^{-1} \operatorname{diag}(\boldsymbol{\mathfrak{c}}^{-1} \circ \boldsymbol{g}(z)) \big[\mathfrak{a}(\tau_s) \boldsymbol{F}_{e,N}^{(d)}(z,z_s) + \mathfrak{b}(\tau_s) \boldsymbol{F}_{e,N}^{(d)}(z,\bar{z}_s) \big] + \mathrm{o}(\boldsymbol{1}_d),$$

According to §G.3.3, we can derive the limiting expressions of $\mathcal{V}_{l,e,N}^{(d)}(z,z_s), \mathcal{U}_{l,e,N}^{(d)}(z,z_s)$, so we have

$$\mathbb{E}[e_{q}(\mathfrak{a}(\tau_{s})\gamma(z_{s}) + \mathfrak{b}(\tau_{s})\gamma(\bar{z}_{s}))] = \sum_{l=1}^{d} \mathbb{E}[e_{q}(\mathfrak{a}(\tau_{s})\gamma_{l}(z_{s}) + \mathfrak{b}(\tau_{s})\gamma_{l}(\bar{z}_{s}))]$$

$$= \sum_{l=1}^{d} \mathfrak{a}(\tau_{s}) \operatorname{Cov}(\gamma_{l}(z_{s}), e_{q}) + \mathfrak{b}(\tau_{s}) \operatorname{Cov}(\gamma_{l}(\bar{z}_{s}), e_{q})$$

$$= i\mathbb{E}[e_{q}] \sum_{r=1}^{q} t_{r} \Big(\mathfrak{a}(\tau_{s}) \mathbf{1}'_{d} \mathbf{\Pi}^{(d)}(z_{s}, z_{s})^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(z_{s})) \big[\mathfrak{a}(\tau_{r}) \boldsymbol{F}_{e,N}^{(d)}(z_{s}, z_{r}) + \mathfrak{b}(\tau_{r}) \boldsymbol{F}_{e,N}^{(d)}(z_{s}, \bar{z}_{r}) \big]$$

$$+ \mathfrak{b}(\tau_{s}) \mathbf{1}'_{d} \mathbf{\Pi}^{(d)}(\bar{z}_{s}, \bar{z}_{s})^{-1} \operatorname{diag}(\mathfrak{c}^{-1} \circ \boldsymbol{g}(\bar{z}_{s})) \big[\mathfrak{a}(\tau_{r}) \boldsymbol{F}_{e,N}^{(d)}(\bar{z}_{s}, z_{r}) + \mathfrak{b}(\tau_{r}) \boldsymbol{F}_{e,N}^{(d)}(\bar{z}_{s}, \bar{z}_{r}) \big] \Big) + o(1)$$

$$: = i\mathbb{E}[e_{q}] \sum_{r=1}^{q} t_{r} A_{rs,N} + o(1),$$

which completes our proof.

G.4.3 Proof of Theorem G.4

By Theorem C.1, it yields that

$$G_N(f) \stackrel{\mathbb{P}}{\longrightarrow} G_N(f) 1_{\|\mathbf{M}\| \leq \mathfrak{v}_d + t} = -\frac{1}{2\pi \mathrm{i}} \oint_{\sigma} f(z) (\mathrm{Tr}(\mathbf{Q}(z)) - Ng(z)) dz,$$

where t>0 is a fixed constant. Next, we split $\mathfrak{C}:=\mathfrak{C}(\eta_0):=\mathfrak{C}^h\cup\mathfrak{C}^v$ by

$$\mathfrak{C}^h := \{ z = E \pm i \eta_0 \in \mathbb{C} : |E| \le E_0 \}, \quad \mathfrak{C}^v := \{ z = \pm E_0 + i \eta \in \mathbb{C} : |\eta| \le \eta_0 \}.$$

In other words, C is a rectangular contour with vertex of $\pm E_0 \pm i\eta_0$, where $E_0 > \max\{\mathfrak{v}_d, \zeta\} + t$ and t > 0 is a constant. According to Theorems G.2, G.3 and G.6, we have shown that $\text{Tr}(\mathbf{Q}(z)) - Ng(z)$ is a Gaussian process with mean of $\mu_N^{(d)}(z)$ and variance of $C_N^{(d)}(z,z)$, which further implies that

$$-\frac{1}{2\pi i} \oint_{\mathfrak{C}^h} f(z) (\operatorname{Tr}(\boldsymbol{Q}(z)) - Ng(z)) dz / \sigma_N^{(d)} - \xi_N^{(d)} / \sigma_N^{(d)} \stackrel{d}{\longrightarrow} \mathcal{N}(0, 1).$$

Next, let's show that

$$\lim_{\eta_0\downarrow 0} \limsup_{N\to\infty} \oint_{\sigma^v} f(z)(\operatorname{Tr}(\boldsymbol{Q}(z)) - Ng(z))dz \stackrel{\mathbb{P}}{\longrightarrow} 0.$$

It is enough to show that

$$\lim_{\eta_0\downarrow 0} \limsup_{N\to\infty} \oint_{\mathcal{C}^v} \mathbb{E}\big[|f(z)(\mathrm{Tr}(\boldsymbol{Q}(z))-Ng(z))|^2\big]dz = 0.$$

Let's first show that

$$\lim_{\eta_0\downarrow 0} \limsup_{N\to\infty} \oint_{\mathcal{C}^v} \left| f(z)(\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}(z))] - Ng(z)) \right|^2 dz = 0.$$

According to Theorem G.3, we know that

$$\mathbb{E}[\operatorname{Tr}(\boldsymbol{Q}(z))] - Ng(z) = \mu_N^{(d)}(z) + \mathcal{O}(C_t N^{-\omega}).$$

In fact, by the definition of g(z) in (B.1), it is easy to see $g_i(z)$ are analytical on \mathfrak{C}^v for all $i=1,\cdots,d$, so does the entries g(z) and $\Pi^{(d)}(z,z)$ due to their definitions in (B.1) and (B.11). Moreover, we have shown that $\Pi^{(d)}(z,z)$ is invertible in Lemma F.1 by (G.19). The mean function $\mu_N^{(d)}(z)$ only depends on g(z) since $W^{(d)}(z)$, $V^{(d)}(z,z)$, $G_{i,N}^{(d)}(z)$ and $H_{i,N}^{(d)}(z)$ also depend on g(z) by their definitions in (G.28) (G.29), (G.21) and (G.22), so does the covariance function $\mathcal{C}_N^{(d)}(z_1,z_2)$ in (G.10), implies that $\mu_N^{(d)}(z)$ and $\mathcal{C}_N^{(d)}(z_1,z_2)$ are analytical on \mathfrak{C}^v , thus, combining with the fact $f \in \mathfrak{F}_d$ is analytic on \mathfrak{C}^v , we have

$$\lim_{\eta_0\downarrow 0} \limsup_{N\to\infty} \oint_{\mathfrak{C}^v} \left| (f(z)\mathbb{E}[\mathrm{Tr}(\boldsymbol{Q}(z))] - Ng(z)) \right|^2 dz = 0.$$

According to Theorem G.2, we know that $Var(Tr(\mathbf{Q}(z))) = C_{t,d,\mathfrak{c}}$ for all $z \in \mathfrak{C}^v$ since $\Re(z) = E_0 > \max\{\mathfrak{v}_d,\zeta\} + t$, then it also conclude that

$$\lim_{\eta_0\downarrow 0} \limsup_{N\to\infty} \oint_{\mathfrak{C}^v} |f(z)|^2 \operatorname{Var}(\operatorname{Tr} \boldsymbol{Q}(z)) dz = 0,$$

which completes our proof.

References

- [1] O. Ajanki, L. Erdős, and T. Krüger. Quadratic vector equations on complex upper half-plane, volume 261. American Mathematical Society, 2019.
- [2] O. H. Ajanki, L. Erdős, and T. Krüger. Stability of the matrix dyson equation and random matrices with correlations. *Probability Theory and Related Fields*, 173(1):293–373, 2019.
- [3] J. Alt, L. Erdős, T. Krüger, and D. Schröder. Correlated random matrices: band rigidity and edge universality. *The Annals of Probability*, 48(2):963–1001, 2020.
- [4] G. B. Arous, S. Mei, A. Montanari, and M. Nica. The landscape of the spiked tensor model. Communications on Pure and Applied Mathematics, 72(11):2282–2330, 2019.
- [5] Z. Bai, D. Jiang, J.-F. Yao, and S. Zheng. Corrections to lrt on large-dimensional covariance matrix by rmt. *The Annals of Statistics*, 37(6 B):3822–3840, 2009.

- [6] Z. Bai and J. W. Silverstein. Clt for linear spectral statistics of large-dimensional sample covariance matrices. Annals of Probability, pages 553–605, 2004.
- [7] Z. Bai and J. W. Silverstein. Spectral analysis of large dimensional random matrices, volume 20. Springer, 2010.
- [8] Z. Bao, X. Ding, J. Wang, and K. Wang. Statistical inference for principal components of spiked covariance matrices. *The Annals of Statistics*, 50(2):1144–1169, 2022.
- [9] G. Ben Arous, R. Gheissari, and A. Jagannath. Algorithmic thresholds for tensor PCA. Annals of Probability, 48(4):2052–2087, 2020.
- [10] G. Ben Arous, D. Z. Huang, and J. Huang. Long random matrices and tensor unfolding. The Annals of Applied Probability, 33(6B):5753–5780, 2023.
- [11] B. Cao, L. He, X. Kong, S. Y. Philip, Z. Hao, and A. B. Ragin. Tensor-based multi-view feature selection with applications to brain diseases. In 2014 IEEE International Conference on Data Mining, pages 40–49. IEEE, 2014.
- [12] Z. Che. Universality of random matrices with correlated entries. Electronic Journal of Probability, 22:1–38, 2017.
- [13] W.-K. Chen. Phase transition in the spiked random tensor with rademacher prior. The Annals of Statistics, 47(5):2734–2756, 2019.
- [14] A. Cichocki. Tensor decompositions: new concepts in brain data analysis? Journal of the Society of Instrument and Control Engineers, 50(7):507–516, 2011.
- [15] J. H. de Morais Goulart, R. Couillet, and P. Comon. A random matrix perspective on random tensors. The Journal of Machine Learning Research, 23(1):12110–12145, 2022.
- [16] F. Götze, H. Sambale, and A. Sinulis. Concentration inequalities for polynomials in α -sub-exponential random variables. *Electronic Journal of Probability*, 26:1–22, 2021.
- [17] M. Hallin, D. Paindaveine, and T. Verdebout. Optimal rank-based testing for principal components. Annals of statistics, 38:3245–3299, 2010.
- [18] Y. Han and C.-H. Zhang. Tensor principal component analysis in high dimensional cp models. *IEEE Transactions on Information Theory*, 69(2):1147–1167, 2022.
- [19] L. He, X. Kong, P. S. Yu, X. Yang, A. B. Ragin, and Z. Hao. Dusk: A dual structure-preserving kernel for supervised tensor learning with applications to neuroimages. In *Proceedings of the* 2014 SIAM International Conference on Data Mining, pages 127–135. SIAM, 2014.
- [20] L. He, C.-T. Lu, H. Ding, S. Wang, L. Shen, P. S. Yu, and A. B. Ragin. Multi-way multi-level kernel modeling for neuroimaging classification. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 356–364, 2017.

- [21] C. J. Hillar and L.-H. Lim. Most tensor problems are np-hard. Journal of the ACM (JACM), 60(6):1–39, 2013.
- [22] J. Huang, D. Z. Huang, Q. Yang, and G. Cheng. Power iteration for tensor PCA. Journal of Machine Learning Research, 23(128):1–47, 2022.
- [23] A. Jagannath, P. Lopatto, and L. Miolane. Statistical thresholds for tensor PCA. The Annals of Applied Probability, 30(4):1910–1933, 2020.
- [24] A. M. Khorunzhy, B. A. Khoruzhenko, and L. A. Pastur. Asymptotic properties of large random matrices with independent entries. *Journal of Mathematical Physics*, 37(10):5033– 5060, 1996.
- [25] T. G. Kolda. Orthogonal tensor decompositions. SIAM Journal on Matrix Analysis and Applications, 23(1):243–255, 2001.
- [26] T. G. Kolda and B. W. Bader. Tensor decompositions and applications. SIAM review, 51(3):455–500, 2009.
- [27] T. Lesieur, L. Miolane, M. Lelarge, F. Krzakala, and L. Zdeborová. Statistical and computational phase transitions in spiked tensor estimation. 2017 IEEE International Symposium on Information Theory (ISIT), pages 511–515, 2017.
- [28] L.-H. Lim. Singular values and eigenvalues of tensors: a variational approach. In 1st IEEE International Workshop on Computational Advances in Multi-Sensor Adaptive Processing, 2005., pages 129–132. IEEE, 2005.
- [29] R. Liu, Z. Wang, and J. Yao. Supplementary materials of "alignment and matching tests for high-dimensional tensor signals by tensor contraction"., 2024+.
- [30] A. Lytova and L. Pastur. Central limit theorem for linear eigenvalue statistics of random matrices with independent entries. The Annals of Probability, 37(5):1778 – 1840, 2009.
- [31] C. McDiarmid et al. On the method of bounded differences. Surveys in combinatorics, 141(1):148–188, 1989.
- [32] A. Naumov, V. Spokoiny, and V. Ulyanov. Bootstrap confidence sets for spectral projectors of sample covariance. *Probability Theory and Related Fields*, 174(3):1091–1132, 2019.
- [33] G. Pan and W. Zhou. Central limit theorem for signal-to-interference ratio of reduced rank linear receiver. *Ann. Appl. Probab.*, pages 1232–1270, 2008.
- [34] A. Perry, A. S. Wein, and A. S. Bandeira. Statistical limits of spiked tensor models. *Annales de lâĂŹInstitut Henri Poincaré*. *Probabilités et Statistiques*, 56(1):230–264, 2020.
- [35] E. Richard and A. Montanari. A statistical model for tensor pca. Advances in Neural Information Processing Systems, 27, 2014.

- [36] M. E. A. Seddik, M. Guillaud, and R. Couillet. When random tensors meet random matrices. Annals of Applied Probability, 34(1 A):203 âĂŞ 248, 2024.
- [37] I. Silin and J. Fan. Hypothesis testing for eigenspaces of covariance matrix. arXiv preprint arXiv:2002.09810, 2020.
- [38] I. Silin and V. Spokoiny. Bayesian inference for spectral projectors of the covariance matrix. Electronic Journal of Statistics, 12(1):1948–1987, 2018.
- [39] W. W. Sun and L. Li. Store: sparse tensor response regression and neuroimaging analysis. The Journal of Machine Learning Research, 18(1):4908–4944, 2017.
- [40] D. Tao, X. Li, W. Hu, S. Maybank, and X. Wu. Supervised tensor learning. In Fifth IEEE International Conference on Data Mining (ICDM'05), pages 8-pp. IEEE, 2005.
- [41] M. Udell and A. Townsend. Why are big data matrices approximately low rank? SIAM Journal on Mathematics of Data Science, 1(1):144–160, 2019.
- [42] S. Zheng, Z. Bai, and J. Yao. Clt for eigenvalue statistics of large-dimensional general Fisher matrices with applications. *Bernoulli*, 23(2):1130–1178, 2017.
- [43] H. Zhou, L. Li, and H. Zhu. Tensor regression with applications in neuroimaging data analysis. Journal of the American Statistical Association, 108(502):540–552, 2013.